DRAFT

PRELIMINARY DOCUMENTATION OF THE SAPRC-16 MECHANISM

Interim Report to California Air Resources Board Contract No. 11-761

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Summary

This document gives a preliminary description of updated the SAPRC gas-phase mechanism that is being developed for California Air Resources Board (CARB) project 11-761. Although not intended to be a comprehensive documentation of all aspects of this mechanism, this describes the general features the mechanism and the mechanism generation system it uses, how they differ from previous versions, and lists the model species, reactions, and rate parameters used. It also gives brief descriptions of the model species, gives the sources of the assigned rate constants and mechanisms, gives a summary of the results of the evaluation and adjustments using chamber data, and compares results of box model simulations of simplified ambient scenarios with simulations using the earlier version of SAPRC. Additional information and files needed to implement the mechanism are available at http://www.cert.ucr.edu/~carter /SAPRC/16, and updated files and documentation will be posted there when available.

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Introduction

The SAPRC gas-phase atmospheric chemical mechanisms are designed to represent the gas-phase reactions of volatile organic compounds (VOCs) and oxides of nitrogen (NO_x) in urban and regional model simulations of the lower troposphere. Previous versions that have been implemented in airshed models include SAPRC-90 (Carter, 1990), SAPRC-99 (Carter, 2000), SAPRC-07 (Carter, 2010a,b), SAPRC-07T (Hutzell et al, 2012), and SAPRC-11 (Carter and Heo, 2013). These previous mechanisms have two versions, the "detailed" versions where as many individual compounds are represented explicitly as necessary for calculation of ozone reactivity scales (e.g., Carter, 1994, 2010c), and various "condensed" versions for use in airshed models. Generally even the condensed versions implement more chemical detail and a lesser amount of condensation than most of the widely-used mechanisms for airshed modeling, with the main exception being the near-explicit "Master Chemical Mechanism" (MCM, see MCM, 2016). The most detailed of the previous SAPRC mechanisms, and the main version currently implemented in the CMAQ model, is SAPRC-07T (Hutzell et al, 2012), which is based on SAPRC-07 but represents several selected individual compounds explicitly rather than using lumped model species, either because of their importance in emissions or because of their importance for assessing formation of toxic compounds. The latest version used in models is SAPRC-11, which is similar to SAPRC-07 in level of detail and reactions for most compounds, but has an updated representation of aromatic chemistry.

None of the current published versions of SAPRC are designed to predict formation of secondary organic aerosol (SOA), though they are used in airshed models in conjunction with separate models designed to predict SOA. A version of SAPRC-11 with additional reactions added to predict SOA from aromatics was developed (Carter et al, 2012), but extension of this approach to other classes of organics was not funded. However, the author believes that reliable and scientifically supportable prediction of SOA requires use of a gas-phase mechanism to predict formation of the condensable species responsible for SOA, rather than by separate and parameterized SOA models that are not informed by the capabilities of the gas-phase mechanism in this regard. Complete separation of SOA models from the gas-phase mechanism as is the current practice is neither scientifically supportable nor necessary. Therefore, modern gas-phase mechanisms need to be developed with the needs for proper predictions of SOA precursors in mind.

The SAPRC mechanisms as used in current models are becoming out of date and need to be updated if they are to continue to be used in regulatory models. In addition to incorporating new data in order to better represent the current state of the science, it needs to have a lumping approach that is more appropriate for SOA modeling. In view of this the California Air Resources Board (CARB) funded the author to develop an update to the SAPRC gas-phase mechanism. This project is nearing completion, and a new version, designated SAPRC-16, has been developed. Although it is condensed in the sense that most organic compounds are represented using lumped model species, it represents more compounds explicitly and uses a greater number of lumped model species for improved chemical detail needed for toxics or SOA modeling. About half of the mass of anthropogenic emissions and most of the mass of biogenic emissions are represented explicitly, and the number of lumped model species representing oxidation products is significantly increased. The objective is to represent explicitly the most important compounds in emissions that have significant reactivity, and to use more lumped model species representing oxidized organic products in order to better simulate NO_x recycling processes as well as formation of SOA precursors. Condensation is employed primarily for compounds of secondary importance or where more explicit representation would result in a significantly larger and more cumbersome mechanism without corresponding improvements in reliability of predictions, and where the additional chemical detail may not be meaningful given available data and knowledge. The result is a larger mechanism than previous versions of SAPRC, though still much smaller than MCM or other near-

explicit or computer generated mechanisms. This is not so large that it cannot be used in 3-D models, and provides a useful reference mechanism against which more condensed mechanisms can be developed and evaluated for specific applications where computational efficiency is a priority.

As the most recent previous versions of SAPRC, SAPRC-16 relies primarily on the SAPRC mechanism generation system to derive explicit mechanisms for the reactions of most organic compounds, with various systematic lumping approaches used to derive the condensed representation more appropriate for modeling. Approximately 75% of the reactions in this mechanism are directly output by this system, a significant increase over previous version of SAPRC. A number of updates to the mechanism generation system were made as part of this project, including the ability to generate mechanisms for aromatic hydrocarbons and some other types of compounds that could not be processed (or processed appropriately) previously, and new types of radical reactions, including peroxy radical isomerizations, that were not represented previously. These generated mechanisms are used not only to predict reactions of the emitted organic compounds, but also for predicting the reactions of predicted oxidation products. These are used to derive mechanisms of compounds that are represented explicitly, but mechanisms of lumped model species based on mechanisms for the compounds they represent. In the case of model species used for oxidation products, the system compiles a list of products predicted to be formed in the reactions of compounds in a representative emissions mixture, uses that to determine a distribution of oxidation product compounds represented by each model species, then generates the mechanisms for those compounds and uses these to derive the mechanisms of the lumped species representing them. Thus the resulting mechanism employs explicitly generated mechanisms for a total of 157 emitted and 212 predicted oxidation product compounds, which are used to derive the mechanisms model species representing 22 explicitly represented compounds and 37 model species representing lumped emitted and organic product compounds. Thus it incorporates available chemical detail from the generated mechanisms for 369 compounds when generating reactions of the 57 model species used to represent them.

As with previous versions of SAPRC, the updated mechanism is being evaluated by comparing its predictions of ozone formation, NO oxidation rates, and radical levels observed in the available database of environmental chamber experiments. These included the experiments used in the SAPRC-07 and SAPRC-11 evaluations, plus additional UCR chamber experiments, primarily with alkenes, carried out subsequently (Yarwood et al, 2012; Heo et al, 2014). The mechanism evaluation experiments included organic - NO_x, mixture - NO_x, and incremental reactivity experiments with a variety of compounds, as well as chamber characterization experiments. Although all experiments to be used in the evaluation have been simulated and SAPRC-16 was found to simulate the data as well or better than previous versions of SAPRC, there are a number of experiments where the fits for SAPRC-16 are not quite as good as for SAPRC-11 and more mechanism adjustments are needed. This evaluation and adjustment work is still underway, but overall the mechanism performs well enough that it can be considered near to its final form in terms of its structure and overall performance in simulating ambient mixtures.

The CARB contracted a peer review of the updated SAPRC mechanism being developed for this project, to be completed by the end of 2016. In order to permit the peer review to begin, we previously submitted a version of the mechanism that is near final and still being evaluated against the chamber data, and with preliminary and incomplete documentation. We believe that reviewer components on this preliminary mechanism and documentation would be useful and could be taken into account when the mechanism is finalized. This version and the available documentation was made available on the SAPRC-16 web site (Carter, 2016). We already received some reviewer comments that resulted in corrections in some errors in the mechanism and documentation.

In the month since the preliminary version of the mechanism was released for peer review, we completed the evaluation against the chamber data and made some revisions to the mechanism and made

it available on the SAPRC-16 web site (Carter, 2016) on October 21. This version corrects some errors and incorporates some revised assignments and estimation methods that gives better fits to chamber data for some compounds. This document describes this updated version of the mechanism and its evaluation against chamber data.

Mechanism Description

Mechanism Structures and Versions for Previous SAPRC Mechanisms

Previous SAPRC mechanisms consisted of both "detailed" and "condensed" versions, where detailed versions were used for calculation of MIR and other ozone reactivity scales (Carter, 1994, 2000c) and condensed versions were used for airshed model calculations. All versions shared the same "base" mechanism for the reactions of the organics and a few low molecular organics such as formaldehyde and ethylene and used a limited number of model species to organic oxidation products, but differed in the representation of primary emitted VOCs. The detailed versions had separate representations of the initial reactions of most of the emitted organics whose ozone reactivities were calculated, while the condensed versions represented explicitly only a few emitted organics such as ethylene, benzene, and acetylene, and used a limited number of lumped model species to represent the others. There are several condensed versions of SAPRC-07, the "standard" version that was originally developed (Carter, 2010a,b), the more condensed version designated CSAPRC-07 that used fewer lumped and explicit model species yet gave essentially the same ozone predictions (Carter, 2010d), and the "Toxics" version, designated SAPRC-07T that has model species to separately represent additional compounds that are relevant to toxics modeling. SAPRC-07T is the version that is currently implemented in the CMAQ model (CMAQ, 2016). SAPRC-11 is similar to standard SAPRC-07 in its level of condensation and most of its reactions, except that it has updated reactions for aromatics (Carter and Heo, 2012, 2013).

Note that the detailed versions of previous SAPRC mechanisms that were actually used to calculate reactivity scales did not include all of the hundreds of compounds whose reactivities were calculated in the mechanism at the same time, but instead used an "adjustable parameter" model species to represent the compound whose reactivity is being calculated, with rate constants and overall product yield parameters being used as input to the calculation. This adjustable model species had a separate reaction for each of the initial consumption processes that may occur, i.e., reaction with OH, etc, and each reaction had parameters specifying overall product yields of all of the possible first-generation product species in the mechanism. These included "chemical operators" that represented the conversion of NO to NO_2 and the consumption of NO in the overall process leading to stable product formation. The parameters giving the rate constants and product yields for each of these compounds were either manually assigned based on considerations of the reactions of the compounds and adjustments to fit chamber data (in the case of the aromatics and a few other compounds) or (for most other compounds) derived using the mechanism generation system, as described in the mechanism documentation (Carter, 2000, 2010a,b; Carter and Heo, 2013). The rate constants and parameters for each of these hundreds of compounds were used not only to calculate their reactivity values, but were also used to derive the rate constants and product yields for the lumped model species that represent these compounds in ambient simulations. The weighting factors used to derive the lumped model species parameters from those of the representative constituent compounds were based on the composition of the mixture that was used to base case anthropogenic VOC emissions the MIR and other reactivity scale calculations (Carter, 1994; Jeffries et al, 1989).

All of these previous SAPRC versions used the simplification that the net effects of the initial atmospheric reactions of an organic compound with OH, etc., can be represented by a single overall process as discussed above. This "reaction lumping" is no approximation if all of the competing

elementary reactions that lead to ultimate first-generation product formation are either unimolecular or with O_2, so their branching ratios do not vary with conditions as long as the temperature is approximately constant. However, the oxidation mechanisms of almost all VOCs involve the intermediacy of peroxy radicals, which in polluted atmospheres react primarily with NO, but can also react with HO_2, NO_3, and other peroxy radicals when NO levels are low. (The reaction with NO_2 can be ignored for peroxy radicals because the peroxynitrate rapidly decomposes. The reactions of NO_2 is non-negligible for acyl peroxy radicals, but the SAPRC mechanisms use separate model species for acyl peroxy radicals so their subsequent reactions are not included in the overall lumped VOC reactions.) For SAPRC-90 and SAPRC-99 the approximation was used that the distribution of oxidation products formed when peroxy + NO reactions dominated could be used for all conditions, and chemical operators were used to predict how NO_x conversions and radical propagation vs. termination changed as NO_x became low. Chemical operators are also used to predict formations of hydroperoxides when peroxy radicals react with HO_2, though this approach requires use of only a single lumped hydroperoxide species, which limits its utility in SOA modeling. This approximation, which is also used in the Carbon Bond mechanisms (Gery et al, 1998; Yarwood et al, 2005), was shown not to significantly affect ozone predictions, but does not permit the predictions of different products being formed when NO_x is low, which may affect SOA predictions. In order to better represent how organic products changed when NO_x levels became low, SAPRC-07 introduced use of separate chemical operators to represent formation of organic product model species in the lumped reactions representing the net effects of initial VOC reactions, with these operators then reacting with NO, NO_3, HO_2, or other peroxy radicals. This permitted the continued use of the reaction lumping and lumped parameter methods employed with previous versions of SAPRC, while giving better predictions of oxidation products under low NO_x conditions.

Note that this representation of the initial reactions of VOCs as a single overall process forming overall products or chemical operators requires the assumption that peroxy radicals do not undergo significant unimolecular reactions and the rate constants for their bimolecular reactions are approximately the same for all radicals. This is clearly not the case for all peroxy + peroxy reactions, but these are generally minor processes and approximating them with the same rate constant for all of them has been shown not to significantly affect results of atmospheric simulations. However, this representation cannot be used if unimolecular reactions of peroxy radicals are non-negligible, especially if they are fast enough to compete with reaction with NO in polluted atmospheres. Previous versions of SAPRC did not consider this possibility, but new data and estimates (e.g., Davis and Francisco, 2010; Crounse et al, 2012; Peeters et al, 2014) indicate that unimolecular reactions of peroxy radicals at rates competing with bimolecular reactions occur in the atmospheric reactions of many compounds, and cannot be neglected. Therefore, a different representation of peroxy radical reactions had to be used in this updated version of the mechanism.

Structure and Versions for the Updated Mechanism

The SAPRC-16 mechanism currently has two versions, one for atmospheric simulations and one used for evaluations against chamber data. At present there is no version for comprehensive reactivity scale calculation, though the version for evaluations against chamber data could be extended for this purpose. They employ the same base mechanism and set of organic product model species and reactions but differ in the number of individual emitted compounds that are represented explicitly. The version for chamber evaluations consists of all the reactions and model species in the version for atmospheric simulations but also includes separate model species and reactions to represent reactions of individual compounds that are important in some of the chamber experiments but that are represented using lumped model species in the version for atmospheric simulations. Therefore, this is referred to as the "extended" version of SAPRC-16, to distinguish it from the "standard" version that is recommended for atmospheric simulations. Using the extended version when testing the mechanism against chamber data permits allows us to test the predictive capabilities of the underlying chemical assumptions, estimates, and

mechanism generation procedures independently of condensation effects. Although many of these compounds are represented in atmospheric simulations using lumped model species, most of the compounds studied in chamber experiments are either important in emissions or representative of compounds that are, and therefore even if they are not explicitly represented, their individual mechanisms are used to derive the mechanisms of the lumped model species representing them.

Extended versions of SAPRC-16 could also be used for calculation of updated MIR and other reactivity scales, though complete reactivity scale updates are beyond the scope of this project. The current extended SAPRC-16 only has the additional compounds needed for chamber evaluation, and not the many hundreds of other compounds that are needed for complete reactivity scales. However, the mechanism generation system could be used to readily add reactions for most of the additional compounds for a complete reactivity scale, should that be desired in the future. This may be appropriate once the mechanism and the underlying mechanism and mechanism generation system are finalized.

As discussed below in the section summarizing updates to the mechanism generation system, it was found that a number of peroxy radical intermediates are predicted to undergo unimolecular reactions at rates that are competitive with their reactions with NO or other bimolecular reactions. This means that the "reaction lumping" procedure employed in previous versions of SAPRC, that requires using the approximation that all peroxy radicals react with the same rate constant and allows the use of a single reaction to represent the overall process of an initial VOC reaction, cannot be used in this version. Instead, it is necessary to use an approach more like that used in the RADM and RACM mechanisms (e.g., Stockwell et al, 1990, 1997; Stockwell and Goliff, 2006; Goliff et al, 2013), where separate model species are used to represent the peroxy radical intermediates in each of the organic compound reactions. Multiple intermediate peroxy radicals can be lumped and represented by a single model species if they all have the same or similar sources and do not have significant unimolecular reactions, but separate model species are needed for peroxy radical intermediates that have non-negligible unimolecular reactions that compete with the bimolecular peroxy reactions such as with NO or HO_2. (Note that if the unimolecular reaction is fast enough to dominate over the NO and other bimolecular reactions then the formation of the peroxy radical can be replaced by its unimolecular reaction products, so it can be removed from the mechanism, just as is the case for alkyl and most alkoxy radicals.) Thus, appropriate representations of reactions of some compounds require multiple model species to represent the reactions of the different types of peroxy radicals involved. The methods used to derive these lumped mechanisms using the mechanism generation system are discussed later in this document.

Both the standard and the extended versions of SAPRC-16 have two types of reactions, those whose rate constants and reaction products are assigned manually based on information in the literature or chemical considerations or estimates, and those that are directly output by the mechanism generation system. The former consists of the inorganic reactions and the reactions of the lower molecular weight compounds that are represented explicitly in the base mechanism, and lumped or parameterized mechanisms for compounds, such as phenols and naphthalenes, whose mechanisms cannot be reliably derived using the current mechanism generation system. The latter are used for the reactions that can be derived using the mechanism generation system and that are output directly by the system. Reactions output by the mechanism generation system account for over 75% of the reactions in the standard mechanism and over 85% of the reactions in the extended mechanism.

Model Species

Table 1 lists the emitted compounds that are represented explicitly in various versions of SAPRC, along with other compounds found to make significant contributions to current anthropogenic and biogenic emissions inventories. To assess their importance in anthropogenic emissions we used the total 2005 U.S. emissions profile provided by the EPA (Luecken, 2013) and to assess their importance in

Table 1. List of major emitted compounds in emissions mixtures that were considered for explicit representation when updating the SAPRC mechanism

Compound [a]	Model Species [b]	Us Emissions [c]		Bio. [e]	Explicit [f]				Notes
		Wt%	MIR % [d]	Wt %	07	07T	Std	Ext	[g]
Primarily Anthropogenic									
toluene	TOLU	7.35%	9.13%	0.14%		y	y		
n-butane	NC4	5.86%	2.09%				y		
isopentane	ALK4	3.34%	1.50%						1
acetone	ACET	3.14%	0.35%	4.35%	y	y	y		
ethene	ETHEN	2.98%	8.31%	2.74%	y	y	y		
benzene	BENZ	2.59%	0.58%		y	y	y		
ethane	ETHAN	2.47%	0.21%	0.03%			y		
ethanol	ETOH	2.46%	1.16%	2.06%		y	y		
propane	PROP	2.22%	0.34%	<0.01%			y		
3-methyl-1-butene	OLE1	2.03%	4.40%						
m-xylene	MXYL	1.98%	5.99%			y	y		
p-xylene	PXYL	1.92%	3.47%			y	y		
n-pentane	ALK4	1.85%	0.75%	<0.01%					1
propene	PROPE	1.70%	6.13%	1.53%			y		
ethyl benzene	C2BEN	1.63%	1.53%				y		
o-xylene	OXYL	1.55%	3.68%			y	y		
formaldehyde	HCHO	1.50%	4.41%	0.50%	y	y	y		
acetylene	ACETL	1.42%	0.42%				y		
acetaldehyde	MECHO	1.28%	2.59%	2.06%	y	y	y		
isobutane	ALK3	1.23%	0.47%		y	y	y		
methanol	MEOH	0.98%	0.21%	9.91%	y	y	y		
methyl ethyl ketone	MEK	0.91%	0.42%	0.03%			y		2
1-butene	OLE1	0.89%	2.67%	0.77%				y	
1,2,4-trimethyl benzene	BZ124	0.89%	2.45%			y			
m-ethyl toluene	ARO2	0.82%	1.89%				y	y	
isopropyl alcohol	OTH3	0.77%	0.15%					y	
2-methyl-1-butene	OLE3	0.72%	1.42%						3
2-methyl-2-butene	OLE4	0.54%	2.37%						3
trans-2-pentene	OLE2	0.43%	1.41%						
1,3-butadiene	BUT13	0.40%	1.58%			y	y		
1,3,5-trimethyl benzene	BZ135	0.39%	1.43%				y		
p-ethyl toluene	ARO2	0.38%	0.52%					y	
1-pentene	OLE1	0.37%	0.84%						
glyoxal	GLY	0.36%	1.38%		y	y	y		
methyl glyoxal	MGLY	0.30%	1.53%						4
o-ethyl toluene	ARO2	0.29%	0.51%					y	
styrene	STYRS	0.29%	0.16%						4
propionaldehyde	ETCHO	0.24%	0.52%				y		
2-pentenenes	OLE2	0.23%	0.75%						
n-propyl benzene	ARO1	0.22%	0.14%					y	
benzaldehyde	BALD	0.21%	<0	<0.01%					4

Table 1 (continued)

Compound [a]	Model Species [b]	Us Emissions [c] Wt%	MIR % [d]	Bio. [e] Wt %	Explicit [f] 07	07T	Std	Ext	Notes [g]
1,2,3-trimethyl benzene	BZ123	0.20%	0.73%				y		
naphthalene	NAPS	0.16%	0.17%	<0.01%					3,4
phenol	PHEN	0.16%	0.14%				y		5
trans-2-butene	OLE2	0.16%	0.75%					y	
isopropyl benzene	ARO1	0.13%	0.10%					y	
cis-2-butene	OLE2	0.13%	0.56%					y	
acrolein	ACRO	0.09%	0.22%			y	y		
methacrolein	MACR	0.06%	0.12%				y		2
isobutene	OLE3	0.05%	0.10%					y	3
biacetyl	BACL	0.04%	0.28%						4
Primarily Biogenic									
isoprene	ISOP	0.03%	0.11%	53.23%		y	y		
a-pinene	APINE	0.10%	0.14%	6.58%		y	y		
b-pinene	BPINE	0.07%	0.07%	1.88%			y		
d-limonene	DLIMO	0.32%	0.45%	1.13%			y		
sabinene	TERP	<0.01%	<0.01%	0.90%				y	
beta-myrcene	TERP	<0.01%	0.01%	0.87%					
3-carene	TERP	0.01%	0.01%	0.71%				y	
acetic acid	AACID	0.03%	0.01%	0.37%	y	y	y		
formic acid	HCOOH	0.02%	<0.01%	0.37%	y	y	y		
2-methyl-3-butene-2-ol	OLEP	0	0	0.22%					3
Fraction explicit									
All listed above		63%	84%	90%					
SAPRC-07		14%	18%	20%					
SAPRC-07T		31%	46%	82%					
Standard SAPRC-16		48%	60%	87%					
Extended SAPRC-16		52%	68%	89%					

[a] Compounds are listed in decreasing order of total for mass fractions for total U.S. or biogenic mixtures.

[b] Name of model species used to represent the compound in the standard SAPRC-16 mechanism. Note that a different, unique model species is used if it is represented explicitly in the extended version.

[c] Total US Emissions based on the 2005ah_tox inventory using the criteria VOC emissions only from all sectors except biogenic & fires. Provided by Deborah Luecken (2013).

[d] Derived using the mass emissions fractions and the SAPRC-07 Maximum Incremental Reactivity scale of Carter (2010c).

[e] Global annual total biogenic VOC emissions for the year 2000 calculated using the using MEGAN 2.1 model algorithms in CLM4 (Guenther et al, 2012; Guenther 2014). "0.00% means emissions are nonzero but lower than 0.005%.

Table 1 (continued)

Compound [a]	Model Species [b]	Us Emissions [c] Wt%	MIR % [d]	Bio. [e] Wt %	Explicit [f] 07	07T	Std	Ext	Notes [g]

[f] Indicates whether this compound is represented explicitly. "Std": y = explicit in the standard mechanism; "Ext": y = explicit in the extended mechanism only.
- 07 Explicit in the standard SAPRC-07 and SAPRC-11 mechanisms
- 07T Explicit in SAPRC-07T
- Std Explicit in the standard and extended versions of SAPRC-16
- Ext Explicit in the current extended version of SAPRC-16 because it is important in some chamber experiments.

[g] Notes for individual compounds
1. Sensitivity calculations indicate that representing most alkanes explicitly has little effect on atmospheric simulation results.
2. This model species is also used to represent other species in SAPRC-07, so it does not represent this compound explicitly.
3. Although not represented explicitly, a new lumped model species is used in SAPRC-16 to better represent compounds of this type.
4. This is used to represent other compounds with a similar mechanism in SAPRC-07 and SAPRC-16, so this model species does not represent this compound explicitly.
5. Represented explicitly in SAPRC-11 but not SAPRC-07 or 07T.

the biogenic emissions we used the total annual biogenic VOC emissions for the year 2000 calculated using the Megan 2.1 model (Guenther et al, 2012; Guenther 2014). These mixtures were also used to derive mechanisms of the lumped model species in the current version SAPRC-16 as discussed below. Note that based on these mixtures SAPRC-07T explicitly represented about a third of the mass and somewhat less than half of the reactivity of anthropogenic emissions explicitly, while standard SAPRC-16 explicitly represents about half of the mass and 60% of the reactivity of these emissions. Most of the biogenic emissions are represented explicitly by both mechanisms because of the importance of explicitly represented isoprene and α-pinene. It was decided that increasing the number of explicit compounds beyond those used in SAPRC-16 would result in only slight changes in the fractions of anthropogenic emissions represented while significantly increasing the size of the mechanism, so no additional explicit species were added to the standard mechanism. However, additional compounds could be made explicit for atmospheric simulations if desired, and would need to be explicit in extended versions of the mechanism to calculate their reactivities or evaluate their mechanisms using chamber data.

Table A-1 lists all the model species in the standard SAPRC-16 mechanism and gives additional information and footnotes describing these species. These include (1) inorganic and organic compounds whose mechanisms were derived manually; model species for emitted or oxidation product compounds represented explicitly, lumped model species, explicit and lumped peroxy and acyl peroxy radical species, model species for several other types of radical intermediates, and various counter species and chemical operators. Note that the mechanism includes a number of peroxy radical model species involved in the generated mechanisms of individual compounds and lumped model species, derived by the mechanism generation system as discussed below. The table indicates which compounds can be held in steady state in order to minimize the number of model species that have to be stored and transported in 3-D model simulations. This includes essentially all of the many peroxy and acyl peroxy radical model species (over half of the species in the mechanism), so use of the steady state approximation is highly recommended.

The chemical operator species in the mechanism include the SumRO2 and SumRCO3 model species that compute the total of peroxy radical and acyl peroxy radical concentrations for the purpose of estimating rates of peroxy + peroxy or peroxy + acyl peroxy reactions. These are treated as active species and each reaction forming a peroxy or acyl peroxy radical also forms the same yield of one of these species, and their loss reactions are treated separately in reactions that affect only these species. This is different than the approach used in SAPRC-07 and SAPRC-11, where the rates of formation of products from peroxy + peroxy and other reactions are computed from relative rates of reactions of a representative peroxy radical model species, and has the advantage over SAPRC-07/11 in that it does not require special treatment when the mechanism is implemented into the model software. However, SAPRC-16 also has the chemical operators RO2C, RO2XC, and various zNitrate model species in order to represent effects of relatively effects of reactions of the relatively minor peroxy radical species predicted in the mechanisms without having to include them as separate model species. These are used for peroxy radicals that are predicted to be formed less than 10% of the time in the initial reactions of a compound and that cannot be lumped with any of the more important peroxy radicals involved. If this approach were not used the mechanism would have a large number of peroxy radical model species representing only very minor pathways.

The model species added to the extended version of the mechanism used in the chamber simulations consist of those representing the 12 compounds indicated in Table 1 as being represented explicitly only in the extended mechanism, plus 62 additional compounds used in the mechanism evaluation chamber species, and the 133 steady-state peroxy radical model species derived by the mechanism generation system to represent their reactions. These model species and their reactions are listed in electronic form in supplementary materials available at the SAPRC-16 web site (Carter, 2016).

As indicated on Table A-1**,** the mechanisms for most of the lumped model species were derived from mechanisms for individual compounds that are represented by these model species, weighed by the mole fractions of the compounds present in representative mixtures. Several different mixtures were employed for this purpose, depending on the model species involved, as follows:

- The "UStot" mixture consists of the total U.S. anthropogenic VOC emissions profile provided by the EPA (Luecken, 2013). The anthropogenic VOC mixture used for previous SAPRC mechanisms for this purpose was not used because it is out of date and also because it is based only on ambient measurements, and does not include many types of compounds present in emissions inventories for which ambient measurements are limited or unavailable. Note that relatively unimportant compounds in the total profile can make non-negligible contributions to some lumped model species in the more detailed mechanisms, such as SAPRC-16, that represents most of the important compounds explicitly. If a compound is represented explicitly, in general it will not be included in mixtures used to derive lumped model species used for non-explicitly-represented compounds. This means that a fairly complete anthropogenic mixture us needed to for this purpose, not one that only has the most important compounds. This was used to derive model species used primarily to represent emitted hydrocarbons, such as the ALKx, OLEx, and AROx species and a few others. It was not used to derive mechanisms for model species that primarily represent oxidized products.
- The "Megan2" mixture consists of total annual biogenic VOC emissions for the year 2000 calculated using the Megan 2.1 model (Guenther et al, 2012; Guenther 2014). This biogenic model was used because it appears to be the most up-to-date and best documented and it has modules that predict emissions of individual compounds rather than lumped model species. It was used to derive the mechanism of the TERP (terpene) model species and also was behind the choice of using the mechanism of β-caryophyllene to represent that of the SESQ species.

- The "UStot OHprods" mixture was derived from the distribution of products predicted to be formed from the reactions of of OH with the compounds in the UStot mixture in the presence of 0.5 ppb of NO, weighted by the mole fraction of the compounds in the mixture and the relative yields of the products. (The choice of 0.5 ppb to estimate branching ratios for unimolecular vs. NO reactions of peroxy radicals that have unimolecular reactions is somewhat arbitrary, but this level is considered to be reasonably representative. It may be revised in future versions of the mechanism if considered appropriate based on analyses of ambient simulations combined with sensitivity studies.) Only the compounds in the UStot mixture whose mechanisms could be processed using the mechanism generation system were used, but these are the major compounds affecting these products. This was used to derive the mechanisms for most of the model species used for organic products, except for hydroperoxy species formed primarily from reactions of peroxy radicals with HO_2, and for the carbonyl nitrates and dinitrates formed primarily from the reactions of NO_3 radicals with some alkenes. Examples include RCHO, KET2, the RNO3 species except for RCNO3 and RDNO3, and the AFGx species. The exceptions include model species used to represent products formed primarily in the isoprene system, discussed below.
- The "UStot NO3prods" mixture was derived as discussed above for UStot OHprods except that it is the predicted products of the reactions of NO_3 with the compounds in the UStot mixture. It was used to derive mechanisms for the carbonyl nitrate (RCNO3) and dinitrate (RDNO3) species that primarily represents these compounds.
- The "UStot HO2prods" mixture was derived from the mixture of hydroperoxide products formed in the reactions of HO_2 with the peroxy radicals predicted to be formed in the reactions of OH with the components of the UStot mixture. This included hydroperoxides formed from second-generation peroxy radicals formed in multi-step mechanisms, with relative yields based on the assumption that the HO_2 or peroxy + peroxy reactions are not important enough to significantly reduce yields of peroxy radical yields in multi-step mechanisms. This was used to derive mechanisms for most of the hydroperoxide model species. The one exception is RUOOH, which represents primarily hydroperoxide products formed from isoprene.
- The "Isoprene OHprods" mixture was derived from the products formed by the reactions of OH with isoprene in the presence of 0.5 ppb of NO. It was used to derive the mechanisms of lumped product model species that primarily represent compounds formed from isoprene. These include OLEP, OLEA1, and HPALD. Note compounds other than isoprene could also form products represented by these species, but for most atmospheric simulations it is expected that most of the moles of oxidized products that are represented by these model species would come from isoprene. The contributions to these compounds in the USTOT OHprods mixture are very low.
- The "Isoprene HO2prods" mixture was derived from the mixture of hydroperoxides formed in the reactions of peroxy radicals formed from the reactions of OH with isoprene, in the same way as used for UStot HO2prods. It was used to derive the mechanism of the RUOOH model species, which represents primarily hydroperoxides formed from isoprene. Compound other than isoprene could also form such compounds, but the contribution from isoprene probably dominates under most conditions. The contributions to these compounds in the USTOT HO2prods mixture are also very low.

Some of these mixtures had many compounds represented by the various model species, but in order to keep the number of generated mechanisms to a manageable level we used only the compounds that contributed to 90% of the total moles, or the top 10 compounds, whichever was fewer. The specific compounds used to derive the mechanisms for each lumped model species, are listed in Table A-2. This table gives the contribution of each compound to the total number mole fractions of compounds represented by the model species in the mixture, and the structure of the compound as used in the

mechanism generation system. Note that many of the compounds in the "prods" mixtures have not been given species names in the SAPRC detailed mechanisms, so they are not included in compound listings for SAPRC or in reactivity scales.

Reactions

Table A-3 lists the all the reactions in the standard SAPRC-16 mechanism, giving the rate constant parameters or files with photolysis information, the products formed, and footnotes giving additional information about the reactions. An Excel file containing the reactions in the extended version of SAPRC-16 used for chamber simulations, files containing the absorption cross sections and quantum yields, and files with the reactions and rate constants in formats used by the SAPRC and CMAQ modeling software, are available at the SAPRC-16 web site (Carter, 2016).

As discussed above, the mechanism consists of reactions that are manually assigned and reactions that were output by the mechanism generation system. The derivations of the rate parameters and products of the manually assigned reactions are indicated in the footnotes to Table A-3. These were updated where appropriate based on the latest evaluations and other published results, primarily the IUPAC (2016), NASA (2015), or Calvert et al, (2000, 2011, 2015). The footnotes in in Table A-3 can be consulted for details.

Table 2 lists the reactions in the base mechanism whose rate constants at 300K or photolysis rates for direct overhead sunlight changed by more than 10% for this update. It can be seen that the changes were relatively small for most reactions, except photolysis rates for new model species added to the mechanism (compared to those of the model species previously used for these compounds), rate constants for some organic + NO_3 reactions, rate constants for reactions involving peroxynitric acid, and the photolysis rate of glyoxal forming stable compounds (the photolysis forming radicals changed by only 2%). Not shown is the rate constant for the important OH + NO_2 reaction, which decreased by about 7%, which may make this a somewhat more reactive mechanism than SAPRC-11 if only this were considered. However, the effects of any of these changes are difficult to assess because of the other changes made to the mechanism. The largest changes concerned photolysis rates of new model species added to the mechanism to better represent photoreactive bifunctional compounds, and photolyses of photoreactive aromatic ring opening products, where the total yields in SAPRC-16 are determined by the mechanism generation system rather than being treated as adjustable products as they are in SAPRC-07 and SAPRC-11.

Approximately 75% of the reactions in the mechanism were derived from the output of the mechanism generation system. As described previously (Carter, 2000, 2010a) this system derives fully explicit mechanisms for the first-generation atmospheric reactions of many types of organics, and uses various "lumping rules" and condensation procedures to derive product yield parameters for compounds and mixtures for incorporation into the mechanism. For previous versions of SAPRC the mechanism generation system output was incorporated by using generic reactions with adjustable rate constants and product yields, whose values were derived by the mechanism generation system for input into the model. This could not be done for this version of the mechanism because of the necessity of having separate peroxy radical model species as discussed above. Instead, the system processed the explicit reactions to generate merged or lumped reactions for a compound or mixture that can be inserted directly in the mechanism. These reactions either form product model species or chemical operators that are part of the base mechanism, or lumped or explicit peroxy species that are used only for the mechanism of the particular compound or mixture. The latter are designated by the VOC's model species name with a suffix _Px or _Ax, where "x" is an index number for this type of radical in the mechanism for this compound or mixture. Species with suffix _Px refer to peroxy radicals that do not isomerize or isomerize slowly enough for peroxy + peroxy reactions to occur so they are included in SumRO2, and species with _Ax refer to peroxy radicals that isomerize fast enough that only isomerization and NO reaction need to

Table 2. Reactions in the base mechanism whose rate constants changed by 10% or more.

Label	Reaction	Rate constant [a]		
		SAPRC-16	SAPRC-11	Change
13	N2O5 + H2O = #2 HNO3	[b]	2.50e-22	
14	N2O5 + H2O + H2O = #2 HNO3 + H2O	[b]	1.80e-39	
H338	AFG2A + HV = Products (compared to AFG1) [c]	3.87e-2	3.87e-1	-90%
H355	AFG2B + HV = Products (compared to AFG1) [c]	3.87e-2	3.87e-1	-90%
C042	MGLY + NO3 = Products	5.66e-16	2.53e-15	-78%
H333	AFG1 + HV = Products [c]	1.35e-1	3.87e-1	-65%
C042	MGLY + NO3 = Products	5.66e-16	2.53e-15	-78%
C037	GLY + NO3 = Products	4.00e-16	1.02e-15	-61%
C035	GLY + HV = HCHO + CO	1.66e-3	3.18e-3	-47%
33	HO2 + NO2 = HNO4	7.40e-13	1.12e-12	-34%
34	HNO4 = HO2 + NO2	7.89e-2	1.07e-1	-26%
24	OH + HONO = H2O + NO2	4.91e-12	5.95e-12	-18%
C041	MGLY + OH = Products	1.29e-11	1.50e-11	-14%
40	NO3 + HO2 =OH + NO2 + O2	3.50e-12	4.00e-12	-13%
C024	MECHO + NO3 = Products	2.49e-15	2.84e-15	-12%
38	HO2 + HO2 = HO2H + O2	2.49e-12	2.84e-12	-12%
39	HO2 + HO2 + H2O = HO2H + O2 + H2O	5.34e-30	6.09e-30	-12%
C010	HCOOH + OH = HO2 + CO2	4.00e-13	4.50e-13	-11%
S002	SumRO2 + HO2 = Products	6.82e-12	7.63e-12	-11%
26	OH + NO3 = HO2 + NO2	2.20e-11	2.00e-11	10%
C049	CRES + OH = Products	4.47e-11	4.06e-11	10%
C023	MECHO + HV = Radical products	4.65e-4	4.16e-4	12%
C006	HCHO + HV = H2 + CO	3.49e-3	3.12e-3	12%
21	O1D + M = O3P + M	3.68e-11	3.28e-11	12%
C048	PHEN + NO3 = Products	4.50e-12	3.80e-12	18%
C036	GLY + OH = Products	1.15e-11	9.63e-12	19%
C046	BALD + NO3 = Products	4.00e-15	2.73e-15	47%
H329	HPALD + HV = Products (was RCHO) [d]	3.95e-3	1.40e-3	182%
H290	RDNO3 + HV = Products (was RNO3) [d]	7.04e-4	2.35e-4	199%
H329	HPALD + HV = Products (was ROOH) [d]	3.95e-3	3.94e-4	903%
H312	CROOH + HV = Products (was ROOH) [d]	3.95e-3	3.94e-4	903%
32	HO2 + NO + H2O = HNO3 + H2O	2.20e-31	[e]	
31	HO2 + NO = HNO3	4.21e-14	[e]	

[a] Thermal rate constant at 300K in cm-molec-sec units or photolysis rate in sec^{-1} for overhead sunlight.

[b] Not included in SAPRC-16 since this is considered to be a heterogeneous reaction.

[c] These model species are used to represent unspecified photoreactive aromatic ring opening products. Their photolysis rates are fixed and yields adjusted in SAPRC-11, while their yields are derived using the mechanism generation system and their photolysis rates adjusted in SAPRC-16.

[d] This model species was added to the mechanism to better represent photoreactive bifunctional products. The model species used for them in the previous mechanism is shown in parentheses.

[e] This reaction route is not included in SAPRC-07 or SAPRC-11.

be included, and they are not part of SumRO2. These generated model species are included at the end of the species listing on Table A-1, which also indicates the compound or mixture each is associated with. Other radical intermediates that are not explicit or represented in the base mechanism are removed and replaced by model species representing the compounds or NO_x conversions that they form.

The specific procedures used to generate explicit and lumped reactions using the mechanism generation system are discussed in the following section.

Mechanism Generation System

Overview

The mechanism generation system was used to derive the reactions of almost all of the organic compounds and lumped mixture model species in the SAPRC-16 mechanism, and significant updates were made to this system for this project. Although preparing comprehensive documentation for this system and subjecting it to peer review is one of the goals of this project, this documentation process is still underway and comprehensive documentation is not yet available. Instead, in this section we will summarize the major features and updates to the system, with emphasis on what has changed relative to the previous version that may affect the resulting mechanism and its predictions. Updates to the documentation describing the system more completely will be provided at the SAPRC-16 web site once they are available, and the reviewers will be notified of their availability.

The major features of the SAPRC mechanism generation system were described in the documentation for the SAPRC-99 mechanism (Carter, 2000), with updates for SAPRC-07 described by Carter et al (2000a). The major types of reactions it generates are summarized in Table 3, which also indicates which updates were made for this version of the mechanism. Although estimates for many types of reactions were added or modified, the following changes are notable.

The ability to generate mechanisms for the reactions of OH with alkylbenzenes, with the subsequent reactions of the OH-aromatic adducts, has been added. This includes (1) estimation of rate constants for OH addition to various positions on alkyl-substituted rings; (2) estimation of branching ratios for the various reactions of the OH-aromatic adducts with O_2; and (3) processing cycloaddition reactions of the OH-aromatic-O_2 adducts, whose subsequent reactions lead to formation of α-dicarbonyl and unsaturated 1,4-dicarbonyl ring opening products. The rate constants or relative branching ratios of the various reactions involved were estimated based on known rate constants and phenolic and α-dicarbonyl product yields for the various methylbenzenes. After adjusting the rate constants of the photoreactive unsaturated 1,4-dicarbonyl aldehydes, the estimated mechanisms perform fairly well simulating results of various methylbenzene - NO_x chamber experiments, though further adjustments and refinements may be needed to improve fits for experiments with ethyl and propyl benzenes. The system does not generate mechanisms for naphthalenes and the mechanisms it generates are not satisfactory for phenols or tetralins (significantly overpredicting reactivity), so parameterized mechanisms are still needed for these types of aromatic compounds.

The system was modified to associate more appropriate photolysis estimates for certain types of bifunctional compounds whose more rapid photolyses may impact simulations of radical levels and NO_x recycling in aged atmospheres. In particular, although the data of Barnes et al (1993) indicated that carbonyl nitrates and photolyze much faster than monofunctional nitrates, this was not incorporated in previous mechanisms. In addition, the data of Wolfe et al (2012) indicates that carbonyl hydroperoxides undergo much more rapid photolyses (forming OH) than monofunctional carbonyls or hydroperoxides, giving higher OH radical sources from low NO_x products of compounds like isoprene. Other bifunctional hydroperoxides may undergo more rapid photolyses for similar reasons The current mechanism lumps these more photoreactive bifunctional compounds into separate model species, and the mechanism

Table 3. Summary of types of reactions supported by the current mechanism generation system and updates relative to SAPRC-07.

Reactant(s)		Type of reactions (* indicates a significant change for this version)	Notes
VOC + OH		H-atom abstraction	1
		Addition to double bonds	1
	*	Addition to aromatic rings.	2, 3
VOC + O_3		Addition to double bonds followed by Criegee biradical formation.	1
		Excited adduct addition to amines, followed by decomposition of adduct forming OH	2
VOC + NO_3		H-atom abstraction	1
		Addition to double bonds	1
VOC + O^3P		Addition to double bonds	1
VOC + hν		Breaking the weakest bond in saturated aldehydes, hydroperoxides, α-dicarbonyls, PAN compounds, and monofunctional organic nitrates	1, 4
		Breaking the weakest bonds in saturated ketones	1, 5
	*	Radical formation from α-unsaturated and β-carbonyl aldehydes	2, 6
		Radical formation or decompositions of other unsaturated carbonyls.	1, 4
	*	More rapid photolysis of carbonyl nitrates and dinitrates	2, 7
	*	Very rapid photolysis of carbonyl hydroperoxides	2, 8
Carbon-centered Radicals		Unimolecular decompositions of radicals with α-nitro, α-nitrato or α-peroxy groups	1
		Reaction with O_2 with H-abstraction from α-OH groups	1
		Addition of O_2 to radicals with allylic resonance	1
	*	Reactions of O_2 with aromatic - OH adducts	2, 9
		Addition of O_2 to other alkyl radicals	1
Peroxy or Acyl peroxy Radicals		Reactions with NO forming the corresponding alkoxy radical or organic nitrate	1
	*	Cyclization of aromatic OH-O2 adducts	2, 9
	*	Unimolecular H-shift reactions forming hydroperoxides	2, 10
	*	Reactions with NO_2 forming the corresponding peroxynitrate or PAN	11
	*	Reaction with HO_2 forming the corresponding hydroperoxide	2, 12
	*	Reaction with NO_3 forming NO_2 and the corresponding alkoxy radical	2, 12
	*	Reaction with SumRO2 and SumRCO3 forming the corresponding alkoxy radical, carbonyl compound, or alcohol, depending on whether the radical has an alpha hydrogen.	2, 12
Alkoxy Radicals		α-H abstraction by O_2 forming the corresponding carbonyl compound	1, 13
		β-scission decompositions	1, 13

Table 3 (continued)

Reactant(s)		Type of reactions (* indicates a significant change for this version)	Notes
		H-shift isomerizations	14
		Ester rearrangement	1
Excited Crigiee biradicals		Decompositions, stabilization, or rearrangements of saturated biradicals	1
	*	Internal addition to the double bond of unsaturated biradicals, followed by O-O scission and epoxide formation.	2, 15

Notes:

1 Estimation methods, generated reactions, and estimated relative or absolute rate constants are generally the same as used in the previous versions.

2 This is new for SAPRC-16.

3 This is implemented for alkylbenzenes only. Naphthalenes, tetralins, and phenolic compounds are not supported

4 Some absorption cross sections and quantum yields were updated in the base mechanism.

5 Overall quantum yields were re-adjusted based on fits to chamber data. Higher quantum yields were used for the higher molecular weight ketones based on this re-evaluation.

6 The α-unsaturated and β-carbonyl aldehydes such as 2-butene 1,4-dial and compounds lumped as AFG1, AFG2A, or AFG2B are believed to be the main radical initiators in the reactions of the aromatic hydrocarbons. Their yields are determined by the mechanism generation system and their overall photolysis rates are adjusted to fit NO oxidation rates observed in aromatic - NO_x chamber experiments.

7 The data of Barnes et al (1993) indicate that carbonyl nitrates and dinitrates photolyze significantly faster than simple nitrates (about 12 and 3 times faster, relatively, for direct overhead sunlight) so they are lumped into different model species and separate sets of absorption cross sections and quantum yields are assigned to them.

8 The data of Wolfe et al (2012) suggest that alpha-unsaturated carbonyls with hydroperoxide groups photolyze at rates consistent with those calculated using absorption cross sections of alpha-unsaturated carbonyls but with unit quantum yields and with the reaction breaking the peroxy bond. This is assumed to be applicable to peroxides, PANs, and nitrates as well. However isoprene and 1,3-butadiene NOx experiments are not well simulated with this high a photolysis rate, so we arbitrarily cut the rate down by a factor of ~10 using an effective quantum yield of 0.1 This is highly uncertain.

9 The system generates three reactions for OH adducts to aromatic rings: (1) H-abstraction forming a phenolic product; (2) O_2 addition to form a peroxy radical that subsequently reacts to ultimately form the α-dicarbonyl and unsaturated dicarbonyl products assumed in previous versions of the mechanism, and (3) H abstraction forming OH and a 7-member ring cyclic ether triene. The latter is highly uncertain but it is necessary to assume that there are additional processes because known yields of phenolic products and α-dicarbonyls cannot account for all of the pathways following OH addition for benzene and alkylbenzenes. The OH-O_2 adduct formed in process (2) is assumed to primarily cyclize to form an allylic radical with a peroxy group in a second 6-member ring, which then adds O_2 and then reacts with NO to form carbonyl ring-opening products. The branching ratios were assigned based on the number of alkyl groups near the radical center and observed yields of phenolic and α-dicarbonyl products for benzene and the methylbenzenes.

10 H-shift isomerizations of peroxy radicals are estimated to be important or non-negligible for many peroxy and acyl peroxy radicals where hydrogen can be abstracted from aldehyde groups or to form

Table 3 (continued)

allylic radicals via 6- or 7-member ring transition states (Davis and Francisco, 2010; Crounse et al, 2012; Peeters et al, 2014). Methods to estimate these rate constants were developed based on the quantum calculated rate constants of Davis and Francisco (2010) and the rate constants in the methacrolein system derived by Crounse et al (2012).

11 These reactions are not needed for mechanism generation for this and previous SAPRC versions because the peroxy nitrate formed from peroxy radicals rapidly decomposes back to the reactants, and acyl peroxy radicals are represented by explicit or lumped model species so their reactions do not need to be generated.

12 These reactions were not needed when generating mechanisms with previous SAPRC versions because the system was only used to determine products formed when peroxy + NO reactions dominate. Since the current mechanism can include these other peroxy radical reactions, these additional reactions are also generated to determine the products formed. In the case of reaction with HO_2, it is assumed that the corresponding hydroperoxide is the only product, and for reaction with NO_3 it is assumed that only the corresponding alkoxy radical is formed (along with NO_2). The reactions with other peroxy or acyl peroxy radicals are represented as a single process with a generic radical, and depend on whether the radical has an abstractable alpha hydrogen.

13 Some estimation methods used for alkoxy radical reactions, and some thermochemical group assignments used for some of these estimates, were updated as part of this work. The most significant change is that new estimates for group contributions to heats of formation were added to allow estimation of more heats of reaction for alkoxy radical reactions where this is required for rate constant estimations, removing the need for manual assignments or estimates of which reactions dominate for many radicals whose heats of reactions could not previously be estimated because of missing thermochemical group additivity values.

14 The procedure used to estimate H-shift isomerizations was modified somewhat, though the estimates are generally similar for radicals formed in alkane oxidations. Rates of 1,4, and 1,6-H shifts were also estimated and their reactions generated if non-negligible, though in most cases they were negligible compared to 1,5-H shifts or competing processes.

15 This appears to be more chemically reasonable than assuming unsaturated biradicals react similarly to saturated radicals, with the overall process estimated to be highly exothermic and the level of excitation estimated to be sufficient to allow formation of a transition state with a four-member ring intermediate.

generation system determines their appropriate absorption cross section and quantum yield assignments as well as generating the appropriate photolysis reaction.

Although H-shift isomerizations of peroxy radicals are known to be important in combustion systems, they have not been considered for atmospheric mechanisms until recently. Davis and Francisco (2010) carried out quantum chemical calculations of rate constants for H-shift reactions of various peroxy radicals and obtained parameters useful for estimating rate constants for such reactions. Crounse et al (2012) proposed that these reactions can be important in the reactions of methacrolein and derived rate constants that were also useful for estimating rates for other compounds. Such reactions are also an important feature of the LIM1 isoprene mechanism of Peeters et al (2014). Based on these data and other estimates we derived procedures for estimating H-shift isomerizations of peroxy radicals, and found they are estimated to dominate over bimolecular reactions in many peroxy and peroxy acyl radicals with aldehyde groups (e.g., HC(O)CH=CHC(O)OO· from 2-butene 1,4-dial) and be non-negligible in radicals where the H-abstraction forms an allylic stabilized radical. These reactions were found to be non-negligible and affect product formation, especially but not only under low NO_x conditions. In many cases bifunctional hydroperoxides are formed that are predicted to be highly photoreactive as discussed above.

Mechanism Generation Procedures

The mechanism generation system is capable of generating fully explicit mechanisms for the atmospheric reactions of many types of organic compounds and their oxidation products. Although in principle it could be used to generate all the reactions of a selected compound and its oxidation products leading either to nonvolatile compounds or CO or CO_2, in practice it is used to generate reactions leading to first generation products, with the subsequent reactions of the non-radical oxidation products not being generated. Reactions of these product compounds are treated by separately, either by generating reactions for selected product compounds, or by representing them using lumped model species derived from generated reactions of representative compounds.

The explicit mechanism generation procedure involves the following steps:

1. The structure of the organic compound whose mechanism is to be estimated is provided as an input to the system. The types of initial reactions that the compound can undergo are assigned based on the type of compound. For example, almost all compounds are assigned as reacting with OH radicals, alkenes are designated as reacting with OH, O_3, NO_3, and O^3P, aldehydes as reacting with OH, NO_3 or by photolysis, etc.

2. All possible modes of initial reactions believed to be potentially important under atmospheric conditions are generated and the rate constant for each route is estimated or an assigned branching ratio is used if data are available. Routes that occur less than 0.5% of the time are ignored. The explicit reactions are added to the list of reactions, along with its estimated relative or absolute rate constants. Each explicit reaction refers to an elementary process, with no lumping or combining consecutive processes. Attempts to react compounds with species whose reactions are not supported, such as photolysis or ozone reactions for alkanes, result in no reactions being generated.

3. The products of the reactions are examined to determine how they are to be processed. If the product is a stable compound or a type of radical that is represented by a model species then they are treated as an end product in the system and their subsequent reactions are not generated. The latter include explicitly represented radicals such as OH, HO_2, methyl peroxy, t-butoxy, or acetyl peroxy radicals. The other radicals are added to the list of species whose subsequent reactions are to be generated.

4. All possible reactions of the next radical in the list are generated and their rate constants or branching ratios are estimated. Routes that occur less than 0.5% of the time are ignored. In the case of peroxy or acyl peroxy radicals, the system first determines whether it undergoes unimolecular reactions, with the subsequent processing depending on the magnitude of the total estimated unimolecular rate constant as shown on Table 4. The reactions and their relative or absolute rate information and products are added to the list of explicit reactions, and products not previously generated are classified as discussed above in Step 3, with reacting intermediates then processed as discussed in this step.

5. This process is complete once the list of radials to be reacted has been completely processed. The result is a list of explicit reactions and their relative or absolute rate constants, and lists of final products and intermediate reactant radicals that were generated. This is referred to as the "explicit mechanism" for first generation reactions of the subject compound. Note that second and subsequent generation reactions can be derived by separately generating explicit mechanisms for subsequent generation products, and this was done for some of the major oxidation products as discussed above. However, second and subsequent generation reactions of non-radical product compounds are not automatically generated by this system.

Table 4. Processing of reactions of peroxy and acyl peroxy radical intermediates in the SAPRC-16 mechanism generation system

Estimated unimolecular rate constant (sec^{-1}) [a]	Processing for Peroxy (RO_2) radicals	Processing for Acyl Peroxy ($RC(O)O_2$) radicals
$< 3.3 \times 10^{-3}$	Unimolecular reactions are ignored. Reactions with NO, HO_2, NO_3, RO_2, and RCO_3 are generated. Radical may be lumped with other peroxy radicals from same reactions of the starting compound. All reactions forming this radical are also indicated as also forming SumRO2.	Reactions are not generated and the radical is treated as an end product in the generated mechanism, to be represented by the peroxy radical model species MECO3, HOCCO3, ETCO3, R2CO3, R2NCO3, BZCO3, ACO3, or MACO3, depending on the radical. All reactions forming these model species are also indicated as forming SumRCO3.
3.3×10^{-3} - 0.33	Unimolecular reactions are not ignored but reactions with NO, HO_2, NO_3, RO_2, and RCO_3 are also generated. Radical is not lumped with other peroxy intermediates from the starting compound. All reactions forming this radical are indicated as also forming SumRO2.	
0.33 - 133.	Unimolecular reactions and reactions with NO are generated. Other bimolecular reactions are assumed not to be important, since the unimolecular reaction is estimated to be fast enough to dominate over these processes when NO is low. Not included in SumRO2 or SumRCO3 because peroxy + peroxy reactions are assumed not to be important.	
> 133.	Only unimolecular reactions are generated, with bimolecular reactions assumed not to be important. Processed in the same way as reactions of alkyl and alkoxy radicals. Not included in SumRO2 or SumRCO3.	

[a] These rate constant limits are somewhat arbitrary but were determined by examining the relative importances of unimolecular vs. bimolecular reactions as a function of unimolecular rate constant for representative atmospheric box model simulations.

In previous versions of SAPRC, these explicit mechanisms were incorporated into the mechanism for airshed or box models by summing up the total yields of final products or NO consumptions or conversions under conditions where reactions of peroxy radicals with NO dominate, and using these for product yield parameters in generalized reactions with adjustable product yield parameters. This requires assuming that peroxy radicals that react with NO or HO_2 do not undergo significant unimolecular reactions, which not the case for many compounds in the current mechanism. As discussed above, it is necessary to represent peroxy radicals involved in the reactions of organics as separate model species in the mechanisms so their competing reactions can be properly simulated. Therefore, the following approach was used for implementing explicitly generated mechanisms into SAPRC-16. Note that reactions with O_2 are treated as unimolecular for the purpose of this analysis, so the processed mechanisms cannot be used for situations where the O_2 concentration varies.

1. All reactions with the same reactants (with reactions with O_2 being treated as unimolecular for this purpose) were combined into a single reaction with variable product yields derived from the branching ratios of the competing reactions.

2. All radical intermediates that do not have generated bimolecular reactions (other than with O_2) are replaced by the set of products they form in the unimolecular or O_2 reactions. This is done recursively until there are no such reactants remaining. Therefore, these species do not need to be considered further. The remaining reactions include reactions of the starting compound and bimolecular and in some cases unimolecular reactions of various peroxy and acyl peroxy radical intermediates. (Note that acyl most acyl peroxy radicals are treated as final products and thus not included as new intermediates except for those represented as reacting unimolecularly or with NO only -- see Table 4). In some cases, this can yield relatively large numbers of model species representing peroxy radical intermediates, many with very low yields and contributions to the overall process.

3. Peroxy radical intermediates that do not have unimolecular reactions or whose unimolecular reactions are slow enough to ignore (see Table 4) and that are formed by the same (or nearly the same) set of reactions are lumped together for representation by a lumped peroxy model species. The yields of products of its bimolecular reactions determined by the relative contributions of the individual radicals that are lumped, multiplied by their product yields. This reduces the number of peroxy radical model species in mechanisms where multiple peroxy radicals that react similarly are formed from reactions of the same compound or set of intermediates. Other peroxy radical intermediates, and acyl peroxy radical intermediates that have generated unimolecular and NO reactions (see Table 4) are represented separately.

4. In order to further reduce the number of peroxy radical model species needed, and eliminate those with only minor contributions to the overall processes, the relative importance of each intermediate peroxy radical is determined from its yields and the yields of its precursors in the various reactions forming them. Those with overall yields of less than 10% relative to the initial reactions of the starting VOCs are eliminated by replacing them with the products they form considering only unimolecular or NO reactions, with the relative importance of unimolecular vs. NO reactions being estimated based on an atmospheric NO concentration of 0.5 ppb, and the peroxy + NO rate constant given for SumRO2 in Table A-3. The reactions of these minor peroxy radicals with NO_3, HO_2, and other peroxy radicals are ignored. Peroxy radicals formed in their reactions are treated in the same way, with their products being added to the products of the starting radical. The NO to NO_2 conversions in multi-step mechanisms are represented using the operator RO2C, the NO consumptions involved with nitrate formation in peroxy + NO reactions are represented by RO2XC, and the nitrates they form are represented by various zRNO3 species, depending on how the nitrate formed is lumped in the mechanism. The latter either react with NO to form the corresponding nitrate model species, or react with HO_2, NO_3, or other peroxy radicals to form model species representing other appropriate products. This is similar to the use of RO2C, RO2XC, and the zRNO3 species in the SAPRC-07 and -11 mechanisms, except that for the earlier mechanisms they are used for essentially all peroxy radical reactions, not just those with relatively low contributions, as is the case for SAPRC-16.

5. The products in the remaining lumped reactions are replaced by the appropriate explicit or lumped model species, based on lumping rules that are specified for use with the mechanism. The peroxy radical model species that remain are given names such as (name)_P1, (name)_P2, (name)_A1, etc, where (name) is the model species name used for the reactant. The $\_P_n$ suffix is used for peroxy radicals that undergo all bimolecular reactions and that are included with SumRO2, and the $\_A_n$ suffix is used for those with only unimolecular and NO reactions and are not included with SumRO2.

6. The merged or lumped mechanisms derived as discussed above are given in the last section of Table A-3. They consist of lumped initial overall reactions of the organic with OH and other applicable species such as O_3, forming model species in the base mechanism and compound-

specific peroxy radical model species, followed by the reactions compound-specific peroxy model species. These can include radical species formed in the initial reactions or in the reactions of some other radical species ultimately formed in the other reactions. The rate constants used for the initial reactions of the organic being processed are either those assigned for the individual compound as indicated in footnotes to Table A-3, or are derived from estimated rate constants of the individual reaction pathways if data are not available. The unimolecular rate constants of the peroxy intermediates are those estimated for the specific radicals, and their bimolecular rate constants are those given on Table A-3 for the corresponding reaction of SumRO2.

An analogous process is used when deriving mechanisms for lumped model species based on generated explicit mechanisms of its components (see Table A-2 for the components used for each mixture, and the derivations of the mixtures). The only difference is that before step 1 all of the initial reactions of the components are merged together with relative yields determined by the fraction of the compound in the mixture multiplied by the relative yields of the initial reaction pathways for the compound, and treated as if they are reactions of the mixture as if it were a single reactant. The subsequent reactions generated for the compounds are then used to locate and process the reactions of the intermediate radicals formed in the initial reactions and the subsequent reactions as they are processed. The processing procedures for the subsequent reactions are exactly the same as used for processing mechanisms of single compounds. The result is a lumped mechanism for the mixture represented as a single model species, including the reactions of the major peroxy radicals formed in the reactions of its components. These reactions are included in Table A-3 for all the lumped model species whose mechanisms were derived this way.

Programming Platform

The mechanism generation system is incorporated into an online MOO system, which was originally developed as a programmable text-base virtual reality system (MOO, 2016, 2014, 1997). This type of text-based system is no longer widely used for online virtual reality experiences and the programming system is no longer being developed or supported, but features of the object-oriented programming language made it much better suited for mechanism generation applications than Fortran or other programming languages that the author is familiar with, so that is why it was used for its initial development. In theory this system could be converted to another platform whose underlying programming system is still being supported. This would allow it to continued to be maintained into the future as a collaborative effort and with more people being available who can program for it. However, this would be a major effort that is well beyond the scope of this project, and there is no urgent incentive to do so since the current system performs satisfactorily. Its online access capabilities, discussed below, provide advantages that may be more difficult to implement using other platforms.

The mechanism generation system is normally accessed using a Telnet client to log in with administrative access to program the system, input its assignment data, generate reactions, process results for mechanism implementation, and download the results in text files for incorporation into the mechanism. Although the MOO system is capable of allowing non-administrative access via Telnet clients for others to work with the system, this capability is not currently implemented in a secure enough fashion to be practical. However, it does have the capability to allow anyone to access the system via a web interface as discussed in the following system. This web interface was developed previously for use with online social MOOs, but its capabilities are used in this system to allow others to access the system and generate reactions online for their own research or review purposes.

Online access

Although the documentation for this system is not complete, those interested in the system can access it online at http://mechgen.cert.ucr.edu:8000. A link to this system is available at the SAPRC-16 mechanism web site at http://www.cert.ucr.edu/~carter/SAPRC/16 (Carter, 2016). It is necessary to log in to access the system, but no registration, username, or password is required for anonymous access. Note that there are two SAPRC mechanism generation systems online, this one that was developed for SAPRC-16 as discussed in this document, and the stable version for SAPRC-07/11 that is available at http://mechgen.cert.ucr.edu (i.e., without the ":8000"). Once logged in, users can create radical or stable reactants (there is help on how to designate structures using the standard MechGen designation, or Smiles notation or detailed model species names can also be used), or one can select compounds to react from a menu listing compounds on the current SAPRC species list. The system can be used to generate reactions of stable compound with atmospheric species such as OH, O_3, NO_3, O^3P, photolysis or by unimolecular reaction where applicable, or atmospheric reactions of radical species, and will output documentation information indicating estimated or assigned rate constants or branching ratios used and the products formed. The system can then be used to react the products, seeing how they are estimated to react and also has the capability of generating full mechanisms online (i.e., without using administrative Telnet access).

Until more comprehensive documentation is available, reviewers of this mechanism can access the system to see how it processes reactions of various types of species. When reactions are run one compound at a time the system outputs documentation text indicating how the estimates were made or if the reaction pathways or rate constants was assigned for the specific compound or radical. Those who are interested can contact the author to get on a mailing list to be notified when new capabilities, such as the capabilities of generating and viewing complete explicit and lumped mechanisms for selected compounds, are implemented. They will also be notified when updates to the documentation, now in preparation, are available.

Evaluation Against Chamber Data

The performance of previous SAPRC mechanisms in simulating O_3 formation, rates of NO oxidation, and other measures of reactivity was evaluated by conducting model simulations of over 2500 environmental chamber experiments carried out in 11 different environmental chambers at 4 different laboratories (Carter, 2000). The experiments used for SAPRC-07 included 682 single VOC experiments, consisting primarily of VOC - NOx or VOC - NO_x experiments with added CO or alkane, 591 incremental reactivity experiments, and 973 experiments with mixtures, though approximately 2/3 of the mixture runs were replicate base case reactivity experiments of various types. The procedures used in the evaluation and descriptions and lists of the experiments used have been described previously (Carter, 2000, 2010a, and the same procedures were used in this work. A number of more recent aromatic-NO_x experiments in the UCR chamber were added for evaluating the SAPRC-11 aromatics mechanism (Carter and Heo, 2013), and a number of new alkene - NO_x and a few other experiments in the UCR chamber (Yarwood et al, 2012; Heo et al, 2014) were subsequently carried out and are available for evaluating SAPRC-16.

Most of these experiments have been simulated using SAPRC-16, and aspects of mechanisms for several types of compounds were adjusted as part of this process. In most cases the results of the simulations are comparable to those for SAPRC-11, but there are some compounds where the simulations using SAPRC-16 are not quite as good as those using SAPRC-11, and there are some compounds where the performance of SAPRC-16 should be improved before reactivity values for the compounds are used in regulatory applications. However, the performance of SAPRC-16 in simulating experiments with the major compounds in mixtures, and most of the other compounds for which experiments have been

carried out is considered to be generally satisfactory and as good as can reasonably be obtained within the scope of the current project.

The primary evaluation metric used in this work was the ability of the model to simulate the amounts of NO oxidized and ozone formed in the experiments. This is measured by the quantity Δ([O3]-[NO]), defined as follows:

$$\Delta([O_3]\text{-}[NO])_t = \{[O_3]_t - [NO]_t\} - \{[O_3]_0 - [NO]_0] = [O_3]_t + [NO]_0 - [NO]_t$$

This gives a measure of reactivity that is useful regardless of whether NO or O_3 is in excess, and has been used in previous evaluations. A secondary metric was the effect of adding the compound on the integrated OH levels, or IntOH, in the incremental reactivity experiments. The integrated OH is derived from the rates of consumption of a reactive compound present in the base case surrogate mixture that reacts significantly with OH radicals, usually m-xylene, given the OH rate constant and the dilution rate if applicable. This is used primarily when evaluating the mechanisms using the incremental reactivity experiments, as discussed below. The derivation and use of these metrics have been discussed in detail in reports describing previous SAPRC evaluations (Carter, 2000, 2010, Carter and Heo, 2012).

Single Compound Experiments

The results of the model simulations of the single compound - NO_x experiments are summarized in Table 5. Results are shown both for SAPRC-16 and, for comparison purposes, for SAPRC-11, the previous version of this mechanism. Footnotes to the table give subjective judgments as to whether the performance of the updated mechanism is better, worse, or about the same as SAPRC-11, and indicate cases where adjustments were made to improve the fits. The footnotes also indicate whether adjustments were made to the mechanism based on the simulations of these experiments (or simulations of incremental reactivity experiments, where applicable).

As indicated on the table, generally the fits to the results of the single compound experiments were reasonably good for both SAPRC-16 and SAPRC-11, considering run-to-run variability and other uncertainties. Note that for the benzene and the methylbenzenes the only adjustments made were the photolysis rates of the model species used to represent the photoreactive ring opening products, and adjustments using data for a subset of the compounds gave satisfactory simulations for most of the others, though the fractions of addition to the aromatic ring vs. abstractions from the side groups had to be adjusted to give satisfactory results for ethyl and the propyl benzenes. The yields of the photoreactive ring opening products relative to addition to the ring in SAPRC-16 were derived using the mechanism generation system and were not adjusted. This contrasts with SAPRC-11, where the yields were adjusted for each aromatic to optimize the fits to these runs. Benzyl alcohol was the only compound where the model performance for SAPRC-16 is significantly worse than for SAPRC-11, and this is because adjustments were not made for this specific compound.

Mixture Experiments

Table 5 also summarizes the performances of the mechanisms in simulating $\Delta([O_3]\text{-}[NO])$ in the various mixture - NO_x experiments. Many but not all of these were used as the "base case" in the incremental reactivity experiments used for mechanism evaluation, discussed below. For most surrogate mixtures the performance of SAPRC-16 was comparable to that of SAPRC-11, though there is a tendency for SAPRC-16 to overpredict $\Delta([O_3]\text{-}[NO])$ in mixture experiments on the average, more than is the case for SAPRC-11. This is despite the fact there does not appear to be a consistent overprediction bias in the single compound experiments, so it is not obvious how to modify the mechanism to reduce this bias for the mixture runs. However, there was no overprediction bias in the simulations of the mixture experiments in the TVA chamber and the biases in simulations of the UCR standard surrogate experiments depended on the initial organic/NO_x ratios, as discussed below.

Table 5. Summary of results of evaluations of SAPRC-16 and SAPRC-11 against single compound and mixture - NO_x chamber experiments.

Compound or Run Type	No. Runs	Average Bias or Error for $\Delta([O_3]-[NO])$. SAPRC-16 Bias	SAPRC-16 Error	SAPRC-11 Bias	SAPRC-11 Error	Change in Error	Notes [b]
Radical source characterization	214	-4%	20%	-7%	20%	0%	Ch
NOx offgasing characterization	42	22%	40%	10%	37%	3%	Ch
Ethene	49	10%	21%	9%	20%	1%	0
Propene	172	15%	21%	4%	16%	4%	0
1-Butene	10	-7%	20%	-2%	25%	-5%	0
1-Pentene	4	5%	9%	4%	8%	1%	0
1-Hexene	8	-8%	12%	18%	18%	-6%	0
Isobutene	7	-25%	25%	-21%	21%	4%	0, A
cis-2-Butene	4	45%	45%	22%	22%	24%	0
trans-2-Butene	9	0%	13%	-3%	13%	0%	0
2-Methyl-2-Butene	5	-5%	9%	-9%	10%	-1%	0
cis-2-Pentene	4	18%	18%	9%	9%	9%	0
1,3-Butadiene	4	-12%	14%	-68%	68%	-54%	+, A
Isoprene	11	-6%	8%	-8%	11%	-3%	0, A
3-Carene	4	5%	17%	-22%	22%	-5%	0, A
a-Pinene	6	3%	6%	0%	10%	-4%	0, A
b-Pinene	5	28%	28%	25%	25%	3%	0, A
d-Limonene	6	7%	17%	47%	47%	-30%	+, A
Sabinene	3	7%	7%	3%	6%	1%	0, A
Acetylene	4	-10%	10%	-11%	11%	-1%	0
Benzene	16	46%	52%	52%	59%	-8%	0, 1, 2
Toluene	81	15%	25%	15%	27%	-1%	0, 3
Ethyl Benzene	14	25%	28%	34%	37%	-9%	+, 1, 4, A
n-Propyl Benzene	4	-7%	7%	-4%	8%	-1%	0, 4, A
Isopropyl Benzene (cumene)	6	3%	8%	-1%	7%	2%	0, 4, A
m-Xylene	134	0%	15%	-1%	20%	-5%	0, 5
o-Xylene	27	16%	19%	0%	14%	5%	0, 3
p-Xylene	29	31%	36%	29%	37%	-1%	0, 6
m-Ethyl Toluene	10	-22%	25%	-11%	21%	5%	0, 3
o-Ethyl Toluene	11	0%	11%	-11%	15%	-4%	0, 3
p-Ethyl Toluene	7	-34%	34%	-15%	33%	1%	0, 3
1,2,3-Trimethyl Benzene	13	10%	14%	-8%	11%	3%	0, 5
1,2,4-Trimethyl Benzene	25	-2%	24%	-4%	27%	-2%	0, 3
1,3,5-Trimethyl Benzene	25	12%	14%	-15%	17%	-4%	0, 7
Tetralin	3	13%	44%	-32%	32%	13%	0
Naphthalene	5	10%	15%	-5%	11%	4%	0, 8, A
2,3-Dimethyl Naphthalene	4	5%	11%	-8%	11%	0%	0, 8, A
phenol	5	13%	18%	0%	24%	-6%	0, 8, A
o-Cresol	7	21%	23%	14%	28%	-5%	0, 8, A
2,4-dimethyl phenol	4	8%	14%	0%	21%	-8%	0, 8, A

Table 5 (continued)

Compound or Run Type	No. Runs	Average Bias or Error for $\Delta([O_3]-[NO])$. SAPRC-16 Bias	SAPRC-16 Error	SAPRC-11 Bias	SAPRC-11 Error	Change in Error	Notes [b]
Benzyl alcohol	6	34%	34%	-1%	8%	26%	*
Formaldehyde	33	-11%	18%	-5%	13%	5%	0
Acetaldehyde	14	6%	15%	3%	13%	2%	0
Acrolein	3	-1%	16%	-4%	22%	-7%	0, A
Methacrolein	12	-7%	24%	-12%	25%	-1%	0, A
Acetone	5	-20%	20%	-18%	19%	1%	0, A
Methyl Ethyl Ketone	6	1%	6%	4%	7%	-1%	0, A
2-Pentanone	1	-1%	1%	8%	8%	-7%	0, A
2-Heptanone	1	-11%	11%	-50%	50%	-39%	+, A
Methylvinyl ketone	6	-3%	26%	-21%	25%	1%	0, A
UCR standard surrogates	454	15%	20%	9%	19%	2%	+, 7
TVA surrogate mixtures	21	-9%	13%	-18%	20%	-7%	0
Non-aromatic UCR surrogates	26	20%	23%	16%	19%	3%	0
UCR "mini surrogate" mixtures	280	34%	36%	5%	17%	19%	--
Older UCR surrogate mixtures	60	36%	52%	33%	53%	-1%	0
Miscellaneous other surrogates	19	53%	56%	31%	36%	20%	--

[a] The NO oxidation rate is the average rate of change of $\Delta([O3]-[NO])$ up to the time of one half the ozone maximum. The average bias is the average of (model - experimental) / experimental for all experiments of this type, and the average error is the average of the absolute values of this quantity.

[b] Notes are as follows:

Ch These were used to derive chamber model parameters, which were adjusted to minimize biases. Errors indicate run-to-run variability and not necessarily mechanism performance issues.

0 No significant change in model performance.

A Adjustments made to improve fits.

+ Updates caused model performance to improve.

-- Updates caused model performance to be slightly worse.

* Adjustments or modifications to the mechanism will be needed for calculating the reactivity value, but this will not significantly affect reactions in the standard atmospheric mechanism.

1 Average bias is positive because experiments indicate that the reactivity increases as NO_x levels are increased, which is not predicted by the mechanism. The mechanism was adjusted to optimize fits for low NO_x conditions that are more representative of most current atmospheres. This problem existed in previous versions of SAPRC and was not corrected with this update.

2 The photolysis rate of the BUDAL model species was adjusted to fit NO oxidation rates in benzene experiments with $NO_x < 100$ ppb.

3 The photolysis rates of the photoreactive fragmentation products adjusted to fit NO oxidation rates benzene and some of the methyllbenzenes gave acceptable fits to the NO oxidation rates for experiments with this compound (for $NO_x < 100$ ppb in the case of toluene) that no adjustments had to be made for this particular compound.

4 The fraction of OH abstracting from the alkyl side group was adjusted upwards in order to optimize model fits to chamber data. The photolysis rates of the photoreactive products were not

Table 5 (continued)

adjusted, but were assumed to be the same as those that fit the methylbenzenes.

5 The photolysis rate of the AFG2A model species was adjusted to fit NO oxidation rates in the m-xylene and 1,2,3-trimethylbenzene experiments.

6 The photolysis rate of the AFG1 model species was adjusted to fit NO oxidation rates for the p-xylene - NO_x experiments.

7 The photolysis rate of the AFG2B model species was adjusted to fit NO oxidation rates for the 1,3,5-trimethylbenzene - NO_x experiments.

8 A parameterized mechanism, similar to that used for SAPRC-11, was used. Parameter values were adjusted to fit chamber data.

9 The tendency for underprediction bias to increase at lower ROG/NO_x ratios was reduced compared to SAPRC-11 but not eliminated. See Figure 1.

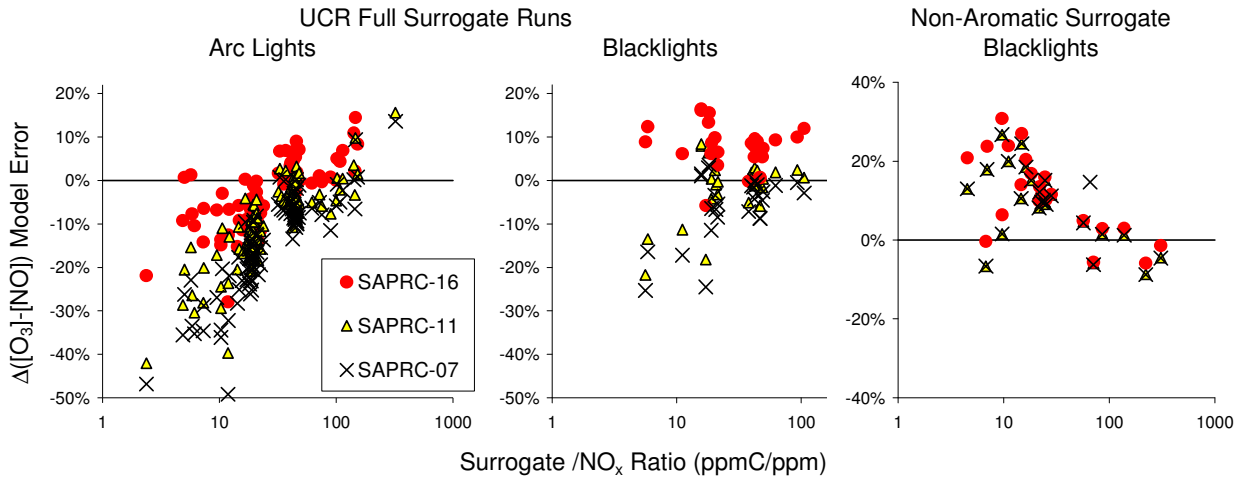

Figure 1. Plots of errors in predictions of final NO oxidation and ozone formation rates against the initial surrogate / NO_x ratios for the various atmospheric surrogates and non-aromatic surrogate - NO_x experiments carried out in the UCR chamber.

It was noted previously that the SAPRC-07 and SAPRC-11 mechanisms tended to underpredict $\Delta([O_3]\text{-}[NO])$ in the UCR standard surrogate experiments at low surrogate/NO_x ratios, with the underprediction becoming less and eventually not occurring if the ratio becomes sufficiently large (Carter et al, 2005, Carter and Heo, 2013). This is associated with the model for the aromatics since this is not observed in simulations when the aromatics are removed from the surrogate. This is shown on Figure 1, which also shows model simulations of these experiments with SAPRC-16. This dependence of underprediction bias on the surrogate/NO_x ratio is also observed with SAPRC-16, but to a much lesser extent than the other two mechanisms, and with the bias being consistently high and independent of the Surrogate/NO_x ratio for the surrogate experiments using blacklights. This can be attributed to changes in the mechanisms for the AFG species used to represent the photoreactive ring opening products, where the previous versions had the photolysis primarily forming unsaturated acyl peroxy radicals that reacted with NO_2 to form PAN analogues, while the updated version has these unsaturated acyl peroxy radicals primarily undergoing relatively rapid unimolecular reactions, forming radicals that ultimately react to form increased levels of OH and other radicals.

Incremental Reactivity Experiments

The mechanism was also evaluated by comparing its ability to predict the incremental reactivities of various compounds with respect to NO oxidation and O_3 formation as measured by $\Delta([O3]\text{-}[NO])$ and on integrated OH levels (IntOH) as measured by rates of consumption of surrogate components that react only with OH. The incremental reactivities IR's relative to $\Delta([O3]\text{-}[NO])$ are derived as follows:

$$\text{IR } \Delta([O_3]\text{-}[NO])_t = \frac{\Delta([O_3]\text{-}[NO]) \text{ at time t in the experiment with the added compound} - \Delta([O_3]\text{-}[NO]) \text{ at time t in the base case experiment}}{\text{Amount of compound added}}$$

$$\text{IR IntOH}_t = \frac{\text{IntOH at time t in the experiment with the added compound} - \text{IntOH at time t in the base case experiment}}{\text{Amount of compound added}}$$

In most cases the incremental reactivity experiments were carried out in a dual chamber, where the base case surrogate and NO_x was injected into both sides of the chamber and mixed, the chambers were closed off and the test compound was added to one side, and the two chamber sides were irradiated together. Some earlier incremental reactivity experiments were carried out in the single reactor "ETC" chamber with base case and added compound experiments alternating, and statistical analyses done to determine base case results corresponding to the conditions of each added compound experiment (Carter et al, 1993). Most of these experiments are described in the SAPRC-07 mechanism evaluation report (Carter, 2010) or references therein.

Table 6 gives a summary of the incremental reactivity experiments used in this mechanism evaluation and gives qualitative indications and comments concerning the fits obtained for both SAPRC-16 and SAPRC-11. Plots of selected experimental and SAPRC-11 and SAPRC-16 model results for each of these experiments are given in tables in Appendix B. These include plots of $\Delta([O3]\text{-}[NO])$ in the base case and test experiments, and the incremental reactivities relative to $\Delta([O_3]\text{-}[NO])$ and integrated OH (IntOH). Table 6 gives the page numbers where the plots can be found in Appendix B for the various compounds.

As discussed on Table 6 and shown in the figures in Appendix B, both mechanisms performed reasonably well in simulating the results of the incremental reactivity experiments, though there were cases of less satisfactory performance for the updated mechanism. SAPRC-16 did not perform as well as SAPRC-11 for some of the branched alkanes, particularly 2,2,4-trimethyl pentane, several of the oxygenated compounds, and some oxygenated compounds. In some cases improvements could be made by adjusting nitrate yields from reactions of NO with the peroxy radicals involved, or by changing

Table 6. Summary of incremental reactivity experiments used for mechanism evaluations. Plots of selected results are given in figures in Appendix B.

Compound	No. Runs	Page	Results [a] Fits	Comments
			Alkanes (See Figure B-1)	
Ethane	7	2	ok	
Propane	3	2	ok	
n-Butane	10	3	ok	
Isobutane	4	4	ok	
n-Hexane	3	4	ok	
Cyclohexane	6	5	ok/+	Slightly better than SAPRC-11 for some runs
n-Octane	13	5-6	ok	
2,2,4-Trimethyl Pentane	2	7	*	SAPRC-11 overpredicts inhibition of IntOH and $\Delta([O_3]-[NO])$ for the two very similar experiments. SAPRC-11 gives much better fits. No simple chemically reasonable adjustment could improve fits.
2,6-Dimethyl Octane	5	7	Var/-	SAPRC-11 is slightly better for some runs
2-Methyl Nonane	5	8	ok	
3,4-Diethyl Hexane	6	8-9	Var/-	SAPRC-11 is slightly better for some runs
n-Dodecane	9	9	ok	
n-Tetradecane	8	10	Var.	Inhibition of Δ([O3]-[NO]) is somewhat overpredicted for some runs
n-Pentadecane	2	10	Var.	Similar to n-tetradecane
n-Hexadecane	5	11	ok	
Hexyl Cyclohexane	6	11-12	ok	
Octyl Cyclohexane	7	12	ok	
			Alkenes and Acetylene (See Figure B-2)	
Ethene	4	13	ok	
Propene	10	14	ok	
Isobutene	3	13	ok	
trans-2-Butene	9	15	ok	
Cyclohexene	1	13	ok	
Isoprene	15	16-17	ok	
a-Pinene	4	17	ok	
b-Pinene	2	17	*	Both SAPRC-11 and SAPRC-16 tend to underpredict underprediction of NO oxidation rates in the middle of the experiments, though reactivities by the end of the runs are predicted.
d-Limonene	3	18	*	SAPRC-11 performs somewhat better for two of the runs but SAPRC-16 does better for the other.
Acetylene	7	18	ok	
			Aromatics (See Figure B-3)	
Styrene	6	19	ok	
Benzene	4	19	Var.	Good fits for low NO_x experiments but significant overprediction for high NO_x runs, consistent with simulations of benzene - NO_x runs.
Toluene	11	20	ok	

Table 6 (continued)

Compound	No. Runs	Page	Results [a] Fits	Comments
m-Xylene	17	21-22	Var.	Some runs are not fit as well by either mechanism but no consistent bias.
o-Xylene	2	22	Var/-	SAPRC-16 has a slight tendency to overpredict for the two very similar runs; SAPRC-11 fits data well.
p-Xylene	1	22	ok	
1,2,3-Trimethyl Benzene	2	23	ok	
1,2,4-Trimethyl Benzene	2	23	ok	
1,3,5-Trimethyl Benzene	1	23	Var/-	Slight tendency to overpredict for the one run
Ethyl Benzene	3	23	?	Amounts added too small for good test of mechanisms
Benzaldehyde	3	24	ok	
m-cresol	1	24	ok	
Benzyl alcohol	3	24	ok	
			Oxygenated Products	
Carbon Monoxide	13	25-26	ok	
Methanol	3	26	ok	
Ethanol	3	26	ok	
Formaldehyde	8	27	Var.	Slight tendency to overpredict in some runs
Acetaldehyde	5	28	ok/+	
Acetone	8	28-29	ok	
Methyl Ethyl Ketone	5	29	Var/-	Slight tendency to underpredict at the end of some experiments could be due to minor discrepancies in simulating the base case.
2-Pentanone	4	30	ok	
2-Heptanone	3	30	ok	
4-Methyl-2-Pentanone	8	31	ok	
Cyclohexanone	9	32	*	SAPRC-16 has a tendency to overpredict inhibition in some experiments and overpredict reactivity in some others, while SAPRC-11 performs generally better.
			Other Oxygenated Compounds	
Dimethyl Ether	4	33	ok	
Diethyl Ether	6	33	ok	
Methyl t-Butyl Ether	4	34	Var/-	SAPRC-16 has a slight tendency to overpredict effects on Δ([O3]-[NO]) and inhibition of IntOH, but may be within experimental variability. SAPRC-11 somewhat better.
Isopropyl Alcohol	10	35	ok	
t-Butyl Alcohol	7	36	Var.	Some variability in fits but both mechanisms perform about the same. Some tendency to overpredict effects on NO oxidation rates and O3 formation and inhibition of IntOH.
1-Octanol	4	37	ok	
2-Octanol	3	37	Var.	Both mechanisms tend to overpredict effects on Δ([O3]-[NO]) in some experiments.
3-Octanol	3	37	Var.	Similar to 2-octanol
Ethylene Glycol	5	38	ok	
Propylene Glycol	12	38-39	ok	

Table 6 (continued)

Compound	No. Runs	Page	Results [a] Fits	Comments
Methyl Acetate	7	40	Var.	Good fits for some runs but tendency to overpredict effect on Δ([O3]-[NO]) in some runs.
Ethyl Acetate	9	41	Var.	Tendency to overpredict inhibition of Δ([O3]-[NO]) in some runs but good fits to others.
Isopropyl Acetate	3	42	ok	
t-Butyl Acetate	6	42	Var/-	SAPRC-16 has tendency to overpredict inhibition of Δ([O3]-[NO]) in some runs where it is inhibited, but fits to runs where it increases Δ([O3]-[NO]) are more variable.
n-Butyl Acetate	8	43	Var/-	Similar to t-butyl acetate
Methyl Isobutyrate	7	44	*	SAPRC-16 has a tendency to overpredict inhibition or underpredict reactivity, while SAPRC-11 performs better. See also comments for methyl pivalate.
Methyl Pivalate	6	44-45	ok	In order to obtain satisfactory simulations for this compound, and improve results for methyl isobutyrate, it was necessary to assume that $CH_3OC(O)\cdot$ radicals primarily add O_2 to ultimately form the PAN analogue $CH_3OC(O)OONO_2$, rather than decomposing to form $CH_3\cdot + CO_2$, which was estimated to be more favorable in the first distributed version of the updated mechanism.
2-Ethoxyethanol	3	45	ok	
2-(2-Ethoxyethoxy) Ethanol	3	45	ok	
1-Methoxy-2-Propanol	6	46	ok	
2-(2-Butoxyethoxy)-Ethanol	3	46	ok	
2-Butoxyethanol	7	47	Var/-	SAPRC-16 tends to overpredict inhibition in runs where the compound inhibits Δ([O3]-[NO]) but generally gives better fits where it has a positive effect on Δ([O_3]-[NO]). SAPRC-11 somewehat better.
Dimethyl Succinate	6	48	Var/-	SAPRC-16 tends to overpredict inhibition or underpredict reactivity in some runs. SAPRC-11 is generally better.
Dimethyl Glutarate	6	49	Var/-	SAPRC-16 gives good fits in runs where the compound inhibits Δ([O3]-[NO]) but underpredicts reactivity in runs where it has a positive effect. SAPRC-11 somewhat better in this regard.
Dimethyl Carbonate	5	50	ok	
Propylene Carbonate	7	50-51	Var.	Tends to overpredict inhibition in runs where the compound inhibits Δ([O3]-[NO]) but gives fair fits to runs where it has a positive effect on zone. SAPRC-11 is similar.
Methyl Isopropyl Carbonate	6	51	ok	
1-Methoxy-2-Propyl Acetate	6	52	Var/-	SAPRC-16 has a slight tendency to overpredict inhibition in runs where it inhibits Δ([O3]-[NO]) but also overpredict its positive effects in runs where it increases Δ([O_3]-[NO]). SAPRC-11 somewhat better.

Table 6 (continued)

Compound	No. Runs	Page	Results [a] Fits	Comments
Texanol® isomers	4	52	ok	
				Amines
Ethanolamine	5	53	Var.	Both mechanisms appropriately predict effects on NO oxidation rates but do not predict experimentally observed tendency of the compound to reduce final O_3 yields in runs achieving an O_3 maximum.
isopropylamine	1	53	Var/-	Does not predict experimentally observed tendency of the compound to reduce final O_3 yields in runs achieving an O_3 maximum. This is also a problem for SAPRC-11 but not as much as SAPRC-16.
t-butyl amine	1	53	ok	
2-Amino-2-Methyl-1-Propanol	7	54	ok	

[a] The "Page" column gives the page number in Appendix B where the data from the experiments with the compound is shown. The "Fits" column gives notes giving a qualitative indication of the quality and acceptability of the of the model calculations to the data, as follows:

ok	Reasonably good fits for both SAPRC-16 and SAPRC-11
ok/+	Reasonably good fits for SAPRC-16. SAPRC-11 not quite as good.
Var.	SAPRC-16 and SAPRC-11 have variable performance depending on the experiment but generally give similar performance
Var/-	SAPRC-16 has variable performance depending on the experiment. SAPRC-11 generally performs better for these runs.
?	The quality of the fits could not be assessed very precisely because the amount of compound added was too small to have a very large effect on measurements.
*	Although the model is not grossly off, the fits for SAPRC-16 is not considered acceptable and the mechanism needs improvement before used for calculating a reactivity value for the compound. No chemically reasonable adjustment could be found to improve simulations and more work is needed.

assumptions concerning some uncertain pathways back to the assumptions used previously. However, the reasons for the reduced performance in simulating reactivities for some of the compounds were more difficult to assess because of the complexity of the mechanisms and the fact that there is more than one uncertain branching ratio, making adjustments difficult and probably ill-advised. In some cases only small changes in highly uncertain estimated rate constants were found to cause changes in reaction pathways that significantly affect reactivity. These will need to be investigated further before the mechanism is used to calculate reactivity scales that include these and related compounds.

Note that in order to obtain satisfactory results of simulations incremental reactivity results for C8+ alkanes it is necessary to assume that alkyl nitrate yields for OH-substituted C8+ peroxy radicals are about the same as those for unsubstituted peroxy radicals. The nitrate yields from peroxy + NO reactions increase with the size of the molecule, and product studies indicate that OH-substituted peroxy radicals such as occur in higher alkane systems following alkoxy H-shift isomerizations have lower nitrate yields than unsubstituted peroxy radicals. In SAPRC-07/11 this was done reducing the effective carbon number

when estimating nitrate yields for OH substituted radicals, which means that the effects of OH substitution is less at higher carbon numbers since the nitrate yields eventually level off as the carbon number increases. However, data given by Yeh (2013) suggested that OH-substitution reduces yields about equally regardless of the size of the molecule, so this was implemented in the first version of SAPRC-16 that was made available for peer review. This version performed much worse than SAPRC-11 in simulating reactivity experiments with higher alkanes and the octanols, significantly overpredicting the inhibition caused by adding these compounds. For that reason, the current version of the mechanism was changed back to use the SAPRC-07/11 nitrate estimation methods, and much better performance in simulating the reactivity data was obtained. It may be that the yields of higher hydroxy nitrates measured by Yeh (2013) had experimental problems due to wall losses, so these data were not used when deriving best-fit parameters to estimate nitrate yields in the mechanism generation system.

Although the evaluation using the reactivity experiments indicated problems with certain compounds that will need to be investigated further before new reactivity scales are calculated, the current mechanism performs reasonably well for the major compounds that are important in ambient simulations. Other mechanisms used in airshed models have not been as extensively evaluated using these data, but it is unlikely that their performance is significantly better.

Examples of Atmospheric Box Model Simulations

The effects of the mechanism updates were examined by conducting multi-day box model simulations of simplified ambient scenarios where both VOCs and NO_x were emitted continuously during the daylight hours. These were similar to the simulations used to test effects of mechanism condensations when developing the condensed versions of SAPRC-07 as discussed by Carter (2010d), and that reference can be consulted for details. These simulations all had the same inputs except for the total amounts of NO_x that was emitted, which were varied such that the ROG/NO_x ratio of emitted reactants (C/N) ranged from approximately 4 to approximately 70 moles carbon per mole nitrogen. In order to place the treatment of heterogeneous reactions on an equal basis, the nonzero N2O5+H2O rate constants in SAPRC-11 were set to zero so they would be the same as used in SAPRC-16, since these reactions are now assumed to be entirely heterogeneous and has zero rate constants in SAPRC-16. The results of these simulations using SAPRC-16 are compared with those using SAPRC-11 on Figure 2 for O_3, H_2O_2, and OH, and on Figure 3 for selected NO_x species.

It can be seen that the updated mechanism gives about the same results for ozone, though it predicts slightly higher O_3 formation rates at lower ROG/NO_x conditions, and slightly lower O_3 at the end of the multi-day simulations using the lowest NO_x levels. However, it is interesting to note that the OH levels are generally higher with the updated mechanism, particularly for the lowest and the highest NO_x scenarios. The updated mechanism also predicts somewhat higher HNO_3 for most conditions, particularly when NO_x is very low. Investigating the reasons for these differences, and of the magnitudes of the differences in 3-D simulations of representative scenarios, is beyond the scope of the current project.

Mechanism Listing Tables

The large tables listing and documenting this mechanism are given in Appendix A of this document. Table A-1 lists and briefly describes all the model species in the mechanism for ambient simulations. Additional information about the model species is given in footnotes to the table. Table A-2 lists the lumped model species whose mechanisms were derived from those of representative compounds and indicates the contributions and structures of the compounds used and how the representative mixtures were derived. Table A-3 lists the reactions and rate parameters in the mechanism for

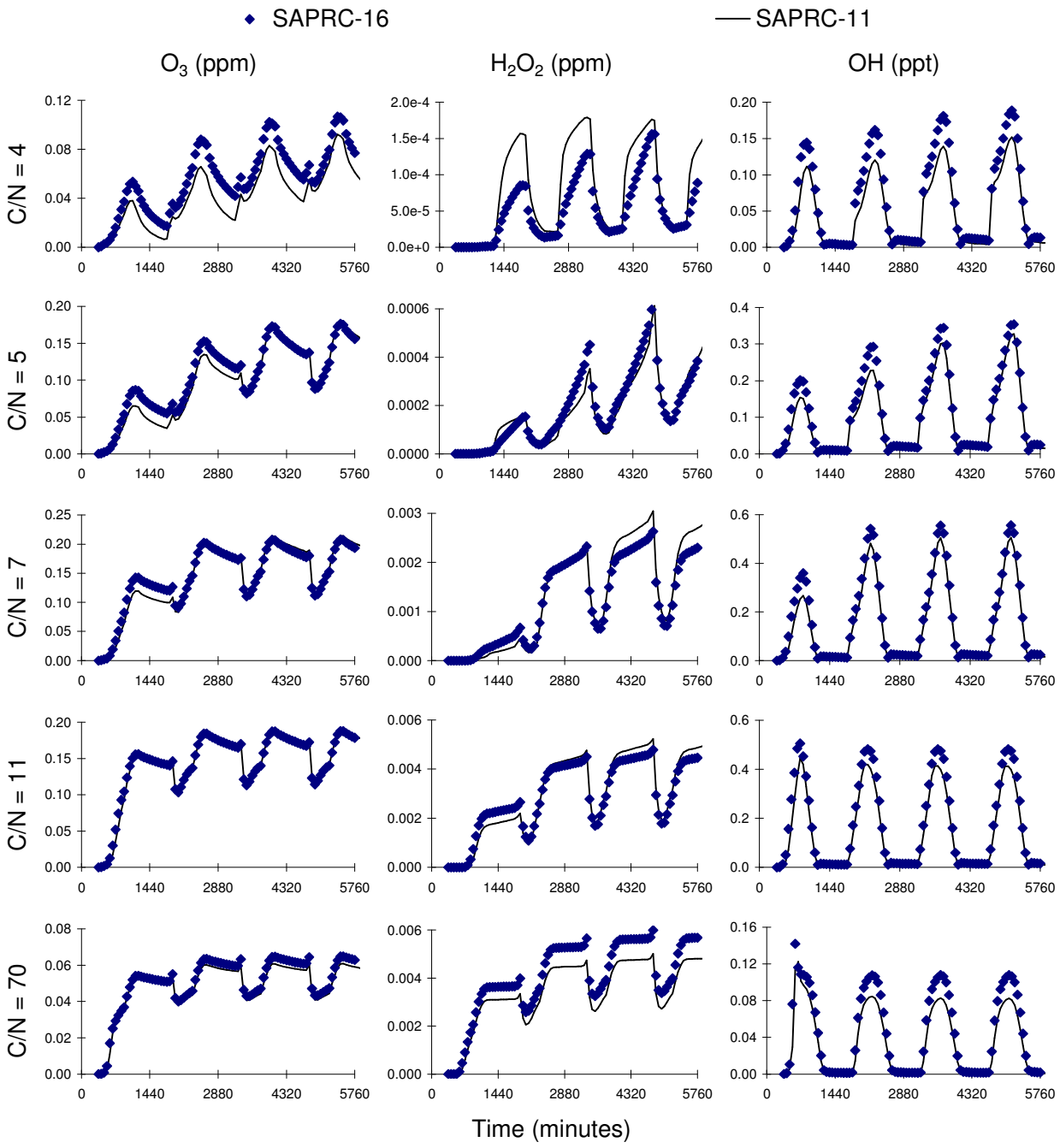

Figure 2. Results of model simulations of O_3, H_2O_2, and OH radicals in the four-day box model ambient simulations using the SAPRC-16 and SAPRC-11 mechanisms.

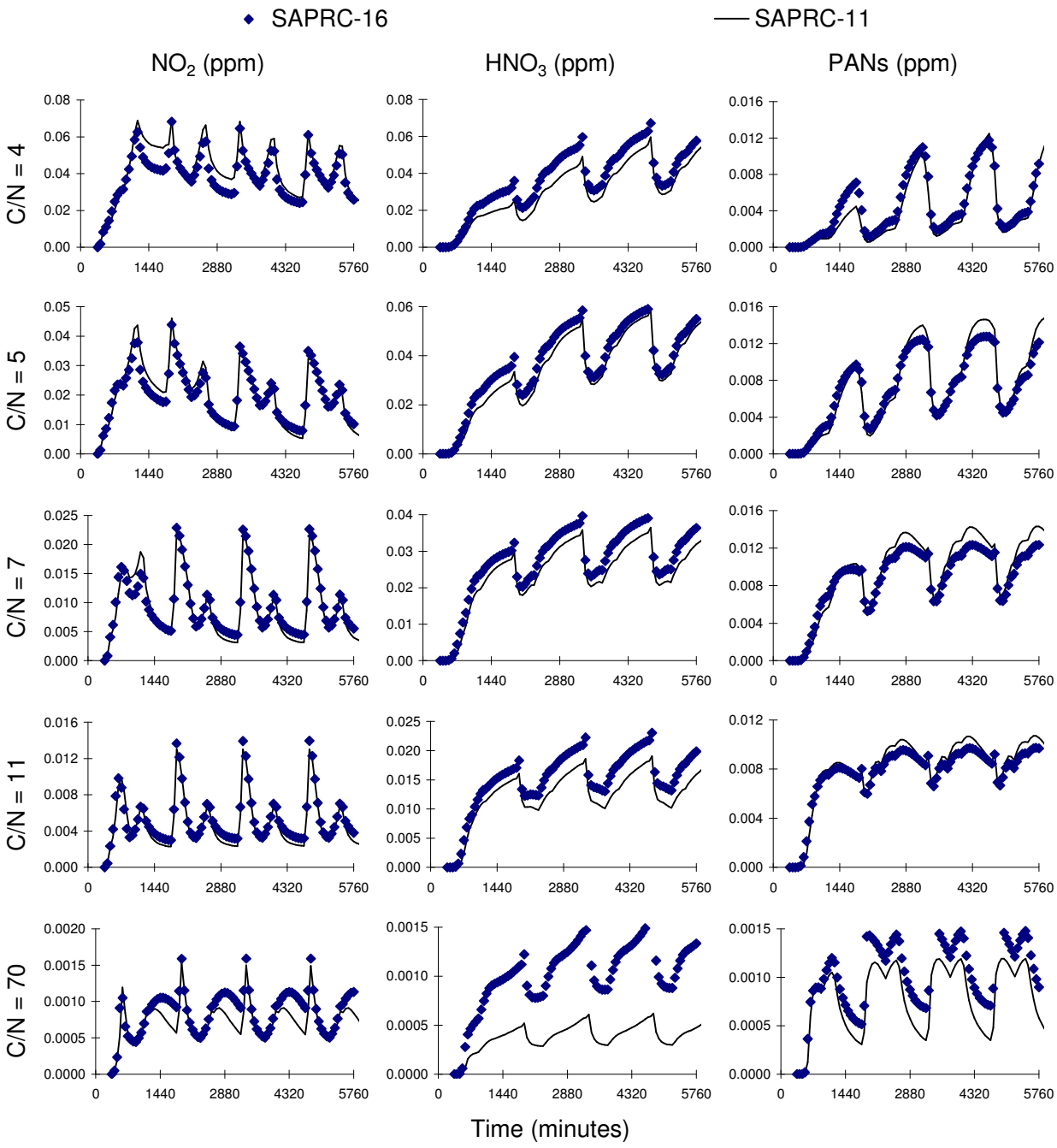

Figure 3. Results of model simulations of selected nitrogen species in the four-day box model ambient simulations using the SAPRC-16 and SAPRC-11 mechanisms.

atmospheric simulations and footnotes to the table describe the sources of the rate parameters and reaction mechanisms that were manually assigned. The table also includes reactions that were output by the mechanism generation system, which were derived as summarized above.

Supplementary Information Available

Additional information about this mechanism is available at the SAPRC-15 mechanism web site at http://www.cert.ucr.edu/~carter/SAPRC/16 (Carter, 2016). Files or data that can be obtained from this site are as follows:

- The latest version of the available mechanism documentation. Currently this consists only of this document, but updates to the documentation will be posted there when available.
- An Excel file (S16desc.xls) containing a complete listing of the model species, mixtures, and reactions in the mechanism. These include not only the information contained in the tables in Appendix A, but also the list of species and reactions used only in the extended version used for simulations of the chamber experiments.
- The file S16desc.xls also has assignments of individual compounds to SAPRC-16 model species. A link to the emissions speciation database files at http://www.cert.ucr.edu/~carter/emitdb/, which includes assignments of compounds in emissions speciation profiles for this and other mechanisms
- A Zip file containing the files containing the absorption cross sections and (where applicable) wavelength-dependent quantum yields for all photolysis reactions in the standard mechanism.
- Mechanism preparation input files containing the reactions of the standard mechanism in both SAPRC and CMAQ format.
- A link to the SAPRC-16 mechanism generation system. Reviewers can access this system to see how reactions for various compounds and species are generated

Additional Work Remaining

Although the current mechanism and mechanism generation system may need some work before it is used to calculate reactivity scales, it should be appropriate for use in atmospheric models if it passes peer review. The peer reviewers may well find problems or ask questions that reveal errors that need to be corrected, so the possibility of changes before it is suitable for regulatory or research modeling cannot be ruled out. In addition, documentation of the mechanism generation system is still incomplete, and it possible that the documentation process may reveal errors, omissions, or better approaches for the mechanism generation estimates or assignments, resulting in changes to the mechanism. We will work on completing this documentation while the existing mechanism and documentation is undergoing review. Reviewers will be notified when updates to the documentation are available, and changes made will be noted so they will not have to re-review portions of the mechanism and documentation that have not been changed.

The latest version of the mechanism will always be available at the SAPRC-16 web site (Carter, 2016), so that site can be consulted to determine if updates are available. Persons who are not on the current list of reviewers for this project can contact the author if they wish to be added to the list of people to be notified when there are updates available.

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Appendix A. Model Species and Mechanism Listing tables

Table A-1. List of model species in the mechanism for atmospheric simulations.

Type Name	Based on [a]	Note [b]	Atoms C	Atoms N	Molec Wt [c]	Description
Constant Species.						
O2			-	-	32.00	Oxygen
M			-	-	28.85	Air
H2O			-	-	18.02	Water
H2			-	-	2.02	Hydrogen Molecules
HV		1	-	-	0.00	Light
Active Inorganic Species.						
O3			-	-	48.00	Ozone
NO			-	1	30.01	Nitric Oxide
NO2			-	1	46.01	Nitrogen Dioxide
NO3			-	1	62.01	Nitrate Radical
N2O5			-	2	108.02	Nitrogen Pentoxide
HONO			-	1	47.02	Nitrous Acid
HNO3			-	1	63.02	Nitric Acid
HNO4			-	1	79.02	Peroxynitric Acid
HO2H			-	-	34.01	Hydrogen Peroxide
CO			1	-	28.01	Carbon Monoxide
SO2			-	-	64.06	Sulfur Dioxide
Active Radical Species and Operators						
OH		2	-	-	17.01	Hydroxyl Radicals
HO2			-	-	33.01	Hydroperoxide Radicals
SumRO2		3	-	-		Total peroxy radical concentration
SumRCO3		3	-	-		Total acyl peroxy radical concentration
Steady State Inorganic Radical Species						
O3P			-	-		Ground State Oxygen Atoms
O1D			-	-		Excited Oxygen Atoms
Explicitly represented organics						
CH4	METHANE		1	-	16.04	Methane
ETHAN	ETHANE		2	-	30.07	Ethane
ETHEN	ETHENE		2	-	28.05	Ethylene
ACETL	ACETYLEN		2	-	26.04	Acetylene
PROP	PROPANE	4	3	-	44.10	Propane
NC4	N-C4	4	4	-	58.12	n-Butane
PROPE	PROPENE	4	3	-	42.08	Propene
BUT13	13-BUTDE	4	4	-	54.09	1,3-Butadiene
ISOP	ISOPRENE	4	5	-	68.12	Isoprene
APINE	A-PINENE	4	10	-	136.23	a-Pinene
BPINE	B-PINENE	4	10	-	136.23	b-Pinene

Table A-1 (continued)

Type Name	Based on [a]	Note [b]	Atoms C	Atoms N	Molec Wt [c]	Description
DLIMO	D-LIMONE	4	10	-	136.23	d-Limonene
BENZ	BENZENE	4	6	-	78.11	Benzene
TOLU	TOLUENE	4	7	-	92.14	Toluene
C2BEN	C2-BENZ	4	8	-	106.17	Ethyl Benzene
MXYL	M-XYLENE	4	8	-	106.17	m-Xylene
OXYL	O-XYLENE	4	8	-	106.17	o-Xylene
PXYL	P-XYLENE	4	8	-	106.17	p-Xylene
BZ123	123-TMB	4	9	-	120.19	1,2,3-Trimethyl Benzene
BZ124	124-TMB	4	9	-	120.19	1,2,4-Trimethyl Benzene
BZ135	135-TMB	4	9	-	120.19	1,3,5-Trimethyl Benzene
HCHO	FORMALD		1	-	30.03	Formaldehyde
MEOH	MEOH		1	-	32.04	Methanol
HCOOH	FORMACID		1	-	46.03	Formic Acid
MEOOH			1	-	48.04	Methyl Hydroperoxide
MECHO	ACETALD		2	-	44.05	Acetaldehyde
GLCHO	GLCLALD		2	-	60.05	Glycolaldehyde
ETOH	ETOH		2	-	46.07	Ethanol
AACID	ACETACID		2	-	60.05	Acetic Acid.
PAA	PAA		2	-	76.05	Peroxyacetic acid
ETOOH			2	-	62.07	Ethyl hydroperoxide
GLY	GLYOXAL		2	-	58.04	Glyoxal
ETCHO	PROPALD		3	-	58.08	Propionaldehyde
ACET	ACETONE		3	-	58.08	Acetone
MGLY	MEGLYOX		3	-	72.07	Methyl Glyoxal
ACRO	ACROLEIN	4	3	-	56.06	Acrolein
MEK	MEK	4	4	-	72.11	Methyl ethyl ketone
BACL	BIACETYL		4	-	86.09	Biacetyl
MACR	METHACRO	4	4	-	70.09	Methacrolein
MVK	MVK	4	4	-	70.09	Methyl Vinyl Ketone
PHEN	PHENOL	5	6	-	94.11	Phenol
BUDAL	BUTEDIAL	4	4		84.07	2-Butene-1,4-dial
Lumped Organic Compounds						
Mechanism for representative compounds or estimated parameterized mechanisms used.						
SESQ	B-CARYOP	4,6	15	-	204.35	Sesquiterpenes
BENX	BENZENE	4,7	6	-	78.11	Aromatics other than benzene that have kOH between 3.4×10^{-13} and 1.7×10^{-12} cm^3 $molec^{-1}$ s^{-1}
NAPS	NAPHTHAL	5,6	11	-	142.20	Naphthalenes, tetralins, and indans
STYRS	STYRENE	4,6	9	-	117.17	Aromatics other than styrene with double bonds outside of the aromatic ring.
ACYLS	ET-ACTYL	4,6	4	-	54.09	Acetylenes other than acetylene
LVKS	See note	4,8	4		86.09	Ketones with at least 1 C=C double bond.
OLEA2	See note	4,9	5	-	116.12	Unsaturated aldehydes with C=C not next to the -CHO

Table A-1 (continued)

Type Name	Based on [a]	Note [b]	Atoms C	Atoms N	Molec Wt [c]	Description
BALD	BENZALD	6	7	-	106.13	Aromatic aldehydes (e.g., benzaldehyde)
CRES	O-CRESOL	5,6	7	-	108.14	Cresols
XYNL	24M-PHEN	5,6	8	-	122.16	Xylenols and higher alkylphenols
NPHE		10	6	1	139.11	Nitrophenols
SVPHE		10	7	-	124.14	Semi-volatile products of reactions of phenols
NAPPRD		10	12		172.22	Phenolic and other products formed from naphthalenes.
IMINE		11	2	1	34.07	Any compound with C=N bond. Assumed to rapidly hydrolize.
INHIB	AMP	12	4	-	89.14	Inhibiting compound such as siloxanes, aromatic isocyanates, alkyl iodides
PHOT		13	4	-	86.09	Unspecified photoreactive compounds such as nitrites or chloropicrin
Lumped Organic Compounds						
Mechanism for representative mixture used, derived using MechGen.						
ALK3	mix=ALK3	14,15	5	-	72.05	Alkanes that have kOH between 1.7 and 3.4 x 10^{-12} cm^3 $molec^{-1}$ s^{-1}
ALK4	mix=ALK4	14,15	6	-	86.12	Alkanes that have kOH between 3.4 and 6.8 x 10^{-12} cm^3 $molec^{-1}$ s^{-1}
ALK5	mix=ALK5	14,15	8	-	113.64	Alkanes that have kOH greater than 6.8 x 10^{-12} cm^3 $molec^{-1}$ s^{-1}
OLE1	mix=OLE1	14,15	5	-	70.13	Monoalkenes with only CH_2=CH- groups or allenes with kOH less than 5 x 10^{-12} cm^3 $molec^{-1}$ s^{-1}
OLE2	mix=OLE2	14,15	5	-	70.13	Monoalkenes with only -CH=CH- groups or allenes with kOH between than 5 x 10^{-12} and 4.8 x 10^{-11} cm^3 $molec^{-1}$ s^{-1}, and no double bonds in rings
OLE3	mix=OLE3	14,15	5	-	70.13	Alkenes other than terpenes or sesquiterpenes with only -CR=CH2 groups.
OLE4	mix=OLE4	14,15	5	-	70.13	Alkenes other than terpenes with non-conjugated -CH=CR- or -CR=CR- groups and possibly other double bonds and no double bonds in rings
OLEC	mix=OLEC	14,15	5	-	68.27	Cycloalkenes other than terpenes and sesquiterpenes with at least one double bond in the ring
OLED	T13PNTDE	14,15	5	-	68.12	Conjugated dialkenes other than terpenes.
TERP	mix=TERP	14,16	10	-	136.23	Terpenes not represented explicitly
AMINS	mix=AMINS	14,15	2	1	43.45	Amines
ARO1	mix=ARO1	14,15	9	-	121.62	Aromatics that have kOH between 1.7 x 10^{-12} and 1.4 x 10^{-11} cm^3 $molec^{-1}$ s^{-1}
ARO2	mix=ARO2	14,15	9	-	120.33	Aromatics other than naphthalenes, tetralins, or indans that have kOH greater than 1.4 x 10^{-11} cm^3 $molec^{-1}$ s^{-1}

Table A-1 (continued)

Type Name	Based on [a]	Note [b]	Atoms C	Atoms N	Molec Wt [c]	Description
OTH1	mix=OTH1	14,17	3	-	77.75	Volatile saturated compounds that react only with OH, and have kOH between 1.4 x 10^{-13} and 1.7 x 10^{-12} cm^3 $molec^{-1}$ s^{-1}
OTH2	mix=OTH2	14,15	3	-	62.09	Volatile saturated compounds that react only with OH, and have kOH between 1.7 and 3.4 x 10^{-12} cm^3 $molec^{-1}$ s^{-1}
OTH3	mix=OTH3	14,15	4	-	79.78	Volatile saturated compounds that react only with OH, and have kOH between 3.4 x 10^{-12} and 1.0 x 10^{-11} cm^3 $molec^{-1}$ s^{-1}
OTH4	mix=OTH4	14,15	4	-	92.61	Volatile saturated compounds that react only with OH, and have kOH greater than 1.0 x 10^{-11} cm^3 $molec^{-1}$ s^{-1}
RCHO	mix=RCHO	14,17	4	-	79.03	C4+ saturated aldehydes
KET2	mix=KET2	14,17	5	-	97.59	Photoreactive saturated ketones
OLEP	mix=OLEP	14,18	5	-	98.10	Non-photoreactive, non-hydrocarbon compounds with C=C double bonds
OLEA1	mix=OLEA1	14,18	5	-	102.27	Unsaturated aldehydes with C=C next to -CHO
RCOOH	mix=RCOOH	14,18	3	-	74.08	C3+ organic acids (mechanism based on propionic acid).
RANO3	mix=RANO3	14,17	8	1	169.17	Aromatic organic nitrates
RCNO3	mix=RCNO3	14,19	3	1	116.27	Volatile organic carbonly nitrates
RHNO3	mix=RHNO3	14,17	6	1	167.95	Volatile organic hydroxy nitrates
RPNO3	mix=RPNO3	14,17	8	1	223.93	Organic nitrates with peroxy groups (formed primarily from aromatics)
RDNO3	mix=RDNO3	14,19	6	2	208.88	Volatile organic dinitrates
R1NO3	mix=R1NO3	14,17	5	1	136.36	Other volatile organic nitrates that react with OH radicals slower than 5 x 10^{-12} cm^3 $molec^{-2}$ sec^{-1}
R2NO3	mix=R2NO3	14,17	8	1	177.57	Other volatile organic nitrates that react with OH radicals faster than 5 x 10^{-12} cm^3 $molec^{-2}$ sec^{-1}
RUOOH	mix=RUOOH	14,20	5	-	125.69	Hydroperoxides with C=C double bonds
RAOOH	mix=RAOOH	14,21	7	-	171.41	Hydroperoxides with other peroxy groups and C=C bonds -- formed primarily from aromatics
HPALD	mix=HPALD	14,18	5	-	120.33	Unsaturated hydroperoxy carbonyls with CO-C=C-OOH structures
CROOH	mix=CROOH	14,21	5	-	126.23	Hydroperoxy carbonyls (other than HPALDs)
ROOH	mix=ROOH	14,21	4	-	93.67	Other hydroperoxides with 3+ carbons and vapor pressure greater than 1 ppb
AFG1	mix=AFG1	14,17	5	-	97.52	Monounsaturated 1,4-dialdehydes formed from aromatics
AFG2A	mix=AFG2A	14,17	5	-	97.17	Monounsaturated 1,4 aldehyde-ketones formed from aromatics, with at no substituents other than the aldehyde on the double bonds
AFG2B	mix=AFG2B	14,17	6	-	111.75	Monounsaturated 1,4 aldehyde-ketones formed from aromatics, with at least one substituent other than the aldehyde on a double bond

Table A-1 (continued)

Type Name	Based on [a]	Note [b]	Atoms C	Atoms N	Molec Wt [c]	Description
AFG3	mix=AFG3	14,17	6	-	111.17	Monounsaturated 1,4-diketone aromatic products
AFG4	mix=AFG4	14,17	7	-	124.13	Tri-unsaturated alpha-hydroxy cyclic ether aromatic fragmentation products.
PAN and PAN Analogues						
PAN			2	1	121.05	Peroxyacetyl nitrate
HOPAN		22	2	1	137.05	PAN analogue from glycolaldehyde, $HOCH_2C(O)OONO_2$
PPN			3	1	135.08	Peroxy propionyl nitrate
PAN2			3	1	135.08	Higher alkyl PAN analogues that react with OH radicals with a rate constant of 1 x 10^{-11} cm^3 $molec^{-1}$ s^{-1} or less
PAN2N		23	2	2	182.05	Pan analogues with nitrate groups -- assumed to be primarily $O_2NOCH_2C(O)OONO_2$
PBZN			7	1	183.13	PAN analogues formed from Aromatic Aldehydes
APAN		22	3	1	133.06	PAN analogue formed from Acrolein
MAPAN			4	1	147.09	PAN analogues formed from Methacrolein and other unsaturated PAN analogues.
Non-Reacting Species (Active for testing -- can be removed if not needed)						
CO2			1	-	44.01	Carbon Dioxide
SULF					98.08	Sulfates (SO_3 or H_2SO_4)
NROG		24	-		1.00	Unreactive mass
NVOL		25	-		1.00	Nonvolatile mass
RNNO3		26	10	1	216.23	Organic nitrates with vapor pressure less than 1 ppb
OTHN		26	12	-	240.28	Other organic products with vapor pressures less than 1 ppb
NAMIN		27	4	2	89.14	Nitramines
IEPOX		28	5		118.13	Any 3-member ring cyclic ether with at least 2 OH groups.
Non-reacting counter species (Set to "dummy" as distributed to avoid numerical problems. Set to "Active" for testing.)						
XC		29	1	-	14.03	Lost Carbon or carbon in unreactive products
XN		30	-	1	46.01	Lost Nitrogen or nitrogen in unreactive products
Peroxy Radical Species in Base Mechanism						
MEO2		31	1	-		Methyl peroxy radicals
ETO2		31	2	-		Ethyl peroxy radicals
ETHEO2		31	2	-		Peroxy radical formed from ethene + OH
ETHEO2N		31	2	1		Peroxy radical formed from ethene + NO3
HCOMEO2		31	2	-		HCO-CH2OO. radicals, formed from acetaldehyde and other compounds.
ACETO2		31	3	-		CH_3-CO-CH_2OO. (formed from acetone)

Table A-1 (continued)

Type Name	Based on [a]	Note [b]	Atoms C	Atoms N	Molec Wt [c]	Description
BZO2		31	6	-		Benzyl peroxy and substituted benzyl peroxy radicals
Acyl peroxy radical species						
MECO3		32	2	-		Acetyl Peroxy Radicals (forms PAN)
HOCCO3		22,32	2	-		Acyl peroxy radicals from glycolaldehyde, HOCH2C(O)OO. (forms HOPAN)
ETCO3		32	3	-		Peroxy propionyl radicals (forms PPN)
R2CO3		32	3	-		Higher saturated peroxy acyl radicals (forms PAN2)
R2NCO3		23,32	2	1		Peroxy acyl radicals with nitrate groups -- assumed to be primarily .OOC(O)CH_2ONO2
BZCO3		32	7	-		Peroxyacyl radical formed from Aromatic Aldehydes (forms PBZN)
ACO3		22,32	3	-		Peroxyacyl radicals formed from acrolein. (forms APAN)
MACO3		32	4	-		Peroxyacyl radicals formed from methacrolein and other unsaturated aldehydes (forms MAPAN)
Other organic radical or reactive intermediate species						
TBUO		33	4	-		t-Butoxy Radicals
BZO		33	6	-		Phenoxy or substituted phenoxy radicals
HCHO2		34	1	-	46.03	Unsubstituted stabilized Criegee biradical
MECHO2		34	2	-	60.05	Methyl substituted stabilized Criegee biradical
RCHO2		34	3	-	74.08	Other stabilized Criegee biradicals
Radical operator species						
RO2C		35	-	-		Peroxy Radical Operator representing NO to NO2 and NO3 to NO2 conversions, and the effects of peroxy radical reactions on acyl peroxy and other peroxy radicals (used in some multi-step mechanisms).
RO2XC		35	-	-		Peroxy Radical Operator representing NO consumption (used in conjunction with organic nitrate formation), and the effects of peroxy radical reactions on NO3, acyl peroxy radicals, and other peroxy radicals. (used in some multi-step mechanisms)
zR1NO3		35	5	-		Formation of R1NO3 after reaction with NO for lumped low yield peroxy reactions
zR2NO3		35	8	-		As above, but for R2NO3
zRANO3		35	8	-		As above, but for RANO3
zRCNO3		35	3	-		As above, but for RCNO3
zRHNO3		35	6	-		As above, but for RHNO3
zRDNO3		35	6	1		As above, but for RDNO3
zRPNO3		35	8	-		As above, but for RPNO3

Table A-1 (continued)

Type Name	Based on [a]	Note [b]	Atoms C	Atoms N	Molec Wt [c]	Description
zRNNO3		35	10	-		As above, but for RNNO3
xNAMIN		27	4	1		Nitramine precursor frormed from amines with no alpha hydrogens
NPRAD		10	12	-		Simplified representative of unknown naphthalene intermediates that react with NO2 forming products
Peroxy radical Intermediates in generated mechanisms (slow or no unimolecular reactions)						
PROP_P1		36	3	-		PROPANE intermediate
NC4_P1		36	4	-		N-C4 intermediate
PROPE_P1		36	3	-		PROPENE intermediate
BUT13_P1		36	4	-		13-BUTDE intermediate
ISOP_P1		36	5	-		ISOPRENE intermediate
APINE_P1		36	10	-		A-PINENE intermediate
BPINE_P1		36	10	-		B-PINENE intermediate
DLIMO_P1		36	10	-		D-LIMONE intermediate
BENZ_P1		36	6	-		BENZENE intermediate
TOLU_P1		36	7	-		TOLUENE intermediate
C2BEN_P1		36	8	-		C2-BENZ intermediate
MXYL_P1		36	8	-		M-XYLENE intermediate
OXYL_P1		36	8	-		O-XYLENE intermediate
PXYL_P1		36	8	-		P-XYLENE intermediate
BZ123_P1		36	9	-		123-TMB intermediate
BZ124_P1		36	9	-		124-TMB intermediate
BZ135_P1		36	9	-		135-TMB intermediate
ACRO_P1		36	3	-		ACROLEIN intermediate
MEK_P1		36	4	-		MEK intermediate
MACR_P1		36	2	-		METHACRO intermediate
MVK_P1		36	4	-		MVK intermediate
SESQ_P1		36	15	-		SESQ intermediate
BENX_P1		36	6	-		BENX intermediate
STYRS_P1		36	8	-		STYRS intermediate
LVKS_P1		36	4	-		LVKS intermediate
OLEA2_P1		36	5	-		OLEA2 intermediate
ALK3_P1		36	5	-		ALK3 intermediate
ALK4_P1		36	6	-		ALK4 intermediate
ALK5_P1		36	8	-		ALK5 intermediate
OLE1_P1		36	5	-		OLE1 intermediate
OLE2_P1		36	5	-		OLE2 intermediate
OLE3_P1		36	5	-		OLE3 intermediate
OLE4_P1		36	5	-		OLE4 intermediate
OLEC_P1		36	5	-		OLEC intermediate
OLED_P1		36	5	-		OLED intermediate
TERP_P1		36	10	-		TERP intermediate
AMINS_P1		36	2	1		AMINS intermediate

Table A-1 (continued)

Type Name	Based on [a]	Note [b]	Atoms C	Atoms N	Molec Wt [c]	Description
ARO1_P1		36	9	-		ARO1 intermediate
ARO2_P1		36	9	-		ARO2 intermediate
OTH1_P1		36	3	-		OTH1 intermediate
OTH2_P1		36	3	-		OTH2 intermediate
OTH3_P1		36	5	-		OTH3 intermediate
OTH4_P1		36	6	-		OTH4 intermediate
RCHO_P1		36	3	-		RCHO intermediate
KET2_P1		36	6	-		KET2 intermediate
OLEP_P1		36	5	-		OLEP intermediate
OLEA1_P1		36	5	-		OLEA1 intermediate
RCOOH_P1		36	3	-		RCOOH intermediate
RANO3_P1		36	8	1		RANO3 intermediate
RCNO3_P1		36	4	1		RCNO3 intermediate
RHNO3_P1		36	7	1		RHNO3 intermediate
RPNO3_P1		36	7	1		RPNO3 intermediate
RDNO3_P1		36	6	2		RDNO3 intermediate(C6N2)
R1NO3_P1		36	5	1		R1NO3 intermediate
R2NO3_P1		36	8	1		R2NO3 intermediate
RUOOH_P1		36	5	-		RUOOH intermediate
CROOH_P1		36	5	-		CROOH intermediate
ROOH_P1		36	4	-		ROOH intermediate
AFG2A_P1		36	5	-		AFG2A intermediate
AFG2B_P1		36	6	-		AFG2B intermediate
AFG3_P1		36	6	-		AFG3 intermediate
AFG4_P1		36	7	-		AFG4 intermediate
APAN_P1		36	3	1		APAN intermediate
MAPAN_P1		36	4	1		MAPAN intermediate
PROPE_P2		36	3	1		PROPENE intermediate
BUT13_P2		36	4	1		13-BUTDE intermediate
ISOP_P2		36	5	1		ISOPRENE intermediate
APINE_P2		36	10	-		A-PINENE intermediate
BPINE_P2		36	9	-		B-PINENE intermediate
DLIMO_P2		36	10	1		D-LIMONE intermediate
ACRO_P2		36	3	1		ACROLEIN intermediate
MACR_P2		36	4	-		METHACRO intermediate
SESQ_P2		36	15	1		SESQ intermediate
STYRS_P2		36	8	1		STYRS intermediate
LVKS_P2		36	2	-		LVKS intermediate
OLEA2_P2		36	5	1		OLEA2 intermediate
ALK3_P2		36	6	-		ALK3 intermediate
ALK4_P2		36	5	-		ALK4 intermediate
ALK5_P2		36	8	-		ALK5 intermediate
OLE1_P2		36	5	1		OLE1 intermediate
OLE2_P2		36	5	1		OLE2 intermediate

Table A-1 (continued)

Type Name	Based on [a]	Note [b]	Atoms C	Atoms N	Molec Wt [c]	Description
OLE3_P2		36	4	-		OLE3 intermediate
OLE4_P2		36	5	1		OLE4 intermediate
OLEC_P2		36	5	1		OLEC intermediate
OLED_P2		36	5	-		OLED intermediate
TERP_P2		36	10	-		TERP intermediate
AMINS_P2		36	2	1		AMINS intermediate
ARO1_P2		36	6	-		ARO1 intermediate
OTH1_P2		36	4	-		OTH1 intermediate
OTH4_P2		36	4	-		OTH4 intermediate
OLEP_P2		36	5	1		OLEP intermediate
OLEA1_P2		36	2	-		OLEA1 intermediate
RHNO3_P2		36	6	-		RHNO3 intermediate
RDNO3_P2		36	4	-		RDNO3 intermediate
R1NO3_P2		36	5	-		R1NO3 intermediate
R2NO3_P2		36	8	-		R2NO3 intermediate
CROOH_P2		36	6	-		CROOH intermediate
AFG2A_P2		36	5	-		AFG2A intermediate
MAPAN_P2		36	3	1		MAPAN intermediate
BUT13_P3		36	4	-		13-BUTDE intermediate
ISOP_P3		36	4	-		ISOPRENE intermediate
APINE_P3		36	10	1		A-PINENE intermediate
BPINE_P3		36	10	1		B-PINENE intermediate
DLIMO_P3		36	10	-		D-LIMONE intermediate
MACR_P3		36	4	1		METHACRO intermediate
SESQ_P3		36	15	-		SESQ intermediate
LVKS_P3		36	3	-		LVKS intermediate
OLEA2_P3		36	4	-		OLEA2 intermediate
ALK3_P3		36	7	-		ALK3 intermediate
ALK5_P3		36	7	-		ALK5 intermediate
OLE1_P3		36	4	-		OLE1 intermediate
OLE3_P3		36	5	1		OLE3 intermediate
OLED_P3		36	5	-		OLED intermediate
TERP_P3		36	10	1		TERP intermediate
OLEA1_P3		36	5	1		OLEA1 intermediate
RHNO3_P3		36	7	-		RHNO3 intermediate
RDNO3_P3		36	6	2		RDNO3 intermediate(C6N2)
R1NO3_P3		36	5	1		R1NO3 intermediate
R2NO3_P3		36	8	1		R2NO3 intermediate
CROOH_P3		36	6	-		CROOH intermediate
BUT13_P4		36	4	-		13-BUTDE intermediate
ISOP_P4		36	5	-		ISOPRENE intermediate
BPINE_P4		36	10	1		B-PINENE intermediate
DLIMO_P4		36	7	-		D-LIMONE intermediate
OLE1_P4		36	4	-		OLE1 intermediate

Table A-1 (continued)

Type Name	Based on [a]	Note [b]	Atoms C	Atoms N	Molec Wt [c]	Description
OLED_P4		36	5	-		OLED intermediate
TERP_P4		36	10	1		TERP intermediate
OLEA1_P4		36	5	-		OLEA1 intermediate
R2NO3_P4		36	7	-		R2NO3 intermediate
BUT13_P5		36	4	-		13-BUTDE intermediate
ISOP_P5		36	5	1		ISOPRENE intermediate
OLED_P5		36	5	1		OLED intermediate
OLEA1_P5		36	4	-		OLEA1 intermediate
OLED_P6		36	5	1		OLED intermediate
OLEA1_P6		36	4	-		OLEA1 intermediate
OLED_P7		36	5	-		OLED intermediate
OLEA1_P7		36	5	1		OLEA1 intermediate
OLEA1_P8		36	4	1		OLEA1 intermediate
Peroxy radical intermediates in generated mechanisms (relatively fast unimolecular and NO reactions only)						
BUT13_A1		37	4	-		13-BUTDE intermediate
ISOP_A1		37	5	-		ISOPRENE intermediate
DLIMO_A1		37	10	-		D-LIMONE intermediate
ACRO_A1		37	3	-		ACROLEIN intermediate
MACR_A1		37	4	-		METHACRO intermediate
BUDAL_A1		37	4	-		BUTEDIAL intermediate
SESQ_A1		37	15	-		SESQ intermediate
LVKS_A1		37	3	-		LVKS intermediate
OLED_A1		37	5	-		OLED intermediate
TERP_A1		37	10	1		TERP intermediate
OLEA1_A1		37	5	-		OLEA1 intermediate
HPALD_A1		37	5	-		HPALD intermediate
AFG1_A1		37	5	-		AFG1 intermediate
AFG2A_A1		37	5	-		AFG2A intermediate
BUT13_A2		37	4	1		13-BUTDE intermediate
ISOP_A2		37	5	-		ISOPRENE intermediate
ACRO_A2		37	3	1		ACROLEIN intermediate
MACR_A2		37	4	1		METHACRO intermediate
OLED_A2		37	5	-		OLED intermediate
OLEA1_A2		37	4	-		OLEA1 intermediate
AFG1_A2		37	5	-		AFG1 intermediate
ISOP_A3		37	5	1		ISOPRENE intermediate
OLED_A3		37	5	-		OLED intermediate
OLEA1_A3		37	4	-		OLEA1 intermediate
ISOP_A4		37	5	1		ISOPRENE intermediate
OLED_A4		37	5	1		OLED intermediate
OLEA1_A4		37	5	1		OLEA1 intermediate
OLED_A5		37	5	1		OLED intermediate
OLEA1_A5		37	4	1		OLEA1 intermediate

Table A-1 (continued)

Type Name	Based on [a]	Note [b]	Atoms C	Atoms N	Molec Wt [c]	Description
OLED_A6		37	5	-		OLED intermediate
OLED_A7		37	5	1		OLED intermediate
OLED_A8		37	5	1		OLED intermediate

[a] Detailed model species or mixture name used to derive the mechanism (organic compounds). See mechanism listing and notes if blank. See "Mixtures" sheet for compounds used to derive mixtures. See "DMS Asst's" sheet for listing of detailed model species.

[b] Notes for individual species

1 Fraction of light intensity relative to maximum or clear sunlight. May not be needed depending on photolyses are handled by the model. It is not included in MEC files prepared for the CMAQ model.

2 It may be appropriate to use the steady state approximation for this species but this is not possible using the way the SAPRC modeling software implements the steady state approximation.

3 These are the sums of total concentrations of peroxy (SumRO2) or acyl peroxy (SumRCO3) radicals that react with other peroxy radicals, and are used to compute the rates of these peroxy + peroxy reactions. Every reaction that forms a peroxy or acyl peroxy radical of this type also forms the corresponding "Sum" species at the same yield, and their loss reactions with NO, NO2 (for SumRCO3), HO2, and each other are included as separate reactions. Note that this gives only an approximation of the rates of these peroxy + peroxy reactions because it ignores loss by unimolecular reactions that are non-negligible for some peroxys and also it neglects the fact that self-reactions involve loss of two rather than one radical. However, tests against a more exact solution give essentially the same results in atmospheric simulations, so the complexity of using a more exact solution is not necessary. Note that peroxy or acyl peroxy radicals that have unimolecular reaction rate constants greater than around 0.33 sec^{-1} are assumed not to have significant bimolecular reactions other than with NO and those that have unimolecular rate constants greater than about 133 sec^{-1} are assumed to have no bimolecular reactions. These are not included in these "Sum" species since they do not react with other peroxy radicals.

4 Mechanism derived using MechGen, the current SAPRC mechanism generation system.

5 The detailed mechanism for this type of compound cannot yet be estimated. A simplified parameterized mechanism that is adjusted to fit chamber data is used.

6 The compound used to derive the mechanism is the most important compound of this type according to the representative anthropogenic and biogenic mixtures.

7 The benzene mechanism may overestimate the reactivity of some compounds of this type, but their contributions to total reactivity is generally negligible.

8 Mechanism based on the representative isoprene product compound $CH_3C(O)CH=CHOH$, which is the major product compound of this type in representative anthropogenic + biogenic mixtures.

9 Mechanism based on the representative isoprene product compound $CH_2=C(CH_2OH)CH(OH)CHO$, which is the major product compound of this type in representative anthropogenic + biogenic mixtures.

10 The detailed mechanism for this type of compound cannot yet be estimated. A simplified parameterized mechanism is used.

11 The main compound of this type is $CH_3CH=NH$, which is assumed to rapidly hydrolyze to form acetaldehyde and ammonia. Therefore it is treated as in steady state and replaced by the

Table A-1 (continued)

formation of MECHO and XN. "Lost nitrogen" is used for ammonia because it is not included in the gas-phase mechanism.

12 Compounds that efficiently inhibit radicals can have very different mechanisms, but amines such as AMP appear to be the most important in emissions so AMP is used to represent their mechanisms. Although this can be highly approximate, it is better than ignoring inhibiting compounds by treating them as unreactive, which is the usual practice for most mechanisms.

13 A highly simplified mechanism is used for photoreactive compounds that are relatively unimportant in emissions and not well represented by other model species.

14 The mechanism for this model species are derived from mechanisms of the individual components of the mixture of representative compounds represented by this model species, which in turn are derived using MechGen. The mixture used is indicated in the other footnote. The compositions and derivations of these mixtures are given in Table ??.

15 The mixture used is the "U.S total" emissions mixture, which is the same as the "US Emit" mixture given by Carter (2015).

16 The mixture used is the "Megan G" biogenic mixture of Guenther (2014), as given by Carter (2015). See also Guenther et al (2012).

17 The mixture used is the mixture of products predicted from the reactions of OH with the components of the "U.S total" emissions mixture.

18 The mixture used is the mixture of products predicted from the reactions of OH with isoprene. This is the main source for compounds represented by this model species in ambient simulations.

19 The mixture used is the mixture of products predicted from the reactions of NO_3 radicals with the components of the "U.S total" emissions mixture. This is the only significant source for compounds represented by this model species in ambient simulations.

20 The mixture used is the mixture of products predicted from the reactions of HO_2 with peroxy radicals formed in the reactions of OH with isoprene. This is the main source for compounds represented by this model species in ambient simulations.

21 The mixture used is the mixture of products predicted from the reactions of HO_2 with peroxy radicals formed in the reactions of OH with the components of the "U.S total" emissions mixture.

22 It may not be a bad approximation for atmospheric simulations to lump HOPAN with PAN or APAN with MAPAN, but they are kept separate for now.

23 This is represented separately from other higher saturated PAN analogues in order to account better for the fate of nitrogen. This is a non-negligible product in the reactions of carbonyl nitrates.

24 This represents unreactive compounds on a mass rather than molar basis, both in emissions and when formed as a product of organic reactions. Note that the yields given for the reactions forming unreactive compounds are given by moles unreactive compound(s) formed x their molecular weights, to give mass yields.

25 The "NVOL" model species is used to represent nonvolatile mass in "gas" emissions profiles and is not used in the gas-phase mechanism. Note that it is not used to represent nonvolatile compounds formed in the gas-phase reactions. These are represented by "RNNO3" on a molar basis if the compound is an organic nitrate and by "OTHN" on a molar basis if not.

26 Compounds represented by these model species are estimated to be non-volatile and their gas-phase reactions are not included in the mechanism. Their molecular weights can be used to estimate their mass contributions to the total SOA formed.

27 These are predicted to be important products in reactions of amines without alpha hydrogens, which are predicted to form radicals that react primarily with NO_2 to form nitramines. Nitramines

Table A-1 (continued)

are not expected to be highly reactive in the gas phase so the mechanism has gas-phase reactions for them.

28 These are believed to be important SOA precursors formed in isoprene reactions under low NOx conditions. They are not expected to be very reactive in the gas phase but are expected to add water in the condensed phase to form highly nonvolatile compounds.

29 This is a counter species used to track carbon imbalance in lumped reactions, and can be formed in non-negligible (positive or negative) yields in some lumped reactions. It is recommended not to use this as an active species in ambient simulations because sometimes it can go negative and cause numerical instability for some solvers. It is not included in MEC files prepared for the CMAQ model.

30 This is a counter species used to track nitrogen imbalance in lumped reactions. Reactions forming or losing it are generally minor but sometimes nonnegligible in ambient simulations, and it is used primarily track nitrate formation in low yield peroxy reactions. It should be minor in ambient simulations but can be used to check this. It should not go negative but if it does it may cause numerical instability for some solvers. If numerical problems are observed, try removing this as an active species.

31 The steady state approximation can be used for all of these peroxy radical model species. Their concentrations are included in SumRO2, so any reaction forming them also forms SumRO2.

32 The steady state approximation can be used for all of these acyl peroxy radical model species. Their concentrations are included in SumRCO3, so any reaction forming them also forms SumRCO3.

33 These react primarily with NO_2, but low NO_x reactions are also included.

34 The mechanism includes reactions of the stabilized Crigiee biradicals is reaction with water, SO_2 and NO_2, with the reaction with water generally dominating. However, the rate constants for the reaction with water are uncertain, and its relative importance may vary with structure in a way that is not represented in the current mechanism.

35 If a peroxy radical is estimated to be formed in less than 10% overall yield in a generated mechanism, it is not represented explicitly but by the mixture of products predicted to be formed from its reactions, and reactions of radicals it form, with NO and unimolecular reactions (if applicable). This reaction lumping approach is similar to the approach used in earlier versions of SAPRC, but is used in this version only for the more minor pathways, to avoid the need for multiple model species only to represent relatively unimportant pathways. The ratio of NO to unimolecular reactions is estimated for this purpose using a representative NO concentration of 0.5 ppb. (Both the fraction reaction where this approximation is used and the representative NO concentration is a mechanism generation option that can be changed.) The model species "RO2C" is used to represent the effects of NO to NO_2 conversions from multi-generational peroxy reactions, and "RO2XC" is used to reflect the consumption of NO to form nitrates. The formation of nitrates in these minor NO reactions are represented by the zRNO3 model species, which primarily react with NO to form the corresponding nitrate but can also react under low NO_x conditions to form non-nitrate products.

36 This is a peroxy radical model species derived by the mechanism generation system to represent reactions of peroxy radicals formed in yields of greater than 10%. Some of these can undergo unimolecular reactions but in all cases the unimolecular rate constant is estimated to be less than 0.33 sec^{-1}, which is sufficiently low that reactions with peroxy radicals may be non-negligible. Peroxy radicals that are formed by the same reactions and that are estimated to have negligible unimolecular reactions (estimated rate constant less than 3.3×10^{-3} sec^{-1}) are lumped together, but those with non-negligible unimolecular reactions are represented separately. The compound

Table A-1 (continued)

whose mechanism uses this radicals is indicated in the "Description" column and also by the name of the radical. The steady state approximation can be used for all of these model species so they do not have to be transported. SumRO2 includes the concentrations of all these species, and any reaction forming them also forms SumRO2 in equal yields.

37 This is a peroxy radical model species derived by the mechanism generation system to represent reactions of peroxy radicals formed in yields of greater than 10%, and that have unimolecular reactions with rate constants between 0.33 and 133 sec^{-1}. Peroxy radicals with lower unimolecular rate constants are assumed to react with other peroxy radicals and are included with "_Pn" model species discussed in the previous footnote, while those with higher unimolecular rate constants are assumed to react only unimolecularly and are replaced by their products. Peroxy radicals with this unimolecular rate constant rang are assumed to react either unimolecularly or with NO but not by other bimolecular reactions, so they are not included in SumRO2. The steady state approximation should be used for all of these model species so they do not have to be transported.

[c] Molecular weights are not assigned for steady state or counter species. They should not be needed.

Table A-2. Mixtures used to derive mechanisms of the mixture-dependent lumped organic model species.

Species	Fac [a]	DMS [b]	Mixture derivation or compound structure [c]
ALK3	99.8%	Total	Derived from UStot Mixture
	62.9%	2-ME-C3	CH3-CH(CH3)-CH3
	25.8%	224TM-C5	CH3-CH(CH3)-CH2-C(CH3)(CH3)-CH3
	11.1%	22-DM-C4	CH3-CH2-C(CH3)(CH3)-CH3
ALK4	99.2%	Total	Derived from UStot Mixture
	33.1%	2-ME-C4	CH3-CH2-CH(CH3)-CH3
	16.0%	N-C5	CH3-CH2-CH2-CH2-CH3
	10.3%	2-ME-C5	CH3-CH2-CH2-CH(CH3)-CH3
	8.3%	N-C6	CH3-CH2-CH2-CH2-CH2-CH3
	6.2%	3-ME-C5	CH3-CH2-CH(CH3)-CH2-CH3
	4.9%	ME-CYCC5	CH3-CH*-CH2-CH2-CH2-CH2*
	3.4%	23-DM-C4	CH3-CH(CH3)-CH(CH3)-CH3
	3.0%	23-DM-C5	CH3-CH2-CH(CH3)-CH(CH3)-CH3
	2.9%	2-ME-C6	CH3-CH2-CH2-CH2-CH(CH3)-CH3
	2.5%	3-ME-C6	CH3-CH2-CH2-CH(CH3)-CH2-CH3
	2.5%	CYCC5	CH2*-CH2-CH2-CH2-CH2*
	2.2%	24-DM-C5	CH3-CH(CH3)-CH2-CH(CH3)-CH3
	1.9%	234TM-C5	CH3-CH(CH3)-CH(CH3)-CH(CH3)-CH3
	0.7%	3E3MC5	CH3-CH2-C(CH3)(CH2-CH3)-CH2-CH3
	0.7%	225TM-C6	CH3-CH(CH3)-CH2-CH2-C(CH3)(CH3)-CH3
	0.6%	13DMCYC5	CH3-CH*-CH2-CH2-CH(CH3)-CH2*
ALK5	95.7%	Total	Derived from UStot Mixture
	21.3%	N-C7	CH3-CH2-CH2-CH2-CH2-CH2-CH3
	13.8%	ME-CYCC6	CH3-CH*-CH2-CH2-CH2-CH2-CH2*
	9.5%	CYCC6	CH2*-CH2-CH2-CH2-CH2-CH2*
	9.2%	N-C8	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH3
	5.8%	3-ME-C7	CH3-CH2-CH2-CH2-CH(CH3)-CH2-CH3
	4.3%	N-C12	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
	4.3%	N-C9	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
	3.9%	N-C10	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
	3.8%	25-DM-C6	CH3-CH(CH3)-CH2-CH2-CH(CH3)-CH3
	3.1%	23-DM-C6	CH3-CH2-CH2-CH(CH3)-CH(CH3)-CH3
	3.0%	N-C11	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
	2.5%	ET-CYCC6	CH3-CH2-CH*-CH2-CH2-CH2-CH2-CH2*
	2.2%	13DMCYC6	CH3-CH*-CH2-CH2-CH2-CH(CH3)-CH2*
	2.1%	3ME-C8	CH3-CH2-CH2-CH2-CH2-CH(CH3)-CH2-CH3
	2.1%	3ET-C5	CH3-CH2-CH(CH2-CH3)-CH2-CH3
	1.4%	ET-CYCC5	CH3-CH2-CH*-CH2-CH2-CH2-CH2*
	1.3%	4-ME-C7	CH3-CH2-CH2-CH(CH3)-CH2-CH2-CH3
	0.8%	25DM-C7	CH3-CH2-CH(CH3)-CH2-CH2-CH(CH3)-CH3
	0.6%	24-DM-C8	CH3-CH2-CH2-CH2-CH(CH3)-CH2-CH(CH3)-CH3
	0.6%	35-DM-C7	CH3-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH3
OLE1	98.6%	Total	Derived from UStot Mixture
	60.8%	3M-1-BUT	CH2=CH-CH(CH3)-CH3

Table A-2. (continued).

Species	Fac [a]	DMS [b]	Mixture derivation or compound structure [c]
	14.3%	1-BUTENE	CH2=CH-CH2-CH3
	13.5%	1-PENTEN	CH2=CH-CH2-CH2-CH3
	3.9%	33M1-BUT	CH2=CH-C(CH3)(CH3)-CH3
	3.6%	1-HEXENE	CH2=CH-CH2-CH2-CH2-CH3
	1.0%	1-HEPTEN	CH2=CH-CH2-CH2-CH2-CH2-CH3
	0.8%	1-C9E	CH2=CH-CH2-CH2-CH2-CH2-CH2-CH2-CH3
	0.7%	3M1-C5E	CH2=CH-CH(CH3)-CH2-CH3
OLE2	99.0%	Total	Derived from UStot Mixture
	35.3%	T-2-PENT	CH3-^CH=CH-^CH2-CH3
	19.1%	T-2-BUTE	CH3-^CH=CH-^CH3
	17.3%	C-2-PENT	CH3-^CH=CH-vCH2-CH3
	15.6%	C-2-BUTE	CH3-^CH=CH-vCH3
	2.7%	T4M2-C5E	CH3-^CH=CH-^CH(CH3)-CH3
	2.2%	T-3-C6E	CH3-CH2-^CH=CH-^CH2-CH3
	1.5%	T-2-C6E	CH3-^CH=CH-^CH2-CH2-CH3
	1.2%	C-2-C6E	CH3-^CH=CH-vCH2-CH2-CH3
	1.0%	C-3-C6E	CH3-CH2-^CH=CH-vCH2-CH3
	0.9%	T-3-C7E	CH3-CH2-^CH=CH-^CH2-CH2-CH3
	0.8%	2MT3C6E	CH3-CH2-^CH=CH-^CH(CH3)-CH3
	0.7%	T-5-C13E	CH3-CH2-CH2-CH2-^CH=CH-^CH2-CH2-CH2-CH2-CH2-CH2-CH3
	0.4%	C-2-C7E	CH3-^CH=CH-vCH2-CH2-CH2-CH3
	0.3%	T-4-C10E	CH3-CH2-CH2-^CH=CH-^CH2-CH2-CH2-CH2-CH3
OLE3	99.3%	Total	Derived from UStot Mixture
	52.8%	2M-1-BUT	CH2=C(CH3)-CH2-CH3
	40.6%	ISOBUTEN	CH2=C(CH3)-CH3
	5.2%	2M1-C5E	CH2=C(CH3)-CH2-CH2-CH3
	0.7%	244M1C5E	CH2=C(CH3)-CH2-C(CH3)(CH3)-CH3
OLE4	99.3%	Total	Derived from UStot Mixture
	82.3%	2M-2-BUT	CH3-CH=C(CH3)-CH3
	9.1%	2M-2-C5E	CH3-CH2-CH=C(CH3)-CH3
	5.8%	C3M2-C5E	CH3-^CH=C(^CH3)-CH2-CH3
	0.6%	24MC2C5E	CH3-C(CH3)=CH-CH(CH3)-CH3
	0.5%	C3M2HEXE	CH3-^CH=C(^CH3)-CH2-CH2-CH3
	0.5%	23M2-C5E	CH3-CH2-C(CH3)=C(CH3)-CH3
	0.5%	2M2C6E	CH3-CH2-CH2-CH=C(CH3)-CH3
OLEC	100.0%	Total	Derived from UStot Mixture
	57.6%	CYC-PNTE	CH*=CH-CH2-CH2-CH2*
	29.1%	3MECC5E	CH3-CH*-CH=CH-CH2-CH2*
	8.4%	CYC-HEXE	CH*=CH-CH2-CH2-CH2-CH2*
	4.9%	1M-CC5E	CH3-C*=CH-CH2-CH2-CH2*
OLED	100.0%	T13PNTDE	CH2=CH-^CH=CH-^CH3
TERP	99.5%	Total	Derived from Megan2 Mixture
	45.1%	A-PINENE	CH3-C*1=CH-CH2-CH*2-CH2-CH*1-C*2(CH3)-CH3
	13.2%	B-OCIMEN	CH2=CH-C(CH3)=CH-CH2-CH=C(CH3)-CH3

Table A-2. (continued).

Species	Fac [a]	DMS [b]	Mixture derivation or compound structure [c]
	12.9%	B-PINENE	CH2=C*1-CH2-CH2-CH*2-CH2-CH*1-C*2(CH3)-CH3
	7.8%	D-LIMONE	CH2=C(CH3)-CH*-CH2-CH=C(CH3)-CH2-CH2*
	6.1%	SABINENE	CH2=C*1-CH2-CH2-C*2(CH2-CH*12)-CH(CH3)-CH3
	5.9%	MYRCENE	CH2=CH-C(=CH2)-CH2-CH2-CH=C(CH3)-CH3
	4.8%	3-CARENE	CH3-C*1=CH-CH2-CH*2-CH(CH2*1)-C*2(CH3)-CH3
	2.8%	CAMPHENE	CH2=C*1-CH*2-CH2-CH2-CH(CH2*2)-C*1(CH3)-CH3
	0.9%	TRPNOLEN	CH3-C(CH3)=C*-CH2-CH=C(CH3)-CH2-CH2*
AMINS	99.7%	Total	Derived from UStot Mixture
	51.6%	ET-AMINE	CH3-CH2-NH2
	39.3%	TM-AMINE	CH3-N(CH3)-CH3
	8.8%	ETOH-NH2	NH2-CH2-CH2-OH
ARO1	99.3%	Total	Derived from UStot Mixture
	43.7%	N-C3-BEN	CH3-CH2-CH2-aC*-aCH-aCH-aCH-aCH-aCH*
	26.6%	2MPR-BEN	CH3-CH(CH3)-CH2-aC*-aCH-aCH-aCH-aCH-aCH*
	20.3%	I-C3-BEN	CH3-CH(CH3)-aC*-aCH-aCH-aCH-aCH-aCH*
	4.3%	BZ-CH2OH	HO-CH2-aC*-aCH-aCH-aCH-aCH-aCH*
	2.1%	T-C4-BEN	CH3-C(CH3)(CH3)-aC*-aCH-aCH-aCH-aCH-aCH*
	1.5%	PTHT-ANH	CO*1-O-CO-aC*2-aCH-aCH-aCH-aCH-aC*12
	0.7%	N-C5-BEN	CH3-CH2-CH2-CH2-CH2-aC*-aCH-aCH-aCH-aCH-aCH*
ARO2	99.2%	Total	Derived from UStot Mixture
	44.2%	M-ET-TOL	CH3-CH2-aC*-aCH-aCH-aCH-aC(CH3)-aCH*
	18.9%	P-ET-TOL	CH3-CH2-aC*-aCH-aCH-aC(CH3)-aCH-aCH*
	14.9%	O-ET-TOL	CH3-CH2-aC*-aCH-aCH-aCH-aCH-aC*-CH3
	8.8%	M-CYMENE	CH3-CH(CH3)-aC*-aCH-aCH-aCH-aC(CH3)-aCH*
	4.2%	12M4ETBN	CH3-CH2-aC*-aCH-aCH-aC(CH3)-aC(CH3)-aCH*
	2.7%	O-CYMENE	CH3-CH(CH3)-aC*-aCH-aCH-aCH-aCH-aC*-CH3
	2.5%	P-C3-TOL	CH3-CH2-CH2-aC*-aCH-aCH-aC(CH3)-aCH-aCH*
	1.8%	13M5ETBN	CH3-CH2-aC*-aCH-aC(CH3)-aCH-aC(CH3)-aCH*
	0.8%	12M3ETBN	CH3-CH2-aC*-aCH-aCH-aCH-aC(CH3)-aC*-CH3
	0.4%	P-CYMENE	CH3-CH(CH3)-aC*-aCH-aCH-aC(CH3)-aCH-aCH*
OTH1	99.8%	Total	Derived from UStot OHprods Mixture
	56.9%	ME-FORM	CH3-O-CHO
	16.3%		CH3-CO-O-CO-CH3
	11.3%		CH3-C(CH3)(CH3)-O-CHO
	6.5%		CH3-CH2-CO-O-CO-CH3
	5.0%	ET-FORM	CH3-CH2-O-CHO
	2.8%	ME-ACET	CH3-CO-O-CH3
	1.0%	ET-ACET	CH3-CH2-O-CO-CH3
OTH2	99.7%	Total	Derived from UStot Mixture
	76.4%	ME-O-ME	CH3-O-CH3
	23.3%	MTBE	CH3-O-C(CH3)(CH3)-CH3
OTH3	99.0%	Total	Derived from UStot Mixture
	60.8%	I-C3-OH	CH3-CH(CH3)-OH
	19.3%	PR-ACET	CH3-CH2-CH2-O-CO-CH3
	4.9%	BU-ACET	CH3-CH2-CH2-CH2-O-CO-CH3

Table A-2. (continued).

Species	Fac [a]	DMS [b]	Mixture derivation or compound structure [c]
	3.4%	IPR-ACET	CH3-CO-O-CH(CH3)-CH3
	2.8%	S-C4-OH	CH3-CH2-CH(CH3)-OH
	2.6%	N-C3-OH	CH3-CH2-CH2-OH
	2.2%	N-C4-OH	CH3-CH2-CH2-CH2-OH
	1.7%	I-C4-OH	CH3-CH(CH3)-CH2-OH
	0.7%	IBU-ACET	CH3-CO-O-CH2-CH(CH3)-CH3
	0.7%	CC6-KET	CH2*-CH2-CH2-CO-CH2-CH2*
OTH4	96.8%	Total	Derived from UStot Mixture
	28.7%	ET-GLYCL	HO-CH2-CH2-OH
	27.7%	PR-GLYCL	CH3-CH(OH)-CH2-OH
	17.6%	BUO-ETOH	CH3-CH2-CH2-CH2-O-CH2-CH2-OH
	4.0%	THF	CH2*-CH2-CH2-O-CH2*
	3.9%	DGBE	CH3-CH2-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
	1.8%	MOEOETOH	CH3-O-CH2-CH2-O-CH2-CH2-OH
	1.7%	DET-GLCL	HO-CH2-CH2-O-CH2-CH2-OH
	1.3%	MEOC3OH	CH3-O-CH2-CH(CH3)-OH
	1.2%	PGME-ACT	CH3-CO-O-CH(CH3)-CH2-O-CH3
	1.0%	DPR-GLCL	CH3-CH(OH)-CH2-O-CH2-CH(CH3)-OH
	1.0%	PROXC3OH	CH3-CH2-CH2-O-CH2-CH(CH3)-OH
	0.9%	GLYCERL	HO-CH2-CH(OH)-CH2-OH
	0.9%	E3EOC3OH	CH3-CH2-O-CH2-CH2-CO-O-CH2-CH3
	0.8%	ET-O-ET	CH3-CH2-O-CH2-CH3
	0.8%	BUOC3OH	CH3-CH2-CH2-CH2-O-CH2-CH(CH3)-OH
	0.8%	CSV-ACET	CH3-CH2-O-CH2-CH2-O-CO-CH3
	0.7%	IAMOH	CH3-CH(CH3)-CH2-CH2-OH
	0.7%	DGEE	CH3-CH2-O-CH2-CH2-O-CH2-CH2-OH
	0.7%	2M24C5OH	CH3-CH(OH)-CH2-C(CH3)(CH3)-OH
	0.6%	ET-O-IPR	CH3-CH2-O-CH(CH3)-CH3
RCHO	73.0%	Total	Derived from UStot OHprods Mixture
	22.7%	2MEC3AL	CH3-CH(CH3)-CHO
	15.9%		HCO-CH2-CH2-CH2-OH
	11.4%	1C4RCHO	CH3-CH2-CH2-CHO
	5.2%		CH3-CH(CHO)-CH2-CH2-OH
	3.5%		CH3-CH(OH)-CH2-CH2-CHO
	3.5%		CH3-CH(CHO)-OH
	3.4%		CH3-CH(CH2-CHO)-CH2-OH
	2.3%	3MC4RCHO	CH3-CH(CH3)-CH2-CHO
	2.0%		CH3-C(CH3)(OH)-CH2-CH2-CHO
	1.8%	GLTRALD	HCO-CH2-CH2-CH2-CHO
	1.4%		HCO-CH2-CH2-O-CHO
KET2	83.5%	Total	Derived from UStot OHprods Mixture
	22.9%	PROD2-1	CH3-CO-CH2-CH2-CH2-OH
	8.2%	DEK	CH3-CH2-CO-CH2-CH3
	8.0%	PROD2-6	CH3-CO-CH2-CH2-CH(CH3)-OH
	7.5%	PROD2-7	CH3-CH2-CO-CH2-CH2-CH2-OH
	6.4%	HOACET	CH3-CO-CH2-OH

Table A-2. (continued).

Species	Fac [a]	DMS [b]	Mixture derivation or compound structure [c]
	4.8%	PROD2-2	CH3-CO-CH2-CH(CH3)-CH2-OH
	4.2%	MPK	CH3-CH2-CH2-CO-CH3
	4.0%		CH3-CO-CH2-O-CO-CH3
	3.0%	PROD2-3	CH3-CH2-CO-CH2-CH2-CH(CH3)-OH
	2.6%	DIACTALC	CH3-CO-CH2-C(CH3)(CH3)-OH
	1.9%	PROD2-10	CH3-CH2-CH(OH)-CH2-CH2-CO-CH3
	1.7%	PROD2-9	CH3-CO-CH2-CH2-C(CH3)(CH3)-OH
	1.5%	MIPRK	CH3-CO-CH(CH3)-CH3
	1.4%		CH3-CH2-CH2-CO-CH2-CH2-CH2-OH
	1.0%	3-C6-KET	CH3-CH2-CH2-CO-CH2-CH3
	1.0%	MIBK	CH3-CO-CH2-CH(CH3)-CH3
	0.9%		CH3-CH2-CH2-CO-CH2-CH2-CH(CH3)-OH
	0.9%		CH3-CH2-CO-CH2-CH(CH3)-CH2-OH
	0.8%		CH3-CH2-CO-CH2-O-CO-CH3
	0.8%		CH3-CO-CH2-C(CH3)(CH3)-CH2-OH
OLEP	67.7%	Total	Derived from Isoprene OHprods Mixture
	51.5%		CH3-C*=CH-O-C(=CH*)-OH
	16.2%		CH3-C*=C(OH)-O-CH=CH*
OLEA1	93.1%	Total	Derived from Isoprene OHprods Mixture
	33.3%	IP-MHY1	CH3-C(CHO)=CH-CH2-OH
	31.3%		CH3-C(CHO)=CH-OH
	28.5%	IP-HMY	CH3-C(=CH-CHO)-CH2-OH
RCOOH	100.0%	Total	Derived from UStot OHprods Mixture
	100.0%	PROPACID	CH3-CH2-CO-OH
R1NO3	56.5%	Total	Derived from UStot OHprods Mixture
	12.2%	2C4-ONO2	CH3-CH2-CH(CH3)-ONO2
	10.2%		CH3-CH2-C(CH3)(CH3)-ONO2
	7.2%	IC3-ONO2	CH3-CH(CH3)-ONO2
	4.3%		CH3-CH(CH3)-CH(CH3)-ONO2
	4.3%		CH3-CH2-CH2-CH(CH3)-ONO2
	4.2%		CH3-C(CH3)(CH3)-ONO2
	3.2%		CH3-CH2-CH2-C(CH3)(CH3)-ONO2
	2.9%		CH3-CH2-CH2-CH(ONO2)-CH2-CH3
	2.8%		CH3-C(CH3)(CH3)-CH2-C(CH3)(CH3)-ONO2
	2.7%		CH3-CH2-CH(ONO2)-CH2-CH3
	2.7%		CH3-CH2-C(CH3)(ONO2)-CH2-CH3
R2NO3	51.4%	Total	Derived from UStot OHprods Mixture
	9.5%		O2NO-CH*-CH2-CH2-CH2-CH2-CH2*
	5.5%		CH3-C*(ONO2)-CH2-CH2-CH2-CH2-CH2*
	5.2%		CH3-CH*-CH2-CH2-CH2-CH(ONO2)-CH2*
	4.8%		CH3-CH2-CH2-CH2-CH2-CH(ONO2)-CH2-CH3
	4.8%		CH3-CH2-CH2-CH2-CH(ONO2)-CH2-CH2-CH3
	4.0%		CH3-CH*-CH2-CH2-CH2-CH2-CH*-ONO2
	3.7%		CH3-CH2-CH2-CH2-CH2-CH2-CH(CH3)-ONO2
	2.6%		CH3-CH*-CH2-CH2-CH(ONO2)-CH2-CH2*

Table A-2. (continued).

Species	Fac [a]	DMS [b]	Mixture derivation or compound structure [c]
	2.1%		CH3-CH2-CH2-CH2-CH2-CH2-CH(ONO2)-CH2-CH3
	2.1%		CH3-CH2-CH2-CH2-CH2-CH(ONO2)-CH2-CH2-CH3
	1.8%		CH3-CH*-CH2-CH2-CH2-C(CH3)(ONO2)-CH2*
	1.7%		CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH(ONO2)-CH2-CH3
	1.7%		CH3-CH2-CH2-CH2-CH2-CH2-CH(ONO2)-CH2-CH2-CH3
	1.7%		CH3-CH2-CH2-CH2-CH2-CH(ONO2)-CH2-CH2-CH2-CH3
RANO3	85.0%	Total	Derived from UStot OHprods Mixture
	32.2%		O2NO-CH2-aC*-aCH-aCH-aCH-aCH-aCH*
	30.9%		CH3-CH(ONO2)-aC*-aCH-aCH-aCH-aCH-aCH*
	5.3%		CH3-aC*-aCH-aCH-aC(CH2-ONO2)-aCH-aCH*
	4.4%		CH3-aC*-aCH-aCH-aCH-aCH-aC*-CH2-ONO2
	3.9%		CH3-aC*-aCH-aCH-aCH-aC(CH2-ONO2)-aCH*
	3.3%		CH3-CH2-CH(ONO2)-aC*-aCH-aCH-aCH-aCH-aCH*
	2.7%		CH3-CH(ONO2)-aC*-aCH-aCH-aCH-aC(CH3)-aCH*
	2.3%		CH3-CH(ONO2)-aC*-aCH-aCH-aC(CH3)-aCH-aCH*
RCNO3	97.2%	Total	Derived from UStot NO3prods Mixture
	47.5%		CH3-CO-CH2-ONO2
	31.0%		HCO-CH2-ONO2
	5.5%		HO-CH2-CH2-CH2-CO-CH2-ONO2
	4.6%		CH3-CH2-CO-CH2-ONO2
	4.1%		O2NO-CH2-CO-aC*-aCH-aCH-aCH-aCH-aCH*
	1.5%		CH3-CH(OH)-CH2-CH2-CO-CH2-ONO2
	1.4%		CH2=CH-CO-CH2-ONO2
	1.0%		CH3-CH(CH3)-CO-CH2-ONO2
	0.6%		CH3-CH2-CH2-CO-CH2-ONO2
RHNO3	26.9%	Total	Derived from UStot OHprods Mixture
	4.4%		CH3-CH(OH)-CH2-CH2-CH2-ONO2
	4.0%		CH3-C(CH3)(OH)-CH2-C(CH3)(CH3)-CH2-ONO2
	3.5%		CH3-CH(CH3)-CH(ONO2)-CH2-OH
	3.3%		CH3-C(CH3)(OH)-CH2-CH2-CH2-ONO2
	3.2%		CH3-C(CH3)(ONO2)-CH2-OH
	3.2%		CH3-CH2-CH(OH)-CH2-CH2-CH2-ONO2
	2.8%		CH3-CH(OH)-CH2-CH2-CH(CH3)-ONO2
	2.6%		CH3-C(OH)(CH2-ONO2)-CH2-CH2-CH2-OH
RPNO3	72.7%	Total	Derived from UStot OHprods Mixture
	17.5%		CH3-C*12-O-O-CH(CH=CH-CH*1-ONO2)-CH*2-OH
	17.5%		CH3-C*12-CH=CH-CH(ONO2)-CH(O-O*1)-CH*2-OH
	10.7%		CH3-C*12-CH=CH-CH(ONO2)-C(CH3)(O-O*1)-CH*2-OH
	4.7%		HO-CH*1-CH*2-CH=CH-CH(ONO2)-CH*1-O-O*2
	3.3%		CH3-C*1=CH-CH(ONO2)-C*2(CH3)-O-O-CH*1-CH*2-OH
	3.3%		CH3-C*1(ONO2)-CH=CH-C*2(CH3)-O-O-CH*1-CH*2-OH
	3.2%		CH3-C*1(OH)-CH*2-CH=CH-CH(ONO2)-C*1(CH3)-O-O*2
	3.2%		CH3-C*1(OH)-CH*2-O-O-C*1(CH3)-CH=CH-CH*2-ONO2
	2.8%		CH3-C*1=CH-C*2(CH3)-O-O-C(CH3)(CH*2-OH)-CH*1-ONO2
	2.2%		CH3-CH2-C*12-O-O-C(CH3)(CH=CH-CH*1-ONO2)-CH*2-OH

Table A-2. (continued).

Species	Fac [a]	DMS [b]	Mixture derivation or compound structure [c]
	2.2%		CH3-CH2-C*12-CH=CH-CH(ONO2)-C(CH3)(O-O*1)-CH*2-OH
	2.0%		CH3-C*1=CH-CH(ONO2)-C*2(CH3)-O-O-C*1(CH3)-CH*2-OH
RDNO3	70.6%	Total	Derived from UStot NO3prods Mixture
	17.4%		CH3-CH(CH3)-CH(ONO2)-CH2-ONO2
	11.9%		O2NO-CH2-CH(ONO2)-aC*-aCH-aCH-aCH-aCH-aCH*
	8.1%		CH3-CH2-CH(ONO2)-CH(CH3)-ONO2
	7.0%		CH3-CH(ONO2)-C(CH3)(CH3)-ONO2
	7.0%		CH2=C(CH3)-CH*-CH2-CH2-C(CH3)(ONO2)-CH(ONO2)-CH2*
	6.4%		CH3-CH2-C(CH3)(ONO2)-CH2-ONO2
	3.9%		CH3-CH2-CH2-CH(ONO2)-CH2-ONO2
	3.1%		HO-CH(CH2-ONO2)-CH2-CH2-CH2-ONO2
	3.1%		CH3-CH(ONO2)-CH(CH3)-ONO2
	2.8%		CH3-C(CH3)(ONO2)-CH2-ONO2
RUOOH	97.0%	Total	Derived from Isoprene HO2prods Mixture
	39.9%		CH2=CH-C(CH3)(CH2-OH)-O-OH
	27.7%		CH2=C(CH3)-CH(CH2-OH)-O-OH
	9.4%		CH3-C(=CH-OH)-CH(CH2-O-OH)-O-OH
	7.8%		CH3-C(CH=CH-OH)(CH2-O-OH)-O-OH
	6.5%		CH3-C(OH)(CH=CH-OH)-CH2-O-OH
	3.2%		CH2=CH-C(CH3)(OH)-CH2-O-OH
	2.5%		CH2=C(CH2-O-OH)-CH(OH)-CH2-O-OH
RAOOH	77.0%	Total	Derived from UStot HO2prods Mixture
	21.2%		CH3-C*12-O-O-CH(CH=CH-CH*1-O-OH)-CH*2-OH
	21.2%		CH3-C*12-CH=CH-CH(O-OH)-CH(O-O*1)-CH*2-OH
	9.5%		CH3-C*12-CH=CH-CH(O-OH)-C(CH3)(O-O*1)-CH*2-OH
	8.2%		HO-O-CH*1-CH=CH-CH*2-O-O-CH*1-CH*2-OH
	3.0%		CH3-C*1=CH-CH(O-OH)-C*2(CH3)-O-O-CH*1-CH*2-OH
	3.0%		CH3-C*1(CH=CH-C*2(CH3)-O-O-CH*1-CH*2-OH)-O-OH
	2.9%		CH3-C*1(OH)-CH*2-CH=CH-CH(O-OH)-C*1(CH3)-O-O*2
	2.9%		CH3-C*1(OH)-CH*2-O-O-C*1(CH3)-CH=CH-CH*2-O-OH
	2.0%		CH3-C*1=CH-C*2(CH3)-O-O-C(CH3)(CH*2-OH)-CH*1-O-OH
	1.7%		CH3-CH2-C*12-CH=CH-CH(O-OH)-CH(O-O*1)-CH*2-OH
	1.7%		CH3-CH2-C*12-O-O-CH(CH=CH-CH*1-O-OH)-CH*2-OH
HPALD	99.8%	Total	Derived from Isoprene OHprods Mixture
	50.9%		CH3-C(CHO)=CH-CH2-O-OH
	36.5%		CH3-C(=CH-CHO)-CH2-O-OH
	8.8%		CH2=C(CHO)-CH(OH)-CH2-O-OH
	3.6%		HCO-CH=C(CH2-OH)-CH2-O-OH
CROOH	71.5%	Total	Derived from UStot HO2prods Mixture
	16.8%		CH3-CH2-CH(O-OH)-O-CO-CH3
	9.7%		CH3-CO-O-CH2-CH(CH3)-O-OH
	8.3%		CH3-CO-CH2-CH2-CH2-CH2-O-OH
	7.0%		CH3-CO-CH(CH2-CH2-CH2-OH)-O-OH
	5.0%		CH3-CO-CH2-C(CH3)(CH3)-O-OH
	4.5%		CH3-CO-O-C(CH3)(CH3)-O-OH

Table A-2. (continued).

Species	Fac [a]	DMS [b]	Mixture derivation or compound structure [c]
	4.4%		CH3-CO-O-CH(CH3)-O-OH
	3.7%		CH3-CO-CH2-CH2-CH2-CH2-CH2-O-OH
	3.0%		CH3-CH2-CH2-CH(O-OH)-O-CO-CH3
	2.4%		HCO-O-CH2-CH2-CH2-O-OH
	2.3%		CH3-CO-CH2-CH(CH2-CH2-CH2-OH)-O-OH
	2.2%		CH3-CH2-CH(CH2-O-CO-CH3)-O-OH
	2.2%		CH3-CO-O-CH2-O-OH
ROOH	47.0%	Total	Derived from UStot HO2prods Mixture
	10.5%		CH3-CH2-CH(CH3)-O-OH
	10.3%		CH3-CH(CH3)-O-OH
	5.9%		CH3-CH2-C(CH3)(CH3)-O-OH
	3.8%		CH3-CH(CH2-OH)-O-OH
	3.6%		CH3-C(CH3)(CH3)-O-OH
	2.5%		CH3-CH(CH3)-CH(CH3)-O-OH
	2.5%		CH3-CH2-CH2-CH(CH3)-O-OH
	2.4%		CH3-CH2-CH2-O-OH
	2.2%		CH3-CH(OH)-CH2-O-OH
	1.9%		CH3-CH(OH)-CH2-CH2-CH2-O-OH
	1.6%		CH3-CH2-CH(CH2-CH3)-O-OH
AFG1	99.1%	Total	Derived from UStot OHprods Mixture
	89.0%	2MBUTDAL	CH3-C(CHO)=CH-CHO
	7.3%		CH3-CH2-C(CHO)=CH-CHO
	2.3%	23MBUDAL	CH3-C(CHO)=C(CH3)-CHO
	0.5%		CH3-CH2-CH2-C(CHO)=CH-CHO
AFG2A	97.6%	Total	Derived from UStot OHprods Mixture
	81.8%	4OX2PEAL	CH3-CO-CH=CH-CHO
	7.4%	2M4OX2PA	CH3-CO-CH=C(CH3)-CHO
	7.4%		CH3-CH2-CO-CH=CH-CHO
	1.0%		CH3-CH(CH3)-CO-CH=CH-CHO
AFG2B	98.7%	Total	Derived from UStot OHprods Mixture
	90.6%	3M4OX2PA	CH3-CO-C(CH3)=CH-CHO
	3.3%		CH3-CH2-C(=CH-CHO)-CO-CH3
	3.1%		CH3-CH2-CO-C(CH3)=CH-CHO
	1.7%	23M4O2PA	CH3-CO-C(CH3)=C(CH3)-CHO
AFG3	99.6%	Total	Derived from UStot OHprods Mixture
	79.8%	3HXE25DO	CH3-CO-CH=CH-CO-CH3
	13.1%		CH3-CH2-CO-CH=CH-CO-CH3
	5.5%	3M3HX25O	CH3-CO-CH=C(CH3)-CO-CH3
	1.2%		CH3-CH2-CH2-CO-CH=CH-CO-CH3
AFG4	81.0%	Total	Derived from UStot OHprods Mixture
	20.6%		CH3-C*=C(OH)-O-CH=CH-CH=CH*
	20.6%		CH3-C*=CH-CH=CH-CH=C(OH)-O*
	19.8%		HO-C*=CH-CH=CH-CH=CH-O*
	7.8%		CH3-C*=CH-CH=CH-C(=C(OH)-O*)-CH3
	2.9%		CH3-C*=CH-O-C(=C(CH3)-CH=CH*)-OH

Table A-2. (continued).

Species	Fac [a]	DMS [b]	Mixture derivation or compound structure [c]
	2.9%		CH3-C*=CH-CH=C(CH3)-O-C(=CH*)-OH
	1.6%		CH3-C*=CH-C(=C(OH)-O-C(=CH*)-CH3)-CH3
	1.6%		CH3-CH2-C*=CH-CH=CH-CH=C(OH)-O*
	1.6%		CH3-CH2-C*=C(OH)-O-CH=CH-CH=CH*
	1.6%		CH3-C*=CH-O-C(=CH-CH=CH*)-OH

[a] Contribution of the compound used when deriving the mechanism of the mixture (molar). Does not always sum to 100% because some compounds in mixtures were not used to derive the mechanisms either because of low yields, because the mechanism generation system is not expected to process them properly, or because of the relatively large number of such compounds in the mixtures. "Total" is total of fractions for compounds used.

[b] See the supplementary material (Carter, 2016) for a description of the detailed model species (DMS). If blank, this is a generated product that is not a regular detailed model species. The "Structure" column indicates the compound that was used.

[c] For compounds, this column gives the structure used in the mechanism generation system. Note that the symbol "*" is used to designate ring closure, and "aC" or "aCH" is used to designate aromatic resonance. For mixtures, this gives the mixture used to obtain the compounds used to derive the mechanisms and the mole fractions. In all cases these are compounds represented by the model species in the first column, listed in descending order of relative importance. Abbreviations used for the mixtures are as follows:

UStot	Total US Emissions based on the 2005ah_tox inventory using the criteria VOC emissions only from all sectors except biogenic and fires (Luecken, 2013).
UStot OHprods	First generation products of the reactions of OH radicals with the compounds in the UStot mixture.
UStot NO3prods	First generation products of the reactions of NO_3 radicals with the compounds in the UStot mixture.
USTOT HO2prods	First generation products of the reactions of HO_2 with the peroxy radicals formed in the reactions of OH radicals with the compounds in the UStot mixture.
Megan2	Global annual total biogenic VOC emissions for the year 2000 calculated using the using MEGAN 2.1 model algorithms in CLM4 (Guenther, 2014; see also Guenther et al 2012).
Isoprene OHprods	First generation products of the reactions of OH radicals with isoprene.
Isoprene HO2prods	First generation products of the reactions of HO_2 with the peroxy radicals formed in the reactions of OH radicals with isoprene.

Table A-3. List of reactions and documentation notes in the version of SAPRC-16 for atmospheric simulations.

Label	Reaction and Products [a]	Rate Parameters [b]				Notes [c]
		k(300)	A	Ea	B	
	Inorganic Reactions					
1	NO2 + HV = NO + O3P	Phot Set= NO2-06				1
2	O3P + O2 + M = O3 + M	6.00e-34	6.00e-34	-	2.40	1
3	O3P + O3 = #2 O2	8.34e-15	8.00e-12	4.09	-	1
4	O3P + NO = NO2	1.64e-12	Falloff, F=0.60, N=1.00			1
		0:	9.00e-32	-	-1.50	
		Inf:	3.00e-11	-	-	
5	O3P + NO2 = NO + O2	1.03e-11	5.10e-12	-0.42	-	1
6	O3P + NO2 = NO3	3.24e-12	Falloff, F=0.60, N=1.00			1
		0:	2.50e-31	-	-1.80	
		Inf:	2.20e-11	-	-0.70	
7	O3 + NO = NO2 + O2	2.02e-14	3.00e-12	2.98	-	1
8	O3 + NO2 = O2 + NO3	3.41e-17	1.20e-13	4.87	-	1
9	NO + NO3 = #2 NO2	2.64e-11	1.50e-11	-0.34	-	1
10	NO + NO + O2 = #2 NO2	1.93e-38	3.30e-39	-1.05	-	2
11	NO2 + NO3 = N2O5	1.24e-12	Falloff, F=0.35, N=1.33			2
		0:	3.60e-30	-	-4.10	
		Inf:	1.90e-12	-	0.20	
12	N2O5 = NO2 + NO3	5.69e-2	Falloff, F=0.35, N=1.33			2
		0:	1.30e-3	-	-3.50	
		Inf:	9.70e+14	22.02	0.10	
13	N2O5 + H2O = #2 HNO3	0.00e+0				3
14	N2O5 + H2O + H2O = #2 HNO3 + H2O	0.00e+0				3
15	NO2 + NO3 = NO + NO2 + O2	6.75e-16	4.50e-14	2.50	-	1
16	NO3 + HV = NO + O2	Phot Set= NO3NO-06				1
17	NO3 + HV = NO2 + O3P	Phot Set= NO3NO2-6				1
18	O3 + HV = O1D + O2	Phot Set= O3O1D-06				1
19	O3 + HV = O3P + O2	Phot Set= O3O3P-06				1
20	O1D + H2O = #2 OH	1.99e-10	1.63e-10	-0.12	-	1
21	O1D + M = O3P + M	3.68e-11	2.65e-11	-0.20	-	4
22	OH + NO = HONO	7.31e-12	Falloff, F=0.60, N=1.00			1
		0:	7.00e-31	-	-2.60	
		Inf:	3.60e-11	-	-0.10	
23	HONO + HV = OH + NO	Phot Set= HONO-06				1
24	OH + HONO = H2O + NO2	4.91e-12	1.80e-11	0.78	-	1
25	OH + NO2 = HNO3	9.73e-12	Falloff, F=0.41, N=1.24			2
		0:	3.20e-30	-	-4.50	
		Inf:	3.00e-11	-	-	
26	OH + NO3 = HO2 + NO2	2.20e-11				1
27	OH + HNO3 = H2O + NO3	1.51e-13	k = k0+k3M/(1+k3M/k2)			1
		k0:	2.40e-14	-0.91	-	
		k2:	2.70e-17	-4.37	-	
		k3:	6.50e-34	-2.65	-	
28	HNO3 + HV = OH + NO2	Phot Set= HNO3				1
29	OH + O3 = HO2 + O2	7.41e-14	1.70e-12	1.87	-	1
30	HO2 + NO = OH + NO2	8.12e-12	3.30e-12	-0.54	-	1
31	HO2 + NO = HNO3	4.21e-14	k = k1 + k2 [M]			5
		k1:	2.39e-12	3.40	-13.77	

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
		k2:	1.83e-32	1.53	-4.85	
32	HO2 + NO + H2O = HNO3 + H2O	2.20e-31	1.20e-35	-5.85	-	6
33	HO2 + NO2 = HNO4	7.40e-13	Falloff, F=0.40, N=1.26			2
		0:	1.40e-31	-	-3.10	
		Inf:	4.00e-12	-	-	
34	HNO4 = HO2 + NO2	7.89e-2	Falloff, F=0.40, N=1.26			2
		0:	4.10e-5	-	-	
		Inf:	6.00e+15	22.20	-	
35	HNO4 + HV = #.8 {HO2 + NO2} + #.2 {OH + NO3}	Phot Set= HNO4-06				1
36	HNO4 + OH = H2O + NO2 + O2	4.61e-12	1.30e-12	-0.76	-	1
37	HO2 + O3 = OH + #2 O2	1.95e-15	1.00e-14	0.97	-	1
38	HO2 + HO2 = HO2H + O2	2.49e-12	k = k1 + k2 [M]			1
		k1:	3.00e-13	-0.91	-	
		k2:	2.10e-33	-1.83	-	
39	HO2 + HO2 + H2O = HO2H + O2 + H2O	5.34e-30	k = k1 + k2 [M]			1
		k1:	4.20e-34	-5.29	-	
		k2:	2.94e-54	-6.20	-	
40	NO3 + HO2 =OH + NO2 + O2	3.50e-12				1
41	NO3 + NO3 = #2 NO2 + O2	2.41e-16	8.50e-13	4.87	-	1
42	HO2H + HV = #2 OH	Phot Set= H2O2				1
43	HO2H + OH = HO2 + H2O	1.80e-12				1
44	OH + HO2 = H2O + O2	1.10e-10	4.80e-11	-0.50	-	1
45	OH + SO2 = HO2 + SULF	9.49e-13	Falloff, F=0.60, N=1.00			1
		0:	3.30e-31	-	-4.30	
		Inf:	1.60e-12	-	-	
46	OH + H2 = HO2 + H2O	6.94e-15	2.80e-12	3.58	-	1
	Reactions of explicit and lumped organic compounds (excluding MechGen-derived reactions)					
C001	CH4 + OH = MEO2 + SumRO2	6.60e-15	2.45e-12	3.53	-	1,7
C002	MEOH + OH = HCHO + HO2	9.18e-13	2.90e-12	0.69	-	1
C003	MEOOH + OH = H2O + #.4 {HCHO + OH} + #.6 {MEO2 + SumRO2}	7.40e-12	3.80e-12	-0.40	-	1,7
C004	MEOOH + HV = HCHO + HO2 + OH	Phot Set= COOH				2
C005	HCHO + HV = #2 HO2 + CO	Phot Set= HCHOR-13				8
C006	HCHO + HV = H2 + CO	Phot Set= HCHOM-13				8
C007	HCHO + OH = HO2 + CO + H2O	8.34e-12	5.50e-12	-0.25	-	1
C008	HCHO + NO3 = HNO3 + HO2 + CO	5.80e-16				1
C009	CO + OH = HO2 + CO2	2.28e-13	k = k1 + k2 [M]			2
		k1:	1.44e-13	-	-	
		k2:	3.43e-33	-	-	
C010	HCOOH + OH = HO2 + CO2	4.00e-13				1
C011	ETHAN + OH = ETO2 + SumRO2	2.56e-13	7.66e-12	2.03	-	1,7
C012	ETHEN + OH = ETHEO2 + SumRO2	7.81e-12	Falloff, F=0.60, N=1.00			1,7
		0:	1.10e-28	-	-3.50	
		Inf:	8.40e-12	-	-1.75	
C013	ETHEN + O3 = #.16 HO2 + #.16 OH + #.51 CO + #.12 CO2 + HCHO + #.37 HCHO2	1.87e-18	1.20e-14	5.23	-	1
C014	ETHEN + NO3 = ETHEO2N + SumRO2	2.24e-16	3.30e-12	5.72	-	2,7
C015	ETHEN + O3P = #4.405 NROG + #.8 HO2 + #.51 CO + #.51 MEO2 + #.29 HCOMEO2 + #.1 MECHO + #.8 SumRO2 + #.2 XC	7.43e-13	1.07e-11	1.59	-	9,7

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
C016	ACETL + OH = #.3 HO2 + #.7 OH + #.3 CO + #.3 HCOOH + #.7 GLY	7.56e-13	Falloff, F=0.60, N=1.00			1
		0:	5.50e-30	-	-	
		Inf:	8.30e-13	-	2.00	
C017	ACETL + O3 = #1.5 HO2 + #.5 OH + #1.5 CO + #.5 CO2	1.16e-20	1.00e-14	8.15	-	1
C018	ETOH + OH = #.95 {HO2 + MECHO} + #.05 ETHEO2 + #0.05 SumRO2	3.32e-12	3.32e-12	-	-	1,7
C019	AACID + OH = H2O + MEO2 + CO2 + SumRO2	6.76e-13	3.15e-14	-1.83	-	1,7
C020	ETOOH + OH = #1.233 NROG + #.594 OH + #.567 MECHO + #.406 ETO2 + #.054 XC + #0.406 SumRO2	6.04e-12				10,7
C021	ETOOH + HV = OH + HO2 + MECHO	Phot Set= COOH				16
C022	MECHO + OH = H2O + #.95 {MECO3 + SumRCO3} + #.05 {HCOMEO2 + SumRO2}	1.49e-11	4.63e-12	-0.70	-	1,7
C023	MECHO + HV = HO2 + #.9 {CO + MEO2 + SumRO2} + #.1 {MECO3 + SumRCO3}	Phot Set= CCHOR-13				11,7
C024	MECHO + NO3 = HNO3 + MECO3 + SumRCO3	2.49e-15	1.40e-12	3.78	-	1,7
C025	ETCHO + OH = H2O + ETCO3 + SumRCO3	1.89e-11	4.90e-12	-0.80	-	2,12,7
C026	ETCHO + NO3 = HNO3 + ETCO3 + SumRCO3	6.53e-15	1.40e-12	3.20	-	2,7
C027	ETCHO + HV = ETO2 + CO + HO2 + SumRO2	Phot Set= C2CHO				2,7
C028	GLCHO + OH = #.2 HO2 + #.8 {HOCCO3 + SumRCO3} + #.2 GLY	8.00e-12				2,7
C029	GLCHO + NO3 = HNO3 + #.991 {HOCCO3 + SumRCO3} + #.009 {CO + HCHO + HO2}	Same k as rxn C026				13,7
C030	GLCHO + HV = #.93 CO + #.1 MEOH + #.07 OH + #1.66 HO2 + #.83 HCHO + #.07 {HCOMEO2 + SumRO2}	Phot Set= GLALD-14				14,7
C031	PAA + OH = H2O + MECO3 + SumRCO3	2.55e-12				10,7
C032	PAA + HV = MEO2 + CO2 + OH + SumRO2	Phot Set= PAA				15,7
C033	GLY + HV = #2 {CO + HO2}	Phot Set= GLY-I13R				1
C035	GLY + HV = HCHO + CO	Phot Set= GLY-I13M				1
C036	GLY + OH = #1.7 CO + #.7 HO2 + #.3 {OH + CO2}	1.15e-11	1.15e-11	-	-	1
C037	GLY + NO3 = HNO3 + #1.7 CO + #.7 HO2 + #.3 {OH + CO2}	4.00e-16				2
C038	ACET + OH = H2O + ACETO2 + SumRO2	1.81e-13	1.46e-12	1.25	-	17,7
C039	ACET + HV = MECO3 + MEO2 + SumRO2	Phot Set= ACET-06, qy= 5.0e-1				18,7
C040	MGLY + HV = HO2 + CO + MECO3 + SumRCO3	Phot Set= MGLY-13				19,7
C041	MGLY + OH = CO + MECO3 + SumRCO3	1.29e-11	1.90e-12	-1.14	-	2,7
C042	MGLY + NO3 = HNO3 + CO + MECO3 + SumRCO3	5.66e-16	1.40e-12	4.66	-	20,7
C043	BACL + HV = #2 MECO3 + #2 SumRCO3	Phot Set= BACL-11				21,7
C044	BALD + OH = BZCO3 + SumRCO3	1.20e-11				2,7
C045	BALD + HV = #7 XC	Phot Set= BALD-11, qy= 9.0e-2				22
C046	BALD + NO3 = HNO3 + BZCO3 + SumRCO3	4.00e-15				23,7
C047	PHEN + OH = #.767 HO2 + #.100 BZO + #.133 OH + #.200 RO2C + #.700 SVPHE + #.067 AFG1 + #.133 OLEA1 + #.067 GLY + #.200 SumRO2 + #-0.634 XC	2.71e-11	4.50e-13	-2.44	-	23,7,24
C048	PHEN + NO3 = #.170 HNO3 + #.770 HO2 + #.100 BZO + #.130 OH + #.200 RO2C + #.830 NPHE + #.070 AFG1 + #.130 OLEA1 + #.070 GLY + #.200 SumRO2 + #-.720 XC	4.50e-12				23,7,24

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
C049	CRES + OH = #.840 HO2 + #.100 BZO + #.060 OH + #.200 RO2C + #.700 SVPHE + #.070 AFG2A + #.070 AFG2B + #.060 OLEA1 + #.070 GLY + #.070 MGLY + #.200 SumRO2 + #.080 XC	4.47e-11	1.60e-12	-1.99	-	23,7,24
C050	CRES + NO3 = #.300 HNO3 + #.900 HO2 + #.100 BZO + #.200 RO2C + #.700 NPHE + #.100 AFG2A + #.100 AFG2B + #.100 GLY + #.100 MGLY + #.200 SumRO2 + #.600 XC	1.40e-11				23,7,24
C051	XYNL + OH = #.870 HO2 + #.100 BZO + #.030 OH + #.330 RO2C + #.570 SVPHE + #.150 AFG2A + #.150 AFG2B + #.030 OLEA1 + #.150 GLY + #.150 MGLY + #.330 SumRO2 + #.860 XC	7.30e-11				23,7,24
C052	XYNL + NO3 = #.430 HNO3 + #.920 HO2 + #.080 BZO + #.350 RO2C + #.570 NPHE + #.175 AFG2A + #.175 AFG2B + #.175 GLY + #.175 MGLY + #.350 SumRO2 + #1.300 XC	3.12e-11				25,7,24
C053	SVPHE + OH = #.600 HO2 + #.200 BZO + #.200 OH + #.400 RO2C + #.400 OTHN + #.100 AFG2A + #.100 AFG2B + #.600 OLEA1 + #.100 GLY + #.100 MGLY + #.400 SumRO2 + #-3.600 XC	2.00e-10				24,7,26
C054	SVPHE + NO3 = #.400 HNO3 + #.600 HO2 + #.200 BZO + #.200 OH + #.400 RO2C + #.200 NPHE + #.400 RNNO3 + #.100 AFG2A + #.100 AFG2B + #.600 OLEA1 + #.100 GLY + #.100 MGLY + #.400 SumRO2 + #-4.000 XC	1.70e-10				24,7,26
C055	NPHE + OH = BZO + NO2	3.50e-12				27
C056	NPHE + HV = HONO + PHEN	Phot Set= NO2-06, qy= 1.5e-3				28
C057	NAPS + OH = #.736 HO2 + #.680 NAPPRD + #.056 RO2C + #.028 AFG2A + #.028 AFG2B + #.056 GLY + #.330 NPRAD + #.250 MACO3 + #.070 SumRO2 + #.250 SumRCO3 + #-2.540 XC	2.29e-11	1.55e-11	-0.23	-	29,7,23
C058	NAPPRD + OH = HO2 + OTHN	Same k as rxn C053				30
C059	NAPPRD + NO3 = HNO3 + OTHN	Same k as rxn C054				30
C060	PHOT + HV = #2 {HO2 + RO2C + SumRO2} + OTH2 + #1 XC	Phot Set= BACL-11				31,7
C061	IMINE = MECHO + XN	1.00e+0				32
	Reactions used to compute loss processes for operators used to represent total RO2 and RCO3 radicals					
S001	SumRO2 + NO = NO	9.05e-12	2.55e-12	-0.76	-	34,33
S002	SumRO2 + HO2 = HO2	6.82e-12	6.40e-13	-1.41	-	34,33
S003	SumRO2 + NO3 = NO3	2.30e-12				34,33
S004	SumRO2 + SumRO2 =	3.50e-14				34,41
S005	SumRCO3 + NO2 = NO2	7.70e-12	7.70e-12	-	-0.20	42,35
S006	SumRCO3 + NO = NO	2.08e-11	6.70e-12	-0.68	-	42,36
S007	SumRCO3 + HO2 = HO2	1.38e-11	4.30e-13	-2.07	-	42,37
S008	SumRCO3 + NO3 = NO3	4.00e-12				42,38
S009	SumRCO3 + SumRO2 =	1.56e-11	4.40e-13	-2.13	-	34,42,39
S010	SumRCO3 + SumRCO3 =	1.70e-11				42,40
	Reactions of peroxy radicals (excluding operator and MechGen-derived reactions)					
P001	MEO2 + NO = NO2 + HCHO + HO2	7.61e-12	2.80e-12	-0.60	-	1

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
P002	MEO2 + HO2 = #.9 MEOOH + #.1 {HCHO + H2O} + O2	5.12e-12	3.80e-13	-1.55	-	2
P003	MEO2 + NO3 = HCHO + HO2 + NO2	1.20e-12				2
P004	MEO2 + SumRO2 = SumRO2 + #.5 HO2 + #.75 HCHO + #.25 MEOH	2.16e-13				34,43
P005	MEO2 + SumRCO3 = SumRCO3 + #.9 {HCHO + HO2} + #.1 {HCHO + O2}	1.06e-11	2.00e-12	-0.99	-	42,44
P006	ETO2 + NO = NO2 + MECHO + HO2		Same k as rxn S001			33
P007	ETO2 + HO2 = ETOOH + O2		Same k as rxn S002			33
P008	ETO2 + NO3 = MECHO + HO2 + NO2		Same k as rxn S003			33
P009	ETO2 + SumRO2 = SumRO2 + #.6 HO2 + #.8 MECHO + #.2 ETOH	7.60e-14				34,45
P010	ETO2 + SumRCO3 = SumRCO3 + MECHO + HO2	1.56e-11	4.40e-13	-2.13	-	43,7
P011	ETHEO2 + NO = NO2 + #1.602 HCHO + #.199 GLCHO + HO2		Same k as rxn S001			33,46
P012	ETHEO2 + NO3 = NO2 + #1.602 HCHO + #.199 GLCHO + HO2		Same k as rxn S002			33,46
P013	ETHEO2 + HO2 = ROOH + #-2 XC		Same k as rxn S003			33
P014	ETHEO2 + SumRO2 = SumRO2 + #.801 HCHO + #.5 HO2 + #.349 GLCHO + #.25 OTH4 + #-.499 XC		Same k as rxn S004			34,41
P015	ETHEO2 + SumRCO3 = SumRCO3 + #.801 HCHO + #.599 GLCHO + #.5 HO2 + #.001 XC		Same k as rxn S009			42,39
P016	HCOMEO2 = RO2C + HOCCO3	7.03e-1	1.64e+11	15.61	-	47
P017	HCOMEO2 + NO = NO2 + #.923 CO + #.923 HCHO + #.077 GLY + HO2		Same k as rxn S001			33,46
P018	HCOMEO2 + NO3 = NO2 + #.923 CO + #.923 HCHO + #.077 GLY + HO2		Same k as rxn S002			33,46
P019	HCOMEO2 + HO2 = ROOH + #-2 XC		Same k as rxn S003			33
P020	HCOMEO2 + SumRO2 = SumRO2 + #.25 GLCHO + #.288 GLY + #.462 CO + #.462 HCHO + #.5 HO2		Same k as rxn S004			34,41
P021	HCOMEO2 + SumRCO3 = SumRCO3 + #.538 GLY + #.462 CO + #.462 HCHO + #.5 HO2		Same k as rxn S009			42,39
P022	ETHEO2N + NO = #1.013 NO2 + #.026 HCHO + #.987 RCNO3 + #.987 HO2 + #-.987 XC		Same k as rxn S001			33,46
P023	ETHEO2N + NO3 = #1.013 NO2 + #.026 HCHO + #.987 RCNO3 + #.987 HO2 + #-.987 XC		Same k as rxn S002			33,46
P024	ETHEO2N + HO2 = RHNO3 + #-4 XC		Same k as rxn S003			33
P025	ETHEO2N + SumRO2 = SumRO2 + #.25 RHNO3 + #.743 RCNO3 + #.007 NO2 + #.013 HCHO + #.493 HO2 + #-1.742 XC		Same k as rxn S004			34,41
P026	ETHEO2N + SumRCO3 = SumRCO3 + #.993 RCNO3 + #.007 NO2 + #.013 HCHO + #.493 HO2 + #-.992 XC		Same k as rxn S009			42,39
P027	ACETO2 + NO = NO2 + MECO3 + HCHO + SumRCO3		Same k as rxn S001			33,46
P028	ACETO2 + NO3 = NO2 + MECO3 + HCHO + SumRCO3		Same k as rxn S002			33,46
P029	ACETO2 + HO2 = ROOH + #-1 XC		Same k as rxn S003			33
P030	ACETO2 + SumRO2 = SumRO2 + #.5 MECO3 + #.5 HCHO + #.25 KET2 + #.25 MGLY + #-0.5 XC + #0.5 SumRCO3		Same k as rxn S004			34,41
P031	ACETO2 + SumRCO3 = SumRCO3 + #.5 MECO3 + #.5 HCHO + #.5 MGLY + #0.5 SumRCO3		Same k as rxn S009			42,39

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
P032	BZO2 + NO = NO2 + BZO		Same k as rxn S001			33,46
P033	BZO2 + HO2 = ROOH + O2 + #2 XC		Same k as rxn S002			33,46
P034	BZO2 + NO3 = BZO + NO2		Same k as rxn S003			33
P035	BZO2 + SumRO2 = SumRO2 + BZO		Same k as rxn S004			34,41
P036	BZO2 + SumRCO3 = SumRCO3 + BZO		Same k as rxn S009			42,39
	Reactions of other peroxy radical operator species used to represent relatively minor processes using a SAPRC-11-like peroxy lumping approach.					
P037	RO2C + NO = NO2		Same k as rxn S001			48
P038	RO2C + HO2 =		Same k as rxn S002			48
P039	RO2C + NO3 = NO2		Same k as rxn S003			48
P040	RO2C + SumRO2 = SumRO2		Same k as rxn S004			48
P041	RO2C + SumRCO3 = SumRCO3		Same k as rxn S009			48
P042	RO2XC + NO = XN		Same k as rxn S001			49
P043	RO2XC + HO2 =		Same k as rxn S002			49
P044	RO2XC + NO3 = NO2		Same k as rxn S003			49
P045	RO2XC + SumRO2 = SumRO2		Same k as rxn S004			49
P046	RO2XC + SumRCO3 = SumRCO3		Same k as rxn S009			49
P047	zR1NO3 + NO = NO + R1NO3 + #-1 XN		Same k as rxn S001			49
P048	zR1NO3 + HO2 = HO2 + ROOH + #1 XC		Same k as rxn S002			49
P049	zR1NO3 + NO3 = NO3 + KET2		Same k as rxn S003			49
P050	zR1NO3 + SumRO2 = SumRO2 + OTH3 + #1 XC		Same k as rxn S004			49
P051	zR1NO3 + SumRCO3 = SumRCO3 + OTH3 + #1 XC		Same k as rxn S009			49
P052	zR2NO3 + NO = NO + R2NO3 + #-1 XN		Same k as rxn S001			49
P053	zR2NO3 + HO2 = HO2 + ROOH + #4 XC		Same k as rxn S002			49
P054	zR2NO3 + NO3 = NO3 + OTH3 + #4 XC		Same k as rxn S003			49
P055	zR2NO3 + SumRO2 = SumRO2 + OTH4 + #4 XC		Same k as rxn S004			49
P056	zR2NO3 + SumRCO3 = SumRCO3 + OTH4 + #4 XC		Same k as rxn S009			49
P057	zRANO3 + NO = NO + RANO3 + #-1 XN		Same k as rxn S001			49
P058	zRANO3 + HO2 = HO2 + ROOH + #4 XC		Same k as rxn S002			49
P059	zRANO3 + NO3 = NO3 + BALD + #1 XC		Same k as rxn S003			49
P060	zRANO3 + SumRO2 = SumRO2 + ARO2 + #-1 XC		Same k as rxn S004			49
P061	zRANO3 + SumRCO3 = SumRCO3 + ARO2 + #-1 XC		Same k as rxn S009			49
P062	zRCNO3 + NO = NO + RCNO3 + #-1 XN		Same k as rxn S001			49
P063	zRCNO3 + HO2 = HO2 + CROOH + #-2 XC		Same k as rxn S002			49
P064	zRCNO3 + NO3 = NO3 + RCHO + #-1 XC		Same k as rxn S003			49
P065	zRCNO3 + SumRO2 = SumRO2 + KET2 + #-2 XC		Same k as rxn S004			49
P066	zRCNO3 + SumRCO3 = SumRCO3 + KET2 + #-2 XC		Same k as rxn S009			49
P067	zRHNO3 + NO = NO + RHNO3 + #-1 XN		Same k as rxn S001			49
P068	zRHNO3 + HO2 = HO2 + ROOH + #2 XC		Same k as rxn S002			49
P069	zRHNO3 + NO3 = NO3 + KET2 + #1 XC		Same k as rxn S003			49
P070	zRHNO3 + SumRO2 = SumRO2 + OTH4 + #2 XC		Same k as rxn S004			49
P071	zRHNO3 + SumRCO3 = SumRCO3 + OTH4 + #2 XC		Same k as rxn S009			49
P072	zRDNO3 + NO = NO + RDNO3 + #-1 XN		Same k as rxn S001			49
P073	zRDNO3 + HO2 = HO2 + RHNO3		Same k as rxn S002			49
P074	zRDNO3 + NO3 = NO3 + RCHO + XN + #2 XC		Same k as rxn S003			49
P075	zRDNO3 + SumRO2 = SumRO2 + RHNO3		Same k as rxn S004			49
P076	zRDNO3 + SumRCO3 = SumRCO3 + RHNO3		Same k as rxn S009			49
P077	zRPNO3 + NO = NO + RPNO3 + #-1 XN		Same k as rxn S001			49
P078	zRPNO3 + HO2 = HO2 + RAOOH + #1 XC		Same k as rxn S002			49
P079	zRPNO3 + NO3 = NO3 + OLEA1 + #3 XC		Same k as rxn S003			49

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
P080	zRPNO3 + SumRO2 = SumRO2 + OLEP + #3 XC		Same k as rxn S004			49
P081	zRPNO3 + SumRCO3 = SumRCO3 + OLEP + #3 XC		Same k as rxn S009			49
P082	zRNNO3 + NO = NO + RNNO3 + #-1 XN		Same k as rxn S001			49
P083	zRNNO3 + HO2 = HO2 + OTHN + #-2 XC		Same k as rxn S002			49
P084	zRNNO3 + NO3 = NO3 + OTHN + #-2 XC		Same k as rxn S003			49
P085	zRNNO3 + SumRO2 = SumRO2 + OTHN + #-2 XC		Same k as rxn S004			49
P086	zRNNO3 + SumRCO3 = SumRCO3 + OTHN + #-2 XC		Same k as rxn S009			49
	Reactions of acyl peroxy radicals and PANs (excluding operator and MechGen-derived reactions)					
Q001	MECO3 + NO2 = PAN	8.59e-12	Falloff, F=0.60, N=1.00			1
		0:	9.70e-29	-	-5.60	
		Inf:	9.30e-12	-	-1.50	
Q002	MECO3 + NO = MEO2 + CO2 + NO2 + SumRO2	1.99e-11	8.10e-12	-0.54	-	1,7
Q003	MECO3 + HO2 = #.44 {OH + MEO2 + CO2} + #.41 PAA + #.15 {O3 + AACID} + #0.44 SumRO2	1.38e-11	4.30e-13	-2.07	-	1,7
Q004	MECO3 + NO3 = MEO2 + CO2 + NO2 + O2 + SumRO2	4.00e-12				2,7
Q005	MECO3 + SumRO2 = SumRO2 + #.9 {MEO2 + CO2} + #.1 AACID + #0.9 SumRO2		Same k as rxn S009			34,39
Q006	MECO3 + SumRCO3 = SumRCO3 + CO2 + MEO2 + SumRO2	1.54e-11	2.90e-12	-0.99	-	42,50
Q007	PAN = MECO3 + NO2 + SumRCO3	5.16e-4	Falloff, F=0.60, N=1.00			1,7
		0:	1.08e+0	-	-5.60	
		Inf:	1.03e+17	27.82	-1.50	
Q008	PAN + HV = #.7 {MECO3 + NO2 + SumRCO3} + #.3 {MEO2 + CO2 + NO3 + SumRO2}		Phot Set= PAN-11			2,7
Q009	HOCCO3 + NO2 = HOPAN		Same k as rxn S005			35
Q010	HOCCO3 + NO = NO2 + HCHO + HO2 + CO2		Same k as rxn S006			36
Q011	HOCCO3 + HO2 = #.44 {OH + HCHO + HO2 + CO2} + #.41 PAA + #.15 {O3 + AACID}		Same k as rxn S007			37
Q012	HOCCO3 + NO3 = NO2 + HCHO + HO2 + CO2 + O2		Same k as rxn S008			38
Q013	HOCCO3 + SumRO2 = SumRO2 + HCHO + HO2 + CO2		Same k as rxn S009			34,39
Q014	HOCCO3 + SumRCO3 = SumRCO3 + HCHO + HO2 + CO2		Same k as rxn S010			42,40
Q015	HOPAN = HOCCO3 + NO2 + SumRCO3		Same k as rxn Q007			51,7
Q016	HOPAN + HV = #.6 {HOCCO3 + NO2 + SumRCO3} + #.4 {HCHO + HO2 + CO2 + NO3}		Phot Set= PPN-11			52,7
Q017	ETCO3 + NO2 = PPN	7.40e-12	Falloff, F=0.60, N=1.00			1
		0:	9.00e-28	-	-8.90	
		Inf:	7.70e-12	-	-0.20	
Q018	ETCO3 + NO = NO2 + ETO2 + CO2 + SumRO2	2.08e-11	6.70e-12	-0.68	-	2,7
Q019	ETCO3 + HO2 = #.44 {OH + ETO2 + CO2} + #.41 ROOH + #.15 {O3 + RCOOH} + #-.41 XC + #0.44 SumRO2		Same k as rxn S007			37
Q020	ETCO3 + NO3 = NO2 + ETO2 + CO2 + O2 + SumRO2		Same k as rxn S008			38
Q021	ETCO3 + SumRO2 = SumRO2 + ETO2 + CO2 + SumRO2		Same k as rxn S009			34,39
Q022	ETCO3 + SumRCO3 = SumRCO3 + ETO2 + CO2 + SumRO2		Same k as rxn S010			42,40

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
Q023	PPN = ETCO3 + NO2 + SumRCO3	4.45e-4	Falloff, F=0.60, N=1.00			53,7
		0:	1.00e+1	-	-8.90	
		Inf:	8.56e+16	27.82	-0.20	
Q024	PPN + HV = #.6 {ETCO3 + NO2} + #.4 {ETO2 + CO2 + NO3} + #0.4 SumRO2		Phot Set= PPN-11			54,7
Q025	ACO3 + NO2 = APAN		Same k as rxn S005			35
Q026	ACO3 + NO = NO2 + HO2 + CO + CO2 + HCHO		Same k as rxn S006			36
Q027	ACO3 + HO2 = #.44 {OH + HO2 + CO + CO2 + HCHO} + #.56 ROOH + #.15 O3 + #-.56 XC		Same k as rxn S007			37
Q028	ACO3 + NO3 = NO2 + HO2 + CO + CO2 + HCHO + O2		Same k as rxn S008			38
Q029	ACO3 + SumRO2 = SumRO2 + HO2 + CO + CO2 + HCHO		Same k as rxn S009			34,39
Q030	ACO3 + SumRCO3 = SumRCO3 + CO2 + HO2 + CO + HCHO + O2		Same k as rxn S010			42,40
Q031	MACO3 + NO2 = MAPAN		Same k as rxn S005			35
Q032	MACO3 + NO = NO2 + CO2 + HCHO + MECO3 + SumRCO3		Same k as rxn S006			36
Q033	MACO3 + HO2 = #.44 {OH + HCHO + MECO3 + CO2} + #.56 ROOH + #.15 O3 + #0.44 SumRCO3		Same k as rxn S007			37
Q034	MACO3 + NO3 = NO2 + CO2 + HCHO + MECO3 + O2 + SumRCO3		Same k as rxn S008			38
Q035	MACO3 + SumRO2 = SumRO2 + CO2 + HCHO + MECO3 + SumRCO3		Same k as rxn S009			34,39
Q036	MACO3 + SumRCO3 = SumRCO3 + CO2 + HCHO + MECO3 + O2 + SumRCO3		Same k as rxn S010			42,40
Q037	R2CO3 + NO2 = PAN2		Same k as rxn S005			35
Q038	R2CO3 + NO = NO2 + PROP_P1 + CO2 + #-1 XC		Same k as rxn S006			36
Q039	R2CO3 + HO2 = #.44 {OH + PROP_P1 + CO2} + #.41 ROOH + #.15 {O3 + RCOOH} + #-.85 XC		Same k as rxn S007			37
Q040	R2CO3 + NO3 = NO2 + PROP_P1 + CO2 + O2 + #-1 XC		Same k as rxn S008			38
Q041	R2CO3 + SumRO2 = SumRO2 + PROP_P1 + CO2 + #-1 XC		Same k as rxn S009			34,39
Q042	R2CO3 + SumRCO3 = SumRCO3 + ETO2 + CO2 + SumRO2		Same k as rxn S010			42,40
Q043	PAN2 = R2CO3 + NO2 + SumRCO3	4.63e-4	8.56e+16	27.82	-0.20	55,7
Q044	PAN2 + HV = #.6 {R2CO3 + NO2} + #.4 {PROP_P1 + CO2 + NO3} + #-.4 XC + #0.6 SumRCO3		Phot Set= PPN-11			56,7
Q045	R2NCO3 + NO2 = PAN2N		Same k as rxn S005			35
Q046	R2NCO3 + NO = #2 NO2 + HCHO + CO2		Same k as rxn S006			36
Q047	R2NCO3 + HO2 = #.44 {OH + NO2 + HCHO + CO2} + #.41 RCNO3 + #.15 {O3 + RCNO3} + #-.56 XC		Same k as rxn S007			37
Q048	R2NCO3 + NO3 = #2 NO2 + HCHO + CO2 + O2		Same k as rxn S008			38
Q049	R2NCO3 + SumRO2 = SumRO2 + NO2 + HCHO + CO2		Same k as rxn S009			34,39
Q050	R2NCO3 + SumRCO3 = SumRCO3 + CO2 + HCHO + NO2		Same k as rxn S010			42,40
Q051	PAN2N = R2NCO3 + NO2 + SumRCO3		Same k as rxn Q023			55,7

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
Q052	PAN2N + HV = #.6 {R2NCO3 + NO2} + #.4 {NO2 + HCHO + CO2 + NO3} + #0.6 SumRCO3		Phot Set= PPN-11			57,7
Q053	BZCO3 + NO2 = PBZN	1.11e-11				58
Q054	BZCO3 + NO = NO2 + CO2 + BZO2 + SumRO2	1.60e-11				58,7
Q055	BZCO3 + HO2 = #.2 {OH + BZO2 + CO2} + #.8 ROOH + #.15 O3 + #2.4 XC + #0.2 SumRO2		Same k as rxn S007			37
Q056	BZCO3 + NO3 = NO2 + CO2 + BZO2 + O2 + SumRO2		Same k as rxn S008			38
Q057	BZCO3 + SumRO2 = SumRO2 + BZO2 + CO2 + SumRO2		Same k as rxn S009			34,39
Q058	BZCO3 + SumRCO3 = SumRCO3 + CO2 + BZO2 + SumRO2		Same k as rxn S010			42,40
Q059	PBZN = BZCO3 + NO2 + SumRCO3	4.31e-4	2.10e+16	27.03	-	58,7
Q060	PBZN + HV = #.6 {BZCO3 + NO2} + #.4 {CO2 + BZO2 + NO3} + #0.3 SumRO2		Phot Set= PPN-11			59,7
	Reactions of non-acylperoxy radicals that react with NO_2					
R001	TBUO + NO2 = R1NO3 + #-1 XC	2.21e-11	3.50e-12	-1.10	-	60
R002	TBUO = ACET + MEO2 + SumRO2	1.66e+3	1.40e+13	13.62	-	61,7
R003	BZO + NO2 = NPHE	2.08e-12				62
R004	BZO + HO2 = CRES + #-1 XC		Same k as rxn S002			63
R005	BZO = CRES + #-1 XC + HO2	1.00e-3				64
R006	NPRAD + NO2 = NPHE + #6 XC		Same k as rxn S005			65
R007	NPRAD + HO2 = NAPPRD		Same k as rxn S007			65
R008	NPRAD = NAPPRD	1.00e-3				64
R009	xNAMIN + NO2 = NAMIN		Same k as rxn S005			66
R010	xNAMIN + HO2 = AMINS + #2 XC		Same k as rxn S007			66
R011	xNAMIN = AMINS + #2 XC	1.00e-3				64
	Reactions of stabilized Criegee biradicals					
CB01	HCHO2 + SO2 = SULF + HCHO	3.80e-11				1,67
CB02	HCHO2 + NO2 = HCHO + NO3	7.00e-12				68,67
CB03	HCHO2 + H2O = HCOOH	2.40e-15				69,67
CB04	MECHO2 + SO2 = SULF + MECHO		Same k as rxn CB01			67
CB05	MECHO2 + NO2 = MECHO + NO3		Same k as rxn CB02			67
CB06	MECHO2 + H2O = AACID		Same k as rxn CB03			67
CB07	RCHO2 + SO2 = SULF + RCHO + #-1 XC		Same k as rxn CB01			67
CB08	RCHO2 + NO2 = RCHO + NO3 + #-1 XC		Same k as rxn CB02			67
CB09	RCHO2 + H2O = RCOOH		Same k as rxn CB03			67
	Reactions of compounds and lumped model species output by the SAPRC mechanism generation system [d]					
G001	PROP + OH = PROP_P1 + SumRO2	1.13e-12	1.00e-11	1.30	0.00	1
G002	PROP_P1 + NO = #.959 HO2 + #.959 NO2 + #.692 ACET + #.267 ETCHO + #.041 R1NO3 + #-0.082 XC		Same k as rxn S001			
G003	PROP_P1 + NO3 = HO2 + NO2 + #.722 ACET + #.278 ETCHO		Same k as rxn S003			
G004	PROP_P1 + HO2 = ROOH + #-1 XC		Same k as rxn S002			
G005	PROP_P1 + SumRO2 = SumRO2 + #.541 ACET + #.5 HO2 + #.25 OTH3 + #.209 ETCHO + #-0.25 XC		Same k as rxn S004			
G006	PROP_P1 + SumRCO3 = SumRCO3 + #.722 ACET + #.5 HO2 + #.278 ETCHO		Same k as rxn S009			
G007	NC4 + OH = NC4_P1 + SumRO2	2.47e-12	1.40e-11	1.03	0.00	1

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
G008	NC4_P1 + NO = #.932 NO2 + #.61 HO2 + #.491 MEK + #.32 MECHO + #.32 ETO2 + #.118 RCHO + #.09 RO2C + #.068 R1NO3 + #.003 RO2XC + #.003 zRHNO3 + #-0.074 XC + #.413 SumRO2		Same k as rxn S001			
G009	NC4_P1 + NO3 = NO2 + #.654 HO2 + #.527 MEK + #.343 MECHO + #.343 ETO2 + #.127 RCHO + #.097 RO2C + #.003 RO2XC + #.003 zRHNO3 + #-0.006 XC + #.443 SumRO2		Same k as rxn S003			
G010	NC4_P1 + HO2 = ROOH		Same k as rxn S002			
G011	NC4_P1 + SumRO2 = SumRO2 + #.481 MEK + #.327 HO2 + #.25 OTH3 + #.172 MECHO + #.172 ETO2 + #.096 RCHO + #.048 RO2C + #.002 RO2XC + #.002 zRHNO3 + #-0.008 XC + #.222 SumRO2		Same k as rxn S004			
G012	NC4_P1 + SumRCO3 = SumRCO3 + #.698 MEK + #.327 HO2 + #.172 MECHO + #.172 ETO2 + #.129 RCHO + #.048 RO2C + #.002 RO2XC + #.002 zRHNO3 + #-0.008 XC + #.222 SumRO2		Same k as rxn S009			
G192	PROPE + OH = PROPE_P1 + SumRO2	2.60e-11	4.85e-12	-1.00	0.00	1
G193	PROPE + O3 = #.525 CO + #.5 MECHO + #.5 HCHO + #.355 MEO2 + #.35 OH + #.215 CO2 + #.185 HCHO2 + #.165 HO2 + #.075 MECHO2 + #.07 CH4 + #.355 SumRO2	1.05e-17	5.51e-15	3.73	0.00	1
G194	PROPE + NO3 = PROPE_P2 + SumRO2	9.79e-15	4.60e-13	2.30	0.00	1
G195	PROPE + O3P = #.5 OTH1 + #.25 ETCHO + #.25 ACET	4.01e-12	1.02e-11	0.56	0.00	9
G196	PROPE_P1 + NO = HO2 + NO2 + #.99 MECHO + #.99 HCHO + #.008 KET2 + #.003 RCHO + #-0.022 XC		Same k as rxn S001			
G197	PROPE_P1 + NO3 = HO2 + NO2 + #.99 MECHO + #.99 HCHO + #.008 KET2 + #.003 RCHO + #-0.022 XC		Same k as rxn S003			
G198	PROPE_P1 + HO2 = ROOH + #-1 XC		Same k as rxn S002			
G199	PROPE_P1 + SumRO2 = SumRO2 + #.5 HO2 + #.495 MECHO + #.495 HCHO + #.25 OTH4 + #.166 KET2 + #.089 RCHO + #-0.671 XC		Same k as rxn S004			
G200	PROPE_P1 + SumRCO3 = SumRCO3 + #.5 HO2 + #.495 MECHO + #.495 HCHO + #.328 KET2 + #.177 RCHO + #-0.833 XC		Same k as rxn S009			
G201	PROPE_P2 + NO = #1.384 NO2 + #.616 RCNO3 + #.616 HO2 + #.384 MECHO + #.384 HCHO		Same k as rxn S001			
G202	PROPE_P2 + NO3 = #1.384 NO2 + #.616 RCNO3 + #.616 HO2 + #.384 MECHO + #.384 HCHO		Same k as rxn S003			
G203	PROPE_P2 + HO2 = RHNO3 + #-3 XC		Same k as rxn S002			
G204	PROPE_P2 + SumRO2 = SumRO2 + #.558 RCNO3 + #.308 HO2 + #.25 RHNO3 + #.192 MECHO + #.192 HCHO + #.192 NO2 + #-0.75 XC		Same k as rxn S004			
G205	PROPE_P2 + SumRCO3 = SumRCO3 + #.808 RCNO3 + #.308 HO2 + #.192 MECHO + #.192 HCHO + #.192 NO2		Same k as rxn S009			
G206	BUT13 + OH = #.533 BUT13_P1 + #.467 BUT13_A1 + #.533 SumRO2	6.59e-11	1.48e-11	-0.89	0.00	1

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
G207	BUT13 + O3 = #.5 ACRO + #.5 RCHO + #.5 HCHO + #.255 CO + #.185 HCHO2 + #.08 HO2 + #.08 OH + #.06 CO2 + #-0.5 XC	6.64e-18	1.34e-14	4.54	0.00	1
G208	BUT13 + NO3 = #.5 BUT13_P2 + #.5 BUT13_A2 + #.5 SumRO2	1.10e-13				1
G209	BUT13 + O3P = #.5 OLEP + #.25 OLEA2 + #.25 MVK + #-0.75 XC	1.98e-11	2.26e-11	0.08	0.00	9
G210	BUT13_P1 + NO = #.99 HO2 + #.99 NO2 + #.869 ACRO + #.869 HCHO + #.121 OLEP + #.01 RHNO3 + #-0.141 XC		Same k as rxn S001			
G211	BUT13_P1 + NO3 = HO2 + NO2 + #.878 ACRO + #.878 HCHO + #.122 OLEP + #-0.122 XC		Same k as rxn S003			
G212	BUT13_P1 + HO2 = RUOOH + #-1 XC		Same k as rxn S002			
G213	BUT13_P1 + SumRO2 = SumRO2 + #.5 HO2 + #.439 ACRO + #.439 HCHO + #.311 OLEP + #.219 LVKS + #.031 OLEA2 + #-0.342 XC		Same k as rxn S004			
G214	BUT13_P1 + SumRCO3 = SumRCO3 + #.5 HO2 + #.439 LVKS + #.439 ACRO + #.439 HCHO + #.061 OLEA2 + #.061 OLEP + #-0.122 XC		Same k as rxn S009			
G215	BUT13_A1 = #.5 HPALD + #.5 HO2 + #.5 BUT13_P3 + #-0.5 XC + #.5 SumRO2	1.72e+0	4.93e+10	14.36	0.00	
G216	BUT13_A1 + NO = #.99 NO2 + #.495 OLEA1 + #.495 HO2 + #.495 BUT13_P4 + #.01 RHNO3 + #-0.515 XC + #.495 SumRO2		Same k as rxn S001			
G217	BUT13_P2 + NO = #1.716 NO2 + #.747 ACRO + #.747 HCHO + #.223 RCNO3 + #.223 HO2 + #.031 RDNO3 + #.157 XC + #-0.001 XN		Same k as rxn S001			
G218	BUT13_P2 + NO3 = #1.77 NO2 + #.77 ACRO + #.77 HCHO + #.23 RCNO3 + #.23 HO2 + #.23 XC		Same k as rxn S003			
G219	BUT13_P2 + HO2 = RHNO3 + #-2 XC		Same k as rxn S002			
G220	BUT13_P2 + SumRO2 = SumRO2 + #.385 ACRO + #.385 HCHO + #.385 NO2 + #.365 RCNO3 + #.25 RHNO3 + #.115 HO2 + #-0.135 XC		Same k as rxn S004			
G221	BUT13_P2 + SumRCO3 = SumRCO3 + #.615 RCNO3 + #.385 ACRO + #.385 HCHO + #.385 NO2 + #.115 HO2 + #.615 XC		Same k as rxn S009			
G222	BUT13_A2 = HPALD + NO2 + #-1 XC	1.72e+0	4.93e+10	14.36	0.00	
G223	BUT13_A2 + NO = #1.441 NO2 + #.497 RCNO3 + #.497 HO2 + #.472 OLEA1 + #.031 RDNO3 + #-0.037 XC		Same k as rxn S001			
G224	BUT13_P3 + NO = #.99 BUT13_P5 + #.99 NO2 + #.01 RHNO3 + #-0.02 XC + #.99 SumRO2		Same k as rxn S001			
G225	BUT13_P3 + NO3 = BUT13_P5 + NO2 + SumRO2		Same k as rxn S003			
G226	BUT13_P3 + HO2 = RUOOH + #-1 XC		Same k as rxn S002			
G227	BUT13_P3 + SumRO2 = SumRO2 + #.5 BUT13_P5 + #.25 HPALD + #.25 RUOOH + #-0.5 XC + #.5 SumRO2		Same k as rxn S004			
G228	BUT13_P3 + SumRCO3 = SumRCO3 + #.5 HPALD + #.5 BUT13_P5 + #-0.5 XC + #.5 SumRO2		Same k as rxn S009			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
G229	BUT13_P4 + NO = #.99 HO2 + #.99 NO2 + #.982 OLEA1 + #.982 HCHO + #.01 RHNO3 + #.008 LVKS + #-1.984 XC		Same k as rxn S001			
G230	BUT13_P4 + NO3 = HO2 + NO2 + #.992 OLEA1 + #.992 HCHO + #.008 LVKS + #-1.984 XC		Same k as rxn S003			
G231	BUT13_P4 + HO2 = RUOOH + #-1 XC		Same k as rxn S002			
G232	BUT13_P4 + SumRO2 = SumRO2 + #.5 HO2 + #.496 OLEA1 + #.496 HCHO + #.254 LVKS + #.25 OLEP + #-1.242 XC		Same k as rxn S004			
G233	BUT13_P4 + SumRCO3 = SumRCO3 + #.504 LVKS + #.5 HO2 + #.496 OLEA1 + #.496 HCHO + #-0.992 XC		Same k as rxn S009			
G234	BUT13_P5 + NO = #.99 OLEP + #.99 HO2 + #.99 NO2 + #.01 RHNO3 + #-1.01 XC		Same k as rxn S001			
G235	BUT13_P5 + NO3 = OLEP + HO2 + NO2 + #-1 XC		Same k as rxn S003			
G236	BUT13_P5 + HO2 = RUOOH + #-1 XC		Same k as rxn S002			
G237	BUT13_P5 + SumRO2 = SumRO2 + #.75 OLEP + #.5 HO2 + #.25 OLEA2 + #-1 XC		Same k as rxn S004			
G238	BUT13_P5 + SumRCO3 = SumRCO3 + #.5 OLEA2 + #.5 OLEP + #.5 HO2 + #-1 XC		Same k as rxn S009			
G281	ISOP + OH = #.618 ISOP_P1 + #.209 ISOP_A2 + #.145 ISOP_A1 + #.026 RO2C + #.02 OLEA2 + #.02 OH + #.007 HO2 + #.006 OLEP + #.002 RO2XC + #.002 zRHNO3 + #-0.002 XC + #.646 SumRO2	9.96e-11	2.54e-11	-0.81	0.00	1
G282	ISOP + O3 = #.4 HCHO + #.39 MACR + #.281 CO + #.204 HCHO2 + #.2 KET2 + #.2 RCHO + #.16 MVK + #.088 HO2 + #.088 OH + #.066 CO2 + #.05 OLEP + #-0.201 XC	1.40e-17	1.09e-14	3.97	0.00	1
G283	ISOP + NO3 = #.5 ISOP_P2 + #.5 ISOP_A3 + #.5 SumRO2	6.69e-13	3.00e-12	0.89	0.00	1
G284	ISOP + O3P = #.75 OLEP + #.25 ISOP_P3 + #.25 MEO2 + #.5 SumRO2	3.50e-11				9
G285	ISOP_A1 = #.887 HO2 + #.823 RO2C + #.5 HPALD + #.387 OLEP + #.093 RO2XC + #.064 zRHNO3 + #.049 LVKS + #.049 HCHO + #.049 OH + #-0.064 XC + #.916 SumRO2	1.72e+0	4.93e+10	14.36	0.00	
G286	ISOP_A1 + NO = #.93 NO2 + #.897 HO2 + #.465 OLEA1 + #.432 RO2C + #.432 LVKS + #.432 HCHO + #.07 RHNO3 + #.033 RO2XC + #.033 zRHNO3 + #-0.103 XC + #.465 SumRO2		Same k as rxn S001			
G287	ISOP_P1 + NO = #.93 HO2 + #.93 NO2 + #.884 HCHO + #.524 MVK + #.359 MACR + #.07 RHNO3 + #.042 OLEP + #.004 LVKS + #-0.062 XC		Same k as rxn S001			
G288	ISOP_P1 + NO3 = HO2 + NO2 + #.95 HCHO + #.564 MVK + #.386 MACR + #.045 OLEP + #.004 LVKS + #.009 XC		Same k as rxn S003			
G289	ISOP_P1 + HO2 = RUOOH		Same k as rxn S002			
G290	ISOP_P1 + SumRO2 = SumRO2 + #.5 HO2 + #.475 HCHO + #.414 OLEP + #.282 MVK + #.193 MACR + #.1 LVKS + #.011 OLEA2 + #.1 XC		Same k as rxn S004			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
G291	ISOP_P1 + SumRCO3 = SumRCO3 + #.782 HO2 + #.757 HCHO + #.564 MVK + #.198 LVKS + #.193 MACR + #.023 OLEA2 + #.023 OLEP + #.193 XC		Same k as rxn S009			
G292	ISOP_A2 = #.5 ISOP_P4 + #.495 HPALD + #.413 HO2 + #.087 OH + #.005 RO2C + #.005 OLEA1 + #.505 SumRO2	2.08e+0				
G293	ISOP_A2 + NO = #.93 NO2 + #.897 HO2 + #.882 OLEA1 + #.427 RO2C + #.422 HCHO + #.07 RHNO3 + #.033 RO2XC + #.033 zRHNO3 + #.011 HPALD + #.005 LVKS + #-0.525 XC + #.46 SumRO2		Same k as rxn S001			
G294	ISOP_P2 + NO = #1.892 NO2 + #.946 MVK + #.946 HCHO + #.054 RDNO3 + #-0.054 XC		Same k as rxn S001			
G295	ISOP_P2 + NO3 = #2 NO2 + MVK + HCHO		Same k as rxn S003			
G296	ISOP_P2 + HO2 = RHNO3 + #-1 XC		Same k as rxn S002			
G297	ISOP_P2 + SumRO2 = SumRO2 + #.5 RHNO3 + #.5 MVK + #.5 HCHO + #.5 NO2 + #-0.5 XC		Same k as rxn S004			
G298	ISOP_P2 + SumRCO3 = SumRCO3 + MVK + HCHO + NO2		Same k as rxn S009			
G299	ISOP_A3 = #.903 NO2 + #.903 HPALD + #.092 RO2C + #.087 RHNO3 + #.087 OH + #.005 RO2XC + #.005 zRDNO3 + #.005 HO2 + #.005 R2NO3 + #-0.107 XC + #.097 SumRO2	2.08e+0				
G300	ISOP_A3 + NO = #1.119 NO2 + #.296 ISOP_A4 + #.296 ISOP_P5 + #.181 RCNO3 + #.181 HO2 + #.172 OLEA1 + #.054 RDNO3 + #.313 XC + #.296 SumRO2		Same k as rxn S001			
G301	ISOP_P3 + NO = #.932 ACO3 + #.932 HCHO + #.932 NO2 + #.068 RCNO3 + #.068 XC + #.932 SumRCO3		Same k as rxn S001			
G302	ISOP_P3 + NO3 = ACO3 + HCHO + NO2 + SumRCO3		Same k as rxn S003			
G303	ISOP_P3 + HO2 = HPALD + #-1 XC		Same k as rxn S002			
G304	ISOP_P3 + SumRO2 = SumRO2 + #.5 ACO3 + #.5 HCHO + #.25 MGLY + #.25 LVKS + #.25 XC + #.5 SumRCO3		Same k as rxn S004			
G305	ISOP_P3 + SumRCO3 = SumRCO3 + #.5 MGLY + #.5 ACO3 + #.5 HCHO + #.5 XC + #.5 SumRCO3		Same k as rxn S009			
G306	ISOP_P4 + NO = #.933 NO2 + #.555 HO2 + #.522 RO2C + #.379 HPALD + #.338 OLEA2 + #.338 OH + #.177 OLEP + #.067 RHNO3 + #.039 RO2XC + #.026 zRNNO3 + #.013 zRHNO3 + #-0.21 XC + #.561 SumRO2		Same k as rxn S001			
G307	ISOP_P4 + NO3 = NO2 + #.595 HO2 + #.56 RO2C + #.406 HPALD + #.363 OLEA2 + #.363 OH + #.19 OLEP + #.042 RO2XC + #.028 zRNNO3 + #.014 zRHNO3 + #-0.159 XC + #.602 SumRO2		Same k as rxn S003			
G308	ISOP_P4 + HO2 = RUOOH		Same k as rxn S002			
G309	ISOP_P4 + SumRO2 = SumRO2 + #.453 HPALD + #.298 HO2 + #.28 RO2C + #.25 RUOOH + #.181 OLEA2 + #.181 OH + #.095 OLEP + #.021 RO2XC + #.014 zRNNO3 + #.007 zRHNO3 + #-0.077 XC + #.301 SumRO2		Same k as rxn S004			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
G310	ISOP_P4 + SumRCO3 = SumRCO3 + #.703 HPALD + #.298 HO2 + #.28 RO2C + #.181 OLEA2 + #.181 OH + #.095 OLEP + #.021 RO2XC + #.014 zRNNO3 + #.007 zRHNO3 + #-0.077 XC + #.301 SumRO2		Same k as rxn S009			
G311	ISOP_A4 = #.901 RHNO3 + #.901 HO2 + #.851 RO2C + #.072 RO2XC + #.05 HCHO + #.051 NO2 + #.027 zRNNO3 + #.025 RCNO3 + #.025 OH + #.025 HPALD + #.023 zRDNO3 + #-1.064 XC + #.923 SumRO2	1.72e+0	4.93e+10	14.36	0.00	
G312	ISOP_A4 + NO = #.974 NO2 + #.918 HO2 + #.473 RHNO3 + #.448 RO2C + #.448 HCHO + #.445 RCNO3 + #.054 RDNO3 + #.025 RO2XC + #.025 zRNNO3 + #.003 LVKS + #-0.207 XC + #.473 SumRO2		Same k as rxn S001			
G313	ISOP_P5 + NO = #.946 RCNO3 + #.946 HO2 + #.946 NO2 + #.936 HCHO + #.054 RDNO3 + #.902 XC		Same k as rxn S001			
G314	ISOP_P5 + NO3 = RCNO3 + HO2 + NO2 + #.989 HCHO + #1.011 XC		Same k as rxn S003			
G315	ISOP_P5 + HO2 = RHNO3 + #-1 XC		Same k as rxn S002			
G316	ISOP_P5 + SumRO2 = SumRO2 + #.75 RCNO3 + #.5 HO2 + #.494 HCHO + #.25 RHNO3 + #.756 XC		Same k as rxn S004			
G317	ISOP_P5 + SumRCO3 = SumRCO3 + RCNO3 + #.5 HO2 + #.494 HCHO + #1.506 XC		Same k as rxn S009			
G441	APINE + OH = APINE_P1 + SumRO2	5.32e-11	1.21e-11	-0.88	0.00	1
G442	APINE + O3 = #.731 OH + #.67 APINE_P2 + #.255 RCHO2 + #.05 RO2C + #.047 R2CO3 + #.047 HCHO + #.029 CO + #.017 zRCNO3 + #.017 RO2XC + #.017 CO2 + #.009 HO2 + #.008 OTH3 + #.003 BACL + #2.206 XC + #.737 SumRO2 + #.047 SumRCO3	8.80e-17	1.01e-15	1.45	0.00	1
G443	APINE + NO3 = APINE_P3 + SumRO2	6.15e-12	1.20e-12	-0.97	0.00	1
G444	APINE + O3P = #.5 OTH3 + #.5 OTH4 + #6 XC	3.20e-11				9
G445	APINE_P1 + NO = #.85 RCHO + #.85 HO2 + #.85 NO2 + #.15 RHNO3 + #5.7 XC		Same k as rxn S001			
G446	APINE_P1 + NO3 = RCHO + HO2 + NO2 + #6 XC		Same k as rxn S003			
G447	APINE_P1 + HO2 = ROOH + #6 XC		Same k as rxn S002			
G448	APINE_P1 + SumRO2 = SumRO2 + #.5 RCHO + #.5 HO2 + #.5 OTH4 + #6 XC		Same k as rxn S004			
G449	APINE_P1 + SumRCO3 = SumRCO3 + #.875 RCHO + #.875 HO2 + #.125 OTH4 + #6 XC		Same k as rxn S009			
G450	APINE_P2 + NO = #.747 NO2 + #.717 OH + #.701 BACL + #.253 RCNO3 + #.026 RCHO + #.022 HO2 + #.021 HCHO + #.016 RO2C + #.016 OTH1 + #.005 RO2XC + #.005 zRCNO3 + #.004 MECO3 + #6.241 XC + #.021 SumRO2 + #.004 SumRCO3		Same k as rxn S001			
G451	APINE_P2 + NO3 = NO2 + #.96 OH + #.938 BACL + #.034 RCHO + #.029 HO2 + #.027 HCHO + #.021 RO2C + #.021 OTH1 + #.006 RO2XC + #.006 zRCNO3 + #.006 MECO3 + #5.992 XC + #.027 SumRO2 + #.006 SumRCO3		Same k as rxn S003			
G452	APINE_P2 + HO2 = CROOH + #5 XC		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
G453	APINE_P2 + SumRO2 = SumRO2 + #.503 RCHO + #.48 OH + #.469 BACL + #.014 HO2 + #.014 OTH3 + #.014 HCHO + #.011 RO2C + #.011 OTH1 + #.003 RO2XC + #.003 zRCNO3 + #.003 MECO3 + #5.994 XC + #.014 SumRO2 + #.003 SumRCO3		Same k as rxn S004			
G454	APINE_P2 + SumRCO3 = SumRCO3 + #.949 OH + #.938 BACL + #.048 RCHO + #.014 HO2 + #.014 HCHO + #.011 RO2C + #.011 OTH1 + #.006 MECO3 + #.003 RO2XC + #.003 zRCNO3 + #5.988 XC + #.014 SumRO2 + #.006 SumRCO3		Same k as rxn S009			
G455	APINE_P3 + NO = #1.482 NO2 + #.714 RCHO + #.231 RDNO3 + #.043 RO2C + #.043 RCNO3 + #.043 OH + #.013 RO2XC + #.013 zRDNO3 + #5.551 XC + #.056 SumRO2		Same k as rxn S001			
G456	APINE_P3 + NO3 = #1.927 NO2 + #.928 RCHO + #.056 RO2C + #.056 RCNO3 + #.056 OH + #.017 RO2XC + #.017 zRDNO3 + #6.018 XC + #.073 SumRO2		Same k as rxn S003			
G457	APINE_P3 + HO2 = RHNO3 + #4 XC		Same k as rxn S002			
G458	APINE_P3 + SumRO2 = SumRO2 + #.5 RHNO3 + #.464 RCHO + #.464 NO2 + #.028 RO2C + #.028 RCNO3 + #.028 OH + #.008 RO2XC + #.008 zRDNO3 + #5.012 XC + #.036 SumRO2		Same k as rxn S004			
G459	APINE_P3 + SumRCO3 = SumRCO3 + #.928 RCHO + #.927 NO2 + #.056 RO2C + #.056 RCNO3 + #.056 OH + #.017 RO2XC + #.017 zRDNO3 + #6.018 XC + #.073 SumRO2		Same k as rxn S009			
G460	BPINE + OH = BPINE_P1 + SumRO2	7.82e-11	2.38e-11	-0.71	0.00	1
G461	BPINE + O3 = #.82 OTH3 + #.418 CO + #.311 OH + #.303 HCHO2 + #.18 BPINE_P2 + #.18 HCHO + #.131 HO2 + #.098 CO2 + #4.101 XC + #.18 SumRO2	1.50e-17				1
G462	BPINE + NO3 = BPINE_P3 + SumRO2	2.60e-12				1
G463	BPINE + O3P = #.5 OTH3 + #.5 RCHO + #6 XC	2.70e-11				9
G464	BPINE_P1 + NO = #.85 OTH3 + #.85 HCHO + #.85 HO2 + #.85 NO2 + #.15 RHNO3 + #4.85 XC		Same k as rxn S001			
G465	BPINE_P1 + NO3 = OTH3 + HCHO + HO2 + NO2 + #5 XC		Same k as rxn S003			
G466	BPINE_P1 + HO2 = ROOH + #6 XC		Same k as rxn S002			
G467	BPINE_P1 + SumRO2 = SumRO2 + #.5 OTH4 + #.5 OTH3 + #.5 HCHO + #.5 HO2 + #5.5 XC		Same k as rxn S004			
G468	BPINE_P1 + SumRCO3 = SumRCO3 + OTH3 + HCHO + HO2 + #5 XC		Same k as rxn S009			
G469	BPINE_P2 + NO = #.76 NO2 + #.459 RO2C + #.405 R2CO3 + #.262 ACET + #.24 RCNO3 + #.231 BACL + #.226 OH + #.162 RO2XC + #.123 zRCNO3 + #.006 HO2 + #.004 HCHO + #4.982 XC + #.621 SumRO2 + #.405 SumRCO3		Same k as rxn S001			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
G470	BPINE_P2 + NO3 = NO2 + #.604 RO2C + #.533 R2CO3 + #.344 ACET + #.304 BACL + #.297 OH + #.213 RO2XC + #.162 zRCNO3 + #.008 HO2 + #.005 HCHO + #4.662 XC + #.817 SumRO2 + #.533 SumRCO3		Same k as rxn S003			
G471	BPINE_P2 + HO2 = CROOH + #4 XC		Same k as rxn S002			
G472	BPINE_P2 + SumRO2 = SumRO2 + #.302 RO2C + #.272 BACL + #.267 R2CO3 + #.261 OTH3 + #.172 ACET + #.148 OH + #.119 OTH4 + #.106 RO2XC + #.081 zRCNO3 + #.004 HO2 + #.003 HCHO + #4.829 XC + #.408 SumRO2 + #.267 SumRCO3		Same k as rxn S004			
G473	BPINE_P2 + SumRCO3 = SumRCO3 + #.604 RO2C + #.543 BACL + #.344 ACET + #.297 OH + #.294 R2CO3 + #.213 RO2XC + #.162 zRCNO3 + #.008 HO2 + #.005 HCHO + #4.423 XC + #.817 SumRO2 + #.294 SumRCO3		Same k as rxn S009			
G474	BPINE_P3 + NO = #.769 BPINE_P4 + #.769 NO2 + #.231 RDNO3 + #.924 XC + #.769 SumRO2		Same k as rxn S001			
G475	BPINE_P3 + NO3 = BPINE_P4 + NO2 + SumRO2		Same k as rxn S003			
G476	BPINE_P3 + HO2 = RHNO3 + #4 XC		Same k as rxn S002			
G477	BPINE_P3 + SumRO2 = SumRO2 + #.5 RHNO3 + #.5 BPINE_P4 + #2 XC + #.5 SumRO2		Same k as rxn S004			
G478	BPINE_P3 + SumRCO3 = SumRCO3 + BPINE_P4 + SumRO2		Same k as rxn S009			
G479	BPINE_P4 + NO = #.769 RCNO3 + #.769 OH + #.769 NO2 + #.231 RDNO3 + #6.307 XC		Same k as rxn S001			
G480	BPINE_P4 + NO3 = RCNO3 + OH + NO2 + #7 XC		Same k as rxn S003			
G481	BPINE_P4 + HO2 = RCNO3 + #7 XC		Same k as rxn S002			
G482	BPINE_P4 + SumRO2 = SumRO2 + RCNO3 + #.5 OH + #7 XC		Same k as rxn S004			
G483	BPINE_P4 + SumRCO3 = SumRCO3 + RCNO3 + #.5 OH + #7 XC		Same k as rxn S009			
G484	DLIMO + OH = #.6 DLIMO_P1 + #.4 DLIMO_A1 + #.6 SumRO2	1.63e-10	4.28e-11	-0.80	0.00	74
G485	DLIMO + O3 = #1.452 OH + #.708 OLEP + #.255 RCHO2 + #.033 RO2C + #.028 CO + #.017 CO2 + #.014 OLEA2 + #.014 HO2 + #.01 RO2XC + #.009 zRCNO3 + #.007 HCHO + #.006 CROOH + #.003 OTHN + #.002 LVKS + #.002 HPALD + #5.462 XC + #.043 SumRO2	2.17e-16	2.95e-15	1.56	0.00	74
G486	DLIMO + NO3 = #.96 DLIMO_P2 + #.031 RO2C + #.031 OH + #.016 RCNO3 + #.015 RNNO3 + #.009 RO2XC + #.009 zRNNO3 + #.112 XC + #.009 XN + SumRO2	1.22e-11				74
G487	DLIMO + O3P = OLEP + #5 XC	7.20e-11				9
G488	DLIMO_A1 = DLIMO_P3 + SumRO2	1.77e+1	9.50e+10	13.36	0.00	
G489	DLIMO_A1 + NO = #.769 NO2 + #.558 DLIMO_P4 + #.558 KET2 + #.231 RHNO3 + #.211 OLEP + #.211 HCHO + #.211 HO2 + #.652 XC + #.558 SumRO2		Same k as rxn S001			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
G490	DLIMO_P1 + NO = #.769 OLEA2 + #.769 HO2 + #.769 NO2 + #.231 RHNO3 + #4.769 XC		Same k as rxn S001			
G491	DLIMO_P1 + NO3 = OLEA2 + HO2 + NO2 + #5 XC		Same k as rxn S003			
G492	DLIMO_P1 + HO2 = RUOOH + #5 XC		Same k as rxn S002			
G493	DLIMO_P1 + SumRO2 = SumRO2 + #.5 OLEP + #.5 OLEA2 + #.5 HO2 + #5 XC		Same k as rxn S004			
G494	DLIMO_P1 + SumRCO3 = SumRCO3 + #.875 OLEA2 + #.875 HO2 + #.125 OLEP + #5 XC		Same k as rxn S009			
G495	DLIMO_P2 + NO = #1.538 NO2 + #.769 OLEA2 + #.231 RDNO3 + #4.769 XC		Same k as rxn S001			
G496	DLIMO_P2 + NO3 = #2 NO2 + OLEA2 + #5 XC		Same k as rxn S003			
G497	DLIMO_P2 + HO2 = RHNO3 + #4 XC		Same k as rxn S002			
G498	DLIMO_P2 + SumRO2 = SumRO2 + #.5 RHNO3 + #.5 OLEA2 + #.5 NO2 + #4.5 XC		Same k as rxn S004			
G499	DLIMO_P2 + SumRCO3 = SumRCO3 + OLEA2 + NO2 + #5 XC		Same k as rxn S009			
G500	DLIMO_P3 + NO = #.769 NO2 + #.767 OH + #.385 LVKS + #.383 OTHN + #.231 RNNO3 + #.002 HPALD + #.002 HO2 + #1.544 XC		Same k as rxn S001			
G501	DLIMO_P3 + NO3 = NO2 + #.997 OH + #.5 LVKS + #.497 OTHN + #.003 HPALD + #.003 HO2 + #2.021 XC		Same k as rxn S003			
G502	DLIMO_P3 + HO2 = OTHN + #-2 XC		Same k as rxn S002			
G503	DLIMO_P3 + SumRO2 = SumRO2 + #.499 OH + #.374 OTHN + #.25 RUOOH + #.25 LVKS + #.126 HPALD + #.001 HO2 + #2.632 XC		Same k as rxn S004			
G504	DLIMO_P3 + SumRCO3 = SumRCO3 + #.749 OH + #.5 LVKS + #.251 HPALD + #.249 OTHN + #.001 HO2 + #3.757 XC		Same k as rxn S009			
G505	DLIMO_P4 + NO = #.815 OLEP + #.815 OH + #.815 NO2 + #.185 R2NO3 + #1.445 XC		Same k as rxn S001			
G506	DLIMO_P4 + NO3 = OLEP + OH + NO2 + #2 XC		Same k as rxn S003			
G507	DLIMO_P4 + HO2 = RUOOH + #2 XC		Same k as rxn S002			
G508	DLIMO_P4 + SumRO2 = SumRO2 + OLEP + #.5 OH + #2 XC		Same k as rxn S004			
G509	DLIMO_P4 + SumRCO3 = SumRCO3 + OLEP + #.5 OH + #2 XC		Same k as rxn S009			
G977	BENZ + OH = #.57 PHEN + #.57 HO2 + #.268 BENZ_P1 + #.162 AFG4 + #.162 OH + #-0.162 XC + #.268 SumRO2	1.22e-12	2.33e-12	0.38	0.00	1
G978	BENZ_P1 + NO = #.916 BUDAL + #.916 GLY + #.916 HO2 + #.916 NO2 + #.084 RPNO3 + #-0.168 XC		Same k as rxn S001			
G979	BENZ_P1 + NO3 = BUDAL + GLY + HO2 + NO2		Same k as rxn S003			
G980	BENZ_P1 + HO2 = RAOOH + #-1 XC		Same k as rxn S002			
G981	BENZ_P1 + SumRO2 = SumRO2 + #.5 BUDAL + #.5 GLY + #.5 HO2 + #.5 OLEP + #.5 XC		Same k as rxn S004			
G982	BENZ_P1 + SumRCO3 = SumRCO3 + #.5 OLEP + #.5 BUDAL + #.5 GLY + #.5 HO2 + #.5 XC		Same k as rxn S009			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
G983	TOLU + OH = #.653 TOLU_P1 + #.198 CRES + #.198 HO2 + #.15 AFG4 + #.15 OH + #-0.007 XC + #.653 SumRO2	5.58e-12	1.81e-12	-0.67	0.00	1
G984	TOLU_P1 + NO = #.871 HO2 + #.871 NO2 + #.405 GLY + #.382 AFG2A + #.371 MGLY + #.371 BUDAL + #.107 RPNO3 + #.095 BALD + #.023 AFG1 + #.022 RANO3 + #-0.129 XC		Same k as rxn S001			
G985	TOLU_P1 + NO3 = HO2 + NO2 + #.461 GLY + #.435 AFG2A + #.422 MGLY + #.422 BUDAL + #.117 BALD + #.026 AFG1		Same k as rxn S003			
G986	TOLU_P1 + HO2 = #.883 RAOOH + #.117 ROOH + #.351 XC		Same k as rxn S002			
G987	TOLU_P1 + SumRO2 = SumRO2 + #.5 HO2 + #.442 OLEP + #.231 GLY + #.217 AFG2A + #.211 MGLY + #.211 BUDAL + #.088 BALD + #.029 ARO2 + #.013 AFG1 + #.824 XC		Same k as rxn S004			
G988	TOLU_P1 + SumRCO3 = SumRCO3 + #.507 HO2 + #.435 OLEP + #.237 GLY + #.224 AFG2A + #.211 MGLY + #.211 BUDAL + #.117 BALD + #.013 AFG1 + #.87 XC		Same k as rxn S009			
H043	C2BEN + OH = #.833 C2BEN_P1 + #.086 XYNL + #.086 HO2 + #.081 AFG4 + #.081 OH + #.081 XC + #.833 SumRO2	7.00e-12				1
H044	C2BEN_P1 + NO = #.803 HO2 + #.803 NO2 + #.469 ARO1 + #.167 AFG2A + #.167 GLY + #.167 MGLY + #.167 BUDAL + #.131 RANO3 + #.066 RPNO3 + #-0.135 XC		Same k as rxn S001			
H045	C2BEN_P1 + NO3 = HO2 + NO2 + #.601 ARO1 + #.2 AFG2A + #.2 GLY + #.2 MGLY + #.2 BUDAL + #-0.209 XC		Same k as rxn S003			
H046	C2BEN_P1 + HO2 = #.601 ROOH + #.399 RAOOH + #2.803 XC		Same k as rxn S002			
H047	C2BEN_P1 + SumRO2 = SumRO2 + #.601 ARO1 + #.5 HO2 + #.2 OLEP + #.1 AFG2A + #.1 GLY + #.1 MGLY + #.1 BUDAL + #.191 XC		Same k as rxn S004			
H048	C2BEN_P1 + SumRCO3 = SumRCO3 + #.601 ARO1 + #.5 HO2 + #.2 OLEP + #.1 AFG2A + #.1 GLY + #.1 MGLY + #.1 BUDAL + #.191 XC		Same k as rxn S009			
G989	MXYL + OH = #.764 MXYL_P1 + #.156 AFG4 + #.156 OH + #.08 XYNL + #.08 HO2 + #.156 XC + #.764 SumRO2	2.31e-11				1
G990	MXYL_P1 + NO = #.833 HO2 + #.833 NO2 + #.719 MGLY + #.719 AFG2A + #.156 RPNO3 + #.075 GLY + #.075 AFG1 + #.039 BALD + #.011 RANO3 + #.114 XC		Same k as rxn S001			
G991	MXYL_P1 + NO3 = HO2 + NO2 + #.861 MGLY + #.861 AFG2A + #.09 GLY + #.09 AFG1 + #.05 BALD + #.132 XC		Same k as rxn S003			
G992	MXYL_P1 + HO2 = #.95 RAOOH + #.05 ROOH + #1.15 XC		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
G993	MXYL_P1 + SumRO2 = SumRO2 + #.5 HO2 + #.475 OLEP + #.43 MGLY + #.43 AFG2A + #.045 GLY + #.045 AFG1 + #.037 BALD + #.012 ARO2 + #1.503 XC		Same k as rxn S004			
G994	MXYL_P1 + SumRCO3 = SumRCO3 + #.5 HO2 + #.475 OLEP + #.43 MGLY + #.43 AFG2A + #.05 BALD + #.045 GLY + #.045 AFG1 + #1.52 XC		Same k as rxn S009			
G995	OXYL + OH = #.851 OXYL_P1 + #.084 XYNL + #.084 HO2 + #.065 AFG4 + #.065 OH + #.065 XC + #.851 SumRO2	1.36e-11				1
G996	OXYL_P1 + NO = #.831 HO2 + #.831 NO2 + #.385 AFG2A + #.385 MGLY + #.267 BACL + #.267 BUDAL + #.152 RPNO3 + #.118 AFG2B + #.118 GLY + #.061 BALD + #.017 RANO3 + #.061 XC		Same k as rxn S001			
G997	OXYL_P1 + NO3 = HO2 + NO2 + #.461 AFG2A + #.461 MGLY + #.319 BACL + #.319 BUDAL + #.142 AFG2B + #.142 GLY + #.079 BALD + #.071 XC		Same k as rxn S003			
G998	OXYL_P1 + HO2 = #.921 RAOOH + #.079 ROOH + #1.237 XC		Same k as rxn S002			
G999	OXYL_P1 + SumRO2 = SumRO2 + #.5 HO2 + #.461 OLEP + #.23 AFG2A + #.23 MGLY + #.16 BACL + #.16 BUDAL + #.071 AFG2B + #.071 GLY + #.059 BALD + #.02 ARO2 + #1.414 XC		Same k as rxn S004			
H000	OXYL_P1 + SumRCO3 = SumRCO3 + #.571 HO2 + #.39 OLEP + #.301 AFG2A + #.301 MGLY + #.16 BACL + #.16 BUDAL + #.079 BALD + #.071 AFG2B + #.071 GLY + #1.241 XC		Same k as rxn S009			
H001	PXYL + OH = #.693 PXYL_P1 + #.158 XYNL + #.158 HO2 + #.148 AFG4 + #.148 OH + #.156 XC + #.693 SumRO2	1.43e-11				1
H002	PXYL_P1 + NO = #.829 HO2 + #.829 NO2 + #.367 MGLY + #.367 AFG1 + #.367 AFG3 + #.367 GLY + #.145 RPNO3 + #.095 BALD + #.027 RANO3 + #.087 XC + #-0.001 XN		Same k as rxn S001			
H003	PXYL_P1 + NO3 = HO2 + NO2 + #.439 MGLY + #.439 AFG1 + #.439 AFG3 + #.439 GLY + #.122 BALD + #.122 XC		Same k as rxn S003			
H004	PXYL_P1 + HO2 = #.878 RAOOH + #.122 ROOH + #1.366 XC		Same k as rxn S002			
H005	PXYL_P1 + SumRO2 = SumRO2 + #.5 HO2 + #.439 OLEP + #.22 MGLY + #.22 AFG1 + #.22 AFG3 + #.22 GLY + #.091 BALD + #.03 ARO2 + #1.378 XC		Same k as rxn S004			
H006	PXYL_P1 + SumRCO3 = SumRCO3 + #.72 HO2 + #.439 AFG3 + #.439 GLY + #.22 OLEP + #.22 MGLY + #.22 AFG1 + #.122 BALD + #.774 XC		Same k as rxn S009			
H007	BZ123 + OH = #.944 BZ123_P1 + #.03 XYNL + #.03 HO2 + #.025 AFG4 + #.025 OH + #.089 XC + #.944 SumRO2	3.27e-11				1

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H008	BZ123_P1 + NO = #.795 HO2 + #.795 NO2 + #.584 BACL + #.584 AFG2A + #.195 RPNO3 + #.178 AFG2B + #.136 MGLY + #.042 GLY + #.033 BALD + #.01 RANO3 + #.313 XC		Same k as rxn S001			
H009	BZ123_P1 + NO3 = HO2 + NO2 + #.733 BACL + #.733 AFG2A + #.223 AFG2B + #.171 MGLY + #.052 GLY + #.044 BALD + #.14 XC		Same k as rxn S003			
H010	BZ123_P1 + HO2 = #.956 RAOOH + #.044 ROOH + #2.132 XC		Same k as rxn S002			
H011	BZ123_P1 + SumRO2 = SumRO2 + #.5 HO2 + #.478 OLEP + #.367 BACL + #.367 AFG2A + #.112 AFG2B + #.085 MGLY + #.033 BALD + #.026 GLY + #.011 ARO2 + #1.998 XC		Same k as rxn S004			
H012	BZ123_P1 + SumRCO3 = SumRCO3 + #.585 HO2 + #.426 BACL + #.426 AFG2A + #.393 OLEP + #.138 AFG2B + #.112 MGLY + #.044 BALD + #.026 GLY + #1.677 XC		Same k as rxn S009			
H013	BZ124 + OH = #.827 BZ124_P1 + #.117 AFG4 + #.117 OH + #.056 XYNL + #.056 HO2 + #.29 XC + #.827 SumRO2	3.25e-11				1
H014	BZ124_P1 + NO = #.795 HO2 + #.795 NO2 + #.592 MGLY + #.321 AFG3 + #.215 AFG2B + #.193 RPNO3 + #.138 AFG1 + #.113 BACL + #.081 AFG2A + #.05 GLY + #.04 BALD + #.013 RANO3 + #.433 XC + #-0.001 XN		Same k as rxn S001			
H015	BZ124_P1 + NO3 = HO2 + NO2 + #.744 MGLY + #.403 AFG3 + #.27 AFG2B + #.173 AFG1 + #.141 BACL + #.102 AFG2A + #.063 GLY + #.052 BALD + #.301 XC		Same k as rxn S003			
H016	BZ124_P1 + HO2 = #.948 RAOOH + #.052 ROOH + #2.156 XC		Same k as rxn S002			
H017	BZ124_P1 + SumRO2 = SumRO2 + #.5 HO2 + #.474 OLEP + #.372 MGLY + #.202 AFG3 + #.135 AFG2B + #.086 AFG1 + #.071 BACL + #.051 AFG2A + #.039 BALD + #.031 GLY + #.013 ARO2 + #2.071 XC		Same k as rxn S004			
H018	BZ124_P1 + SumRCO3 = SumRCO3 + #.717 HO2 + #.558 MGLY + #.403 AFG3 + #.257 OLEP + #.135 AFG2B + #.086 AFG1 + #.071 BACL + #.067 AFG2A + #.063 GLY + #.052 BALD + #1.274 XC		Same k as rxn S009			
H019	BZ135 + OH = #.792 BZ135_P1 + #.158 AFG4 + #.158 OH + #.05 XYNL + #.05 HO2 + #.366 XC + #.792 SumRO2	5.67e-11				1
H020	BZ135_P1 + NO = #.795 HO2 + #.795 NO2 + #.772 MGLY + #.772 AFG2A + #.197 RPNO3 + #.024 BALD + #.008 RANO3 + #1.016 XC		Same k as rxn S001			
H021	BZ135_P1 + NO3 = HO2 + NO2 + #.969 MGLY + #.969 AFG2A + #.031 BALD + #1.031 XC		Same k as rxn S003			
H022	BZ135_P1 + HO2 = #.969 RAOOH + #.031 ROOH + #2.093 XC		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H023	BZ135_P1 + SumRO2 = SumRO2 + #.5 HO2 + #.484 MGLY + #.484 AFG2A + #.484 OLEP + #.023 BALD + #.008 ARO2 + #2.475 XC	Same k as rxn S004				
H024	BZ135_P1 + SumRCO3 = SumRCO3 + #.5 HO2 + #.484 OLEP + #.484 MGLY + #.484 AFG2A + #.031 BALD + #2.491 XC	Same k as rxn S009				
G566	ACRO + OH = #.68 ACO3 + #.26 ACRO_A1 + #.06 RO2C + #.043 MGLY + #.043 HCHO + #.043 HO2 + #.017 R2CO3 + #-0.043 XC + #.06 SumRO2 + #.697 SumRCO3	2.15e-11	7.10e-12	-0.66	0.00	1
G567	ACRO + O3 = #1.005 CO + #.83 HO2 + #.5 GLY + #.5 HCHO + #.33 OH + #.31 CO2 + #.185 HCHO2	2.90e-19				1
G568	ACRO + NO3 = #.885 ACO3 + #.885 HNO3 + #.115 ACRO_A2 + #.885 SumRCO3	1.10e-15				1
G569	ACRO + HV = #1.243 CO + #.526 HO2 + #.32 MEO2 + #.25 ETHEN + #.243 OH + #.15 HCHO + #.15 ACO3 + #.14 CO2 + #.068 MECHO2 + #.063 CH4 + #-0.002 XC + #.32 SumRO2 + #.15 SumRCO3	Phot Set= ACROL-16				
G570	ACRO_A1 = ACRO_P1 + SumRO2	7.15e-1	1.64e+11	15.60	0.00	
G571	ACRO_A1 + NO = GLCHO + CO + HO2 + NO2	Same k as rxn S001				
G572	ACRO_A2 = ACRO_P2 + SumRO2	7.15e-1	1.64e+11	15.60	0.00	
G573	ACRO_A2 + NO = RCNO3 + CO + HO2 + NO2 + #-1 XC	Same k as rxn S001				
G574	ACRO_P1 + NO = NO2 + #.953 GLCHO + #.953 OH + #.953 CO2 + #.047 R2CO3 + #.047 SumRCO3	Same k as rxn S001				
G575	ACRO_P1 + NO3 = NO2 + #.953 GLCHO + #.953 OH + #.953 CO2 + #.047 R2CO3 + #.047 SumRCO3	Same k as rxn S003				
G576	ACRO_P1 + HO2 = CROOH + #-2 XC	Same k as rxn S002				
G577	ACRO_P1 + SumRO2 = SumRO2 + #.477 GLCHO + #.477 OH + #.477 CO2 + #.25 BACL + #.25 CROOH + #.023 R2CO3 + #-0.75 XC + #.023 SumRCO3	Same k as rxn S004				
G578	ACRO_P1 + SumRCO3 = SumRCO3 + #.5 BACL + #.477 GLCHO + #.477 OH + #.477 CO2 + #.023 R2CO3 + #-0.5 XC + #.023 SumRCO3	Same k as rxn S009				
G579	ACRO_P2 + NO = NO2 + #.859 OH + #.859 RCNO3 + #.859 CO2 + #.141 R2CO3 + #-0.859 XC + #.141 XN + #.141 SumRCO3	Same k as rxn S001				
G580	ACRO_P2 + NO3 = NO2 + #.859 OH + #.859 RCNO3 + #.859 CO2 + #.141 R2CO3 + #-0.859 XC + #.141 XN + #.141 SumRCO3	Same k as rxn S003				
G581	ACRO_P2 + HO2 = RCNO3	Same k as rxn S002				
G582	ACRO_P2 + SumRO2 = SumRO2 + #.93 RCNO3 + #.43 OH + #.43 CO2 + #.07 R2CO3 + #-0.43 XC + #.07 XN + #.07 SumRCO3	Same k as rxn S004				
G583	ACRO_P2 + SumRCO3 = SumRCO3 + #.93 RCNO3 + #.43 OH + #.43 CO2 + #.07 R2CO3 + #-0.43 XC + #.07 XN + #.07 SumRCO3	Same k as rxn S009				
G629	MEK + OH = MEK_P1 + SumRO2	1.11e-12	3.02e-13	-0.78	2.00	1
G630	MEK + HV = ETCO3 + MEO2 + SumRO2 + SumRCO3	Phot Set= MEK-06, qy= 1.75e-1				

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
G631	MEK_P1 + NO = #.932 NO2 + #.604 MECO3 + #.604 MECHO + #.198 RCHO + #.198 HO2 + #.13 HCHO + #.068 RCNO3 + #.066 ETCO3 + #.062 ACETO2 + #.002 RO2C + #.002 R2CO3 + #.068 XC + #.064 SumRO2 + #.672 SumRCO3		Same k as rxn S001			
G632	MEK_P1 + NO3 = NO2 + #.648 MECO3 + #.648 MECHO + #.213 RCHO + #.213 HO2 + #.14 HCHO + #.071 ETCO3 + #.066 ACETO2 + #.002 RO2C + #.002 R2CO3 + #-0.001 XC + #.068 SumRO2 + #.721 SumRCO3		Same k as rxn S003			
G633	MEK_P1 + HO2 = CROOH + #-1 XC		Same k as rxn S002			
G634	MEK_P1 + SumRO2 = SumRO2 + #.324 MECO3 + #.324 MECHO + #.25 KET2 + #.177 RCHO + #.162 BACL + #.106 HO2 + #.07 HCHO + #.035 ETCO3 + #.033 ACETO2 + #.018 MGLY + #.001 RO2C + #.001 R2CO3 + #-0.233 XC + #.034 SumRO2 + #.36 SumRCO3		Same k as rxn S004			
G635	MEK_P1 + SumRCO3 = SumRCO3 + #.324 BACL + #.324 MECO3 + #.324 MECHO + #.247 RCHO + #.106 HO2 + #.07 HCHO + #.035 MGLY + #.035 ETCO3 + #.033 ACETO2 + #.001 RO2C + #.001 R2CO3 + #.038 XC + #.034 SumRO2 + #.36 SumRCO3		Same k as rxn S009			
G598	MACR + OH = #.5 MACO3 + #.44 MACR_A1 + #.058 RO2C + #.058 BACL + #.058 HCHO + #.058 HO2 + #.002 RO2XC + #.002 zRCNO3 + #-0.056 XC + #.06 SumRO2 + #.5 SumRCO3	3.19e-11	9.00e-12	-0.76	0.00	1
G599	MACR + O3 = #.9 MGLY + #.559 CO + #.333 HCHO2 + #.244 OH + #.144 HO2 + #.108 CO2 + #.1 HCHO + #.1 MACR_P1 + #.1 SumRO2	1.10e-18				1
G600	MACR + NO3 = #.5 HNO3 + #.5 MACO3 + #.5 MACR_A2 + #.5 SumRCO3	3.40e-15				1
G601	MACR + HV = #.67 HO2 + #.67 CO + #.34 MECO3 + #.34 HCHO + #.33 MACO3 + #.33 ACETO2 + #.33 OH + #.33 SumRO2 + #.67 SumRCO3		Phot Set= MACR-06			
G602	MACR_A1 = MACR_P2 + SumRO2	7.15e-1	1.64e+11	15.60	0.00	
G603	MACR_A1 + NO = #.969 KET2 + #.969 CO + #.969 HO2 + #.969 NO2 + #.031 RHNO3 + #-2 XC		Same k as rxn S001			
G604	MACR_P1 + NO = HOCCO3 + NO2 + SumRCO3		Same k as rxn S001			
G605	MACR_P1 + NO3 = HOCCO3 + NO2 + SumRCO3		Same k as rxn S003			
G606	MACR_P1 + HO2 = CROOH + #-3 XC		Same k as rxn S002			
G607	MACR_P1 + SumRO2 = SumRO2 + #.5 HOCCO3 + #.25 MGLY + #.25 CROOH + #-1 XC + #.5 SumRCO3		Same k as rxn S004			
G608	MACR_P1 + SumRCO3 = SumRCO3 + #.5 MGLY + #.5 HOCCO3 + #-0.5 XC + #.5 SumRCO3		Same k as rxn S009			
G609	MACR_A2 = MACR_P3 + SumRO2	7.15e-1	1.64e+11	15.60	0.00	
G610	MACR_A2 + NO = #.969 RCNO3 + #.969 CO + #.969 HO2 + #.969 NO2 + #.031 RDNO3 + #-0.062 XC		Same k as rxn S001			
G611	MACR_P2 + NO = #.969 KET2 + #.969 OH + #.969 CO2 + #.969 NO2 + #.031 RCNO3 + #-1.907 XC		Same k as rxn S001			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
G612	MACR_P2 + NO3 = KET2 + OH + CO2 + NO2 + #-2 XC	Same k as rxn S003				
G613	MACR_P2 + HO2 = CROOH + #-1 XC	Same k as rxn S002				
G614	MACR_P2 + SumRO2 = SumRO2 + #.5 CROOH + #.5 KET2 + #.5 OH + #.5 CO2 + #-1.5 XC	Same k as rxn S004				
G615	MACR_P2 + SumRCO3 = SumRCO3 + KET2 + OH + CO2 + #-2 XC	Same k as rxn S009				
G616	MACR_P3 + NO = #.969 RCNO3 + #.969 OH + #.969 CO2 + #.969 NO2 + #.031 RDNO3 + #-0.062 XC	Same k as rxn S001				
G617	MACR_P3 + NO3 = RCNO3 + OH + CO2 + NO2	Same k as rxn S003				
G618	MACR_P3 + HO2 = RCNO3 + XC	Same k as rxn S002				
G619	MACR_P3 + SumRO2 = SumRO2 + RCNO3 + #.5 OH + #.5 CO2 + #.5 XC	Same k as rxn S004				
G620	MACR_P3 + SumRCO3 = SumRCO3 + RCNO3 + OH + CO2	Same k as rxn S009				
G621	MVK + OH = MVK_P1 + SumRO2	2.00e-11	2.60e-12	-1.22	0.00	1
G622	MVK + O3 = #.95 MGLY + #.534 CO + #.351 HCHO2 + #.202 OH + #.152 HO2 + #.114 CO2 + #.05 HCHO + #.05 RO2C + #.05 HOCCO3 + #.001 XC + #.05 SumRO2 + #.05 SumRCO3	5.00e-18				1
G623	MVK + HV = #.6 PROPE + #.6 CO + #.4 ACO3 + #.4 MEO2 + #.4 SumRO2 + #.4 SumRCO3	Phot Set= MVK-16				
G624	MVK_P1 + NO = #.969 NO2 + #.679 MECO3 + #.679 GLCHO + #.291 HO2 + #.289 MGLY + #.289 HCHO + #.031 RCNO3 + #.001 RCHO + #.031 XC + #.679 SumRCO3	Same k as rxn S001				
G625	MVK_P1 + NO3 = NO2 + #.7 MECO3 + #.7 GLCHO + #.3 HO2 + #.298 MGLY + #.298 HCHO + #.002 RCHO + #.7 SumRCO3	Same k as rxn S003				
G626	MVK_P1 + HO2 = CROOH + #-1 XC	Same k as rxn S002				
G627	MVK_P1 + SumRO2 = SumRO2 + #.35 MECO3 + #.35 GLCHO + #.25 KET2 + #.175 BACL + #.15 HO2 + #.149 MGLY + #.149 HCHO + #.076 RCHO + #-0.25 XC + #.35 SumRCO3	Same k as rxn S004				
G628	MVK_P1 + SumRCO3 = SumRCO3 + #.35 BACL + #.35 MECO3 + #.35 GLCHO + #.151 RCHO + #.15 HO2 + #.149 MGLY + #.149 HCHO + #.35 SumRCO3	Same k as rxn S009				
G924	BUDAL + OH = #.69 OH + #.56 AFG3 + #.31 BUDAL_A1 + #.13 CROOH + #-1.25 XC	5.29e-11				80
G925	BUDAL + HV = AFG3 + OH + HO2 + #-2 XC	Phot Set= AFGS, qy= 2.50e-1				
G926	BUDAL_A1 = CROOH + OH + #-1 XC	7.15e-1	1.64e+11	15.60	0.00	
G927	BUDAL_A1 + NO = #.969 NO2 + #.853 HO2 + #.439 GLY + #.439 MGLY + #.414 CROOH + #.414 CO + #.116 OTH2 + #.116 OH + #.031 RCNO3 + #-1.12 XC	Same k as rxn S001				
H275	SESQ + OH = SESQ_P1 + SumRO2	1.51e-10				

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H276	SESQ + O3 = #.806 OH + #.607 SESQ_A1 + #.247 RCHO2 + #.052 OTHN + #.051 RO2C + #.04 HCHO + #.032 CO + #.029 MACO3 + #.023 RO2XC + #.018 OLEP + #.018 CO2 + #.015 CROOH + #.015 zRCNO3 + #.012 LVKS + #.009 HO2 + #.005 zRNNO3 + #.005 HCHO2 + #4.011 XC + #.074 SumRO2 + #.029 SumRCO3	4.24e-16				
H277	SESQ + NO3 = SESQ_P2 + SumRO2	9.76e-12				
H278	SESQ + O3P = #.872 OLEP + #.128 OLEA2 + #10 XC	6.82e-11				
H279	SESQ_P1 + NO = #.729 NO2 + #.434 HO2 + #.427 OLEA2 + #.275 SESQ_P3 + #.259 RHNO3 + #.018 OH + #.013 HCHO + #.013 OLEP + #.012 R2NO3 + #.008 OLEA1 + #.003 LVKS + #.002 OTHN + #.001 RO2XC + #.001 zRCNO3 + #6.933 XC + #.276 SumRO2	Same k as rxn S001				
H280	SESQ_P1 + NO3 = NO2 + #.596 HO2 + #.585 OLEA2 + #.378 SESQ_P3 + #.025 OH + #.017 HCHO + #.017 OLEP + #.011 OLEA1 + #.004 LVKS + #.003 OTHN + #.001 RO2XC + #.001 zRCNO3 + #6.193 XC + #.379 SumRO2	Same k as rxn S003				
H281	SESQ_P1 + HO2 = #.812 OTHN + #.188 RUOOH + #4.316 XC	Same k as rxn S002				
H282	SESQ_P1 + SumRO2 = SumRO2 + #.503 OLEP + #.298 HO2 + #.293 OLEA2 + #.189 SESQ_P3 + #.012 OH + #.009 HCHO + #.008 LVKS + #.005 OLEA1 + #.002 OTHN + #.001 RO2XC + #.001 zRCNO3 + #8.092 XC + #.19 SumRO2	Same k as rxn S004				
H283	SESQ_P1 + SumRCO3 = SumRCO3 + #.524 HO2 + #.51 OLEA2 + #.374 SESQ_P3 + #.093 OLEP + #.017 HCHO + #.015 LVKS + #.014 OH + #.005 OLEA1 + #.002 OTHN + #.001 RO2XC + #.001 zRCNO3 + #6.246 XC + #.375 SumRO2	Same k as rxn S009				
H284	SESQ_A1 = OTHN + OH + #3 XC	1.26e+1	2.47e+10	12.76	0.00	
H285	SESQ_A1 + NO = #.726 OLEA2 + #.726 MECO3 + #.726 NO2 + #.274 RCNO3 + #9.096 XC + #.726 SumRCO3	Same k as rxn S001				
H286	SESQ_P2 + NO = #1.428 NO2 + #.699 OLEA2 + #.293 RNNO3 + #.021 RO2C + #.021 OH + #.008 RO2XC + #.008 zRNNO3 + #8.495 XC + #.279 XN + #.029 SumRO2	Same k as rxn S001				
H287	SESQ_P2 + NO3 = #1.971 NO2 + #.96 OLEA2 + #.029 RO2C + #.029 RNNO3 + #.029 OH + #.011 RO2XC + #.011 zRNNO3 + #9.8 XC + #.04 SumRO2	Same k as rxn S003				
H288	SESQ_P2 + HO2 = RNNO3 + #5 XC	Same k as rxn S002				
H289	SESQ_P2 + SumRO2 = SumRO2 + #.5 RHNO3 + #.48 OLEA2 + #.485 NO2 + #.015 RO2C + #.015 RNNO3 + #.015 OH + #.005 RO2XC + #.005 zRNNO3 + #9.4 XC + #.02 SumRO2	Same k as rxn S004				

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H290	SESQ_P2 + SumRCO3 = SumRCO3 + #.96 OLEA2 + #.971 NO2 + #.029 RO2C + #.029 RNNO3 + #.029 OH + #.011 RO2XC + #.011 zRNNO3 + #9.8 XC + #.04 SumRO2		Same k as rxn S009			
H291	SESQ_P3 + NO = #.729 NO2 + #.723 OH + #.698 OTHN + #.259 RNNO3 + #.015 LVKS + #.012 RCNO3 + #.011 OLEP + #.005 HO2 + #.004 OLEA1 + #.002 RO2C + #.001 RO2XC + #.001 zRNNO3 + #3.853 XC + #.003 SumRO2		Same k as rxn S001			
H292	SESQ_P3 + NO3 = NO2 + #.992 OH + #.958 OTHN + #.02 LVKS + #.015 OLEP + #.007 HO2 + #.006 OLEA1 + #.003 RO2C + #.001 RO2XC + #.001 zRNNO3 + #3.309 XC + #.004 SumRO2		Same k as rxn S003			
H293	SESQ_P3 + HO2 = #.98 OTHN + #.02 HPALD + #3.14 XC		Same k as rxn S002			
H294	SESQ_P3 + SumRO2 = SumRO2 + #.718 OTHN + #.496 OH + #.249 OLEP + #.019 LVKS + #.014 OLEA1 + #.003 HO2 + #.002 RO2C + #.001 RO2XC + #.001 zRNNO3 + #4.983 XC + #.003 SumRO2		Same k as rxn S004			
H295	SESQ_P3 + SumRCO3 = SumRCO3 + #.496 OH + #.485 OLEP + #.479 OTHN + #.02 LVKS + #.015 OLEA1 + #.003 HO2 + #.002 RO2C + #.001 RO2XC + #.001 zRNNO3 + #6.662 XC + #.003 SumRO2		Same k as rxn S009			
H309	BENX + OH = #.57 PHEN + #.57 HO2 + #.268 BENX_P1 + #.162 AFG4 + #.162 OH + #-0.162 XC + #.268 SumRO2	1.22e-12				
H310	BENX_P1 + NO = #.916 BUDAL + #.916 GLY + #.916 HO2 + #.916 NO2 + #.084 RPNO3 + #-0.168 XC		Same k as rxn S001			
H311	BENX_P1 + NO3 = BUDAL + GLY + HO2 + NO2		Same k as rxn S003			
H312	BENX_P1 + HO2 = RAOOH + #-1 XC		Same k as rxn S002			
H313	BENX_P1 + SumRO2 = SumRO2 + #.5 BUDAL + #.5 GLY + #.5 HO2 + #.5 OLEP + #.5 XC		Same k as rxn S004			
H314	BENX_P1 + SumRCO3 = SumRCO3 + #.5 OLEP + #.5 BUDAL + #.5 GLY + #.5 HO2 + #.5 XC		Same k as rxn S009			
H332	STYRS + OH = #.915 STYRS_P1 + #.102 RO2C + #.06 HO2 + #.051 HCHO + #.051 BALD + #.032 RO2XC + #.022 zRHNO3 + #.009 STYRS + #.003 AFG4 + #.003 OH + #1.038 XC + #1.049 SumRO2	5.80e-11				
H333	STYRS + O3 = #.5 BALD + #.5 RCHO2 + #.5 HCHO + #.255 CO + #.185 HCHO2 + #.08 HO2 + #.08 OH + #.06 CO2 + #3 XC	1.76e-17				
H334	STYRS + NO3 = STYRS_P2 + XC + SumRO2	1.50e-13				
H335	STYRS_P1 + NO = #.836 NO2 + #.83 HO2 + #.762 HCHO + #.756 BALD + #.15 RHNO3 + #.039 GLY + #.033 AFG2A + #.026 RO2C + #.021 OLEA1 + #.014 RPNO3 + #.007 HPALD + #.007 ARO1 + #.007 RO2XC + #.005 AFG1 + #.003 zRPNO3 + #.002 zRNNO3 + #.419 XC + #.033 SumRO2		Same k as rxn S001			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H336	STYRS_P1 + NO3 = NO2 + #.994 HO2 + #.912 HCHO + #.905 BALD + #.046 GLY + #.04 AFG2A + #.032 RO2C + #.025 OLEA1 + #.009 HPALD + #.009 ARO1 + #.008 RO2XC + #.006 AFG1 + #.004 zRPNO3 + #.003 zRNNO3 + #.118 XC + #.04 SumRO2		Same k as rxn S003			
H337	STYRS_P1 + HO2 = #.914 ROOH + #.086 RAOOH + #3.742 XC		Same k as rxn S002			
H338	STYRS_P1 + SumRO2 = SumRO2 + #.497 HO2 + #.456 HCHO + #.453 BALD + #.228 ARO2 + #.153 ARO1 + #.08 RCHO + #.043 OLEP + #.023 GLY + #.02 AFG2A + #.016 RO2C + #.012 OLEA1 + #.004 HPALD + #.004 RO2XC + #.003 AFG1 + #.002 zRPNO3 + #.001 zRNNO3 + #.142 XC + #.02 SumRO2		Same k as rxn S004			
H339	STYRS_P1 + SumRCO3 = SumRCO3 + #.497 HO2 + #.456 HCHO + #.453 BALD + #.301 ARO1 + #.161 RCHO + #.043 OLEP + #.023 GLY + #.02 AFG2A + #.016 RO2C + #.012 OLEA1 + #.004 HPALD + #.004 RO2XC + #.003 AFG1 + #.002 zRPNO3 + #.001 zRNNO3 + #.538 XC + #.02 SumRO2		Same k as rxn S009			
H340	STYRS_P2 + NO = #1.076 NO2 + #.594 RCNO3 + #.594 HO2 + #.242 HCHO + #.242 BALD + #.165 RDNO3 + #3.292 XC		Same k as rxn S001			
H341	STYRS_P2 + NO3 = #1.289 NO2 + #.711 RCNO3 + #.711 HO2 + #.289 HCHO + #.289 BALD + #3.555 XC		Same k as rxn S003			
H342	STYRS_P2 + HO2 = RHNO3 + #2 XC		Same k as rxn S002			
H343	STYRS_P2 + SumRO2 = SumRO2 + #.605 RCNO3 + #.355 HO2 + #.25 RHNO3 + #.145 HCHO + #.145 BALD + #.145 NO2 + #3.525 XC		Same k as rxn S004			
H344	STYRS_P2 + SumRCO3 = SumRCO3 + #.855 RCNO3 + #.355 HO2 + #.145 HCHO + #.145 BALD + #.145 NO2 + #4.275 XC		Same k as rxn S009			
H296	ACYLS + OH = #.67 MGLY + #.67 OH + #.33 HCOOH + #.33 ETCO3 + #.67 XC + #.33 SumRCO3	8.00e-12				
H396	LVKS + OH = #.495 RCHO + #.495 HO2 + #.495 LVKS_P1 + #.01 OLEA1 + #-0.01 XC + #.495 SumRO2	4.15e-11				
H397	LVKS + O3 = #.5 LVKS_P2 + #.5 OH + #.5 CO + #.5 HCOOH + #.5 MGLY + #.5 RCHO2 + #-1 XC + #.5 SumRO2	3.32e-17				
H398	LVKS + HV = LVKS_A1 + MEO2 + SumRO2		Phot Set= MVK-16			
H399	LVKS_P1 + NO = #.969 MECO3 + #.969 RCHO + #.969 NO2 + #.031 RCNO3 + #-1.907 XC + #.969 SumRCO3		Same k as rxn S001			
H400	LVKS_P1 + NO3 = MECO3 + RCHO + NO2 + #-2 XC + SumRCO3		Same k as rxn S003			
H401	LVKS_P1 + HO2 = CROOH + #-1 XC		Same k as rxn S002			
H402	LVKS_P1 + SumRO2 = SumRO2 + #.5 MECO3 + #.5 RCHO + #.25 BACL + #.25 KET2 + #-1.25 XC + #.5 SumRCO3		Same k as rxn S004			
H403	LVKS_P1 + SumRCO3 = SumRCO3 + #.5 BACL + #.5 MECO3 + #.5 RCHO + #-1 XC + #.5 SumRCO3		Same k as rxn S009			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H404	LVKS_P2 + NO = HOCCO3 + NO2 + SumRCO3		Same k as rxn S001			
H405	LVKS_P2 + NO3 = HOCCO3 + NO2 + SumRCO3		Same k as rxn S003			
H406	LVKS_P2 + HO2 = CROOH + #-3 XC		Same k as rxn S002			
H407	LVKS_P2 + SumRO2 = SumRO2 + #.5 HOCCO3 + #.25 MGLY + #.25 CROOH + #-1 XC + #.5 SumRCO3		Same k as rxn S004			
H408	LVKS_P2 + SumRCO3 = SumRCO3 + #.5 MGLY + #.5 HOCCO3 + #-0.5 XC + #.5 SumRCO3		Same k as rxn S009			
H409	LVKS_A1 = LVKS_P3 + SumRO2	7.15e-1	1.64e+11	15.60	0.00	
H410	LVKS_A1 + NO = R2CO3 + NO2 + SumRCO3		Same k as rxn S001			
H411	LVKS_P3 + NO = R2CO3 + NO2 + SumRCO3		Same k as rxn S001			
H412	LVKS_P3 + NO3 = R2CO3 + NO2 + SumRCO3		Same k as rxn S003			
H413	LVKS_P3 + HO2 = OTHN + #-9 XC		Same k as rxn S002			
H414	LVKS_P3 + SumRO2 = SumRO2 + #.5 R2CO3 + #.25 BACL + #.25 CROOH + #-0.75 XC + #.5 SumRCO3		Same k as rxn S004			
H415	LVKS_P3 + SumRCO3 = SumRCO3 + #.5 BACL + #.5 R2CO3 + #-0.5 XC + #.5 SumRCO3		Same k as rxn S009			
H483	OLEA2 + OH = #.667 OLEA2_P1 + #.264 MACO3 + #.045 HO2 + #.024 OLEA1 + #.024 OLEP + #.024 OH + #.021 MGLY + #.021 CO + #.285 XC + #.667 SumRO2 + #.264 SumRCO3	8.84e-11				
H484	OLEA2 + O3 = #.723 HO2 + #.723 OH + #.67 MGLY + #.67 HCHO + #.33 RCHO + #.168 CO + #.122 HCHO2 + #.04 CO2 + #.67 XC	1.41e-17				
H485	OLEA2 + NO3 = #.972 OLEA2_P2 + #.028 MACO3 + #.028 HNO3 + #.028 XC + #.972 SumRO2 + #.028 SumRCO3	4.06e-13				
H486	OLEA2 + HV = #1.5 HO2 + CO + #.5 OLEA1 + #.5 OLEA2_P3 + #-0.5 XC + #.5 SumRO2		Phot Set= C2CHO			
H487	OLEA2_P1 + NO = #.947 NO2 + #.917 HO2 + #.892 KET2 + #.892 MGLY + #.055 CROOH + #.053 RNNO3 + #.03 OH + #.03 CO2 + #.025 HCHO + #-2.996 XC		Same k as rxn S001			
H488	OLEA2_P1 + NO3 = NO2 + #.969 HO2 + #.943 KET2 + #.943 MGLY + #.057 CROOH + #.031 OH + #.031 CO2 + #.026 HCHO + #-2.886 XC		Same k as rxn S003			
H489	OLEA2_P1 + HO2 = OTHN + #-7 XC		Same k as rxn S002			
H490	OLEA2_P1 + SumRO2 = SumRO2 + #.5 OTHN + #.484 HO2 + #.471 KET2 + #.471 MGLY + #.029 CROOH + #.016 OH + #.016 CO2 + #.013 HCHO + #-4.942 XC		Same k as rxn S004			
H491	OLEA2_P1 + SumRCO3 = SumRCO3 + #.969 HO2 + #.943 KET2 + #.943 MGLY + #.057 CROOH + #.031 OH + #.031 CO2 + #.026 HCHO + #-2.886 XC		Same k as rxn S009			
H492	OLEA2_P2 + NO = #.946 RCNO3 + #.946 HO2 + #.946 NO2 + #.934 MGLY + #.054 RNNO3 + #.013 HCHO + #-1.193 XC + #.054 XN		Same k as rxn S001			
H493	OLEA2_P2 + NO3 = RCNO3 + HO2 + NO2 + #.986 MGLY + #.014 HCHO + #-0.972 XC		Same k as rxn S003			
H494	OLEA2_P2 + HO2 = RNNO3 + #-5 XC		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H495	OLEA2_P2 + SumRO2 = SumRO2 + #.5 RNNO3 + #.5 RCNO3 + #.5 HO2 + #.493 MGLY + #.007 HCHO + #-2.986 XC		Same k as rxn S004			
H496	OLEA2_P2 + SumRCO3 = SumRCO3 + RCNO3 + HO2 + #.986 MGLY + #.014 HCHO + #-0.972 XC		Same k as rxn S009			
H497	OLEA2_P3 + NO = #.969 OLEA1 + #.969 HO2 + #.969 NO2 + #.031 RHNO3 + #-1.031 XC		Same k as rxn S001			
H498	OLEA2_P3 + NO3 = OLEA1 + HO2 + NO2 + #-1 XC		Same k as rxn S003			
H499	OLEA2_P3 + HO2 = RUOOH + #-1 XC		Same k as rxn S002			
H500	OLEA2_P3 + SumRO2 = SumRO2 + #.75 OLEA1 + #.5 HO2 + #.25 OLEP + #-1 XC		Same k as rxn S004			
H501	OLEA2_P3 + SumRCO3 = SumRCO3 + OLEA1 + #.5 HO2 + #-1 XC		Same k as rxn S009			
H345	INHIB + OH = #.535 xNAMIN + #.435 HO2 + #.411 RCHO + #.078 HCHO + #.078 RO2C + #.053 AMINS + #.029 MEO2 + #.001 RO2XC + #.001 zRHNO3 + #-0.003 XC + #-0.588 XN + #.108 SumRO2	2.80e-11				
H346	INHIB + O3 = xNAMIN + OH + #-1 XN	7.40e-21				
H066	ALK3 + OH = ALK3_P1 + SumRO2	2.49e-12				
H067	ALK3_P1 + NO = #.885 NO2 + #.485 TBUO + #.345 ALK3_P2 + #.115 R1NO3 + #.112 RCHO + #.074 HCHO + #.06 MECHO + #.055 HO2 + #.005 ACET + #-0.242 XC + #.345 SumRO2		Same k as rxn S001			
H068	ALK3_P1 + NO3 = NO2 + #.52 TBUO + #.421 ALK3_P2 + #.132 RCHO + #.082 HCHO + #.07 MECHO + #.059 HO2 + #.007 ACET + #-0.377 XC + #.421 SumRO2		Same k as rxn S003			
H069	ALK3_P1 + HO2 = ROOH + XC		Same k as rxn S002			
H070	ALK3_P1 + SumRO2 = SumRO2 + #.26 OTH1 + #.26 TBUO + #.21 ALK3_P2 + #.115 RCHO + #.069 OTH2 + #.044 OTH4 + #.042 OTH3 + #.041 HCHO + #.036 KET2 + #.035 MECHO + #.03 HO2 + #.003 ACET + #.609 XC + #.21 SumRO2		Same k as rxn S004			
H071	ALK3_P1 + SumRCO3 = SumRCO3 + #.592 TBUO + #.385 RO2C + #.217 HCHO + #.193 RCHO + #.167 HO2 + #.15 KET2 + #.093 RO2XC + #.055 ACET + #.05 zRHNO3 + #.035 MECHO + #.011 ETO2 + #.009 zR1NO3 + #.001 MEO2 + #.001 MEK + #.286 XC + #.49 SumRO2		Same k as rxn S009			
H072	ALK3_P2 + NO = #.893 NO2 + #.314 TBUO + #.291 ALK3_P3 + #.232 HO2 + #.209 HCHO + #.193 ACET + #.094 RCHO + #.068 RHNO3 + #.053 ETO2 + #.039 R1NO3 + #.004 MEK + #.004 MEO2 + #.814 XC + #.348 SumRO2		Same k as rxn S001			
H073	ALK3_P2 + NO3 = NO2 + #.347 ALK3_P3 + #.337 TBUO + #.253 HO2 + #.249 HCHO + #.206 ACET + #.109 RCHO + #.059 ETO2 + #.004 MEK + #.004 MEO2 + #.782 XC + #.41 SumRO2		Same k as rxn S003			
H074	ALK3_P2 + HO2 = ROOH + #2 XC		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H075	ALK3_P2 + SumRO2 = SumRO2 + #.173 ALK3_P3 + #.168 OTH1 + #.168 TBUO + #.151 OTH3 + #.149 RCHO + #.139 ACET + #.127 HO2 + #.125 HCHO + #.032 OTH2 + #.029 ETO2 + #.017 OTH4 + #.002 MEK + #.002 MEO2 + #.001 KET2 + #1.634 XC + #.204 SumRO2		Same k as rxn S004			
H076	ALK3_P2 + SumRCO3 = SumRCO3 + #.337 TBUO + #.277 RCHO + #.206 ACET + #.178 ALK3_P3 + #.159 HO2 + #.125 HCHO + #.059 ETO2 + #.004 MEK + #.004 MEO2 + #.001 KET2 + #1.412 XC + #.241 SumRO2		Same k as rxn S009			
H077	ALK3_P3 + NO = #.871 NO2 + #.752 HO2 + #.679 HCHO + #.638 KET2 + #.535 RO2C + #.125 RHNO3 + #.087 ACET + #.073 RO2XC + #.072 RCHO + #.071 zRHNO3 + #.044 TBUO + #.004 R1NO3 + #.004 ETHEO2 + #.001 zRNNO3 + #1.192 XC + #.612 SumRO2		Same k as rxn S001			
H078	ALK3_P3 + NO3 = NO2 + #.867 HO2 + #.781 HCHO + #.735 KET2 + #.609 RO2C + #.099 ACET + #.085 RCHO + #.083 RO2XC + #.081 zRHNO3 + #.047 TBUO + #.004 ETHEO2 + #.001 zRNNO3 + #1.215 XC + #.696 SumRO2		Same k as rxn S003			
H079	ALK3_P3 + HO2 = #.934 ROOH + #.066 OTHN + #2.472 XC		Same k as rxn S002			
H080	ALK3_P3 + SumRO2 = SumRO2 + #.434 HO2 + #.39 HCHO + #.367 KET2 + #.331 OTH2 + #.304 RO2C + #.096 RCHO + #.081 OTH4 + #.05 ACET + #.041 RO2XC + #.041 zRHNO3 + #.024 OTH1 + #.024 TBUO + #.011 OTH3 + #.002 ETHEO2 + #2.462 XC + #.347 SumRO2		Same k as rxn S004			
H081	ALK3_P3 + SumRCO3 = SumRCO3 + #.762 HO2 + #.696 HCHO + #.651 KET2 + #.599 RO2C + #.17 RCHO + #.099 ACET + #.081 RO2XC + #.08 zRHNO3 + #.047 TBUO + #.004 ETHEO2 + #.001 zRNNO3 + #1.386 XC + #.684 SumRO2		Same k as rxn S009			
H082	ALK4 + OH = ALK4_P1 + SumRO2	4.76e-12				
H083	ALK4_P1 + NO = #.872 NO2 + #.511 ALK4_P2 + #.237 ETO2 + #.236 ACET + #.127 R1NO3 + #.097 MECHO + #.06 HO2 + #.058 KET2 + #.057 MEK + #.049 OH + #.048 OTH2 + #.045 ETCHO + #.017 RCHO + #.014 MEO2 + #.004 HCHO + #.002 OTH3 + #.001 R2NO3 + #.535 XC + #.762 SumRO2		Same k as rxn S001			
H084	ALK4_P1 + NO3 = NO2 + #.595 ALK4_P2 + #.268 ACET + #.266 ETO2 + #.11 MECHO + #.068 HO2 + #.067 MEK + #.067 KET2 + #.056 OH + #.055 OTH2 + #.051 ETCHO + #.02 RCHO + #.015 MEO2 + #.004 HCHO + #.002 OTH3 + #.441 XC + #.876 SumRO2		Same k as rxn S003			
H085	ALK4_P1 + HO2 = ROOH + #2 XC		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H086	ALK4_P1 + SumRO2 = SumRO2 + #.298 ALK4_P2 + #.145 OTH2 + #.143 OTH3 + #.138 KET2 + #.134 ACET + #.133 ETO2 + #.114 OTH4 + #.055 MECHO + #.034 HO2 + #.033 MEK + #.032 RCHO + #.028 OH + #.026 ETCHO + #.008 MEO2 + #.002 HCHO + #1.231 XC + #.439 SumRO2		Same k as rxn S004			
H087	ALK4_P1 + SumRCO3 = SumRCO3 + #.44 RO2C + #.382 ACET + #.378 KET2 + #.355 HO2 + #.263 ETO2 + #.124 RCHO + #.083 MECHO + #.081 MEK + #.047 RO2XC + #.047 OTH2 + #.043 HCHO + #.039 ETCHO + #.029 OH + #.024 zRHNO3 + #.016 MECO3 + #.015 MEO2 + #.011 OTH3 + #.009 zR1NO3 + #.005 zRCNO3 + #.001 TBUO + #.852 XC + #.765 SumRO2 + #.016 SumRCO3		Same k as rxn S009			
H088	ALK4_P2 + NO = #.928 NO2 + #.853 HO2 + #.371 KET2 + #.286 ACET + #.173 RCHO + #.154 RO2C + #.069 HCHO + #.056 MECHO + #.045 RHNO3 + #.039 MEK + #.029 ETO2 + #.028 MECO3 + #.025 ETCHO + #.021 R1NO3 + #.015 RO2XC + #.011 zRHNO3 + #.006 RCNO3 + #.003 TBUO + #.003 zRCNO3 + #.001 zR1NO3 + #.001 OTH2 + #.001 OH + #.581 XC + #.198 SumRO2 + #.028 SumRCO3		Same k as rxn S001			
H089	ALK4_P2 + NO3 = NO2 + #.916 HO2 + #.404 KET2 + #.301 ACET + #.188 RCHO + #.174 RO2C + #.077 HCHO + #.062 MECHO + #.043 MEK + #.032 ETO2 + #.031 MECO3 + #.026 ETCHO + #.017 RO2XC + #.012 zRHNO3 + #.003 zRCNO3 + #.003 TBUO + #.001 zR1NO3 + #.001 OTH2 + #.001 OH + #.001 ETHEO2 + #.645 XC + #.224 SumRO2 + #.031 SumRCO3		Same k as rxn S003			
H090	ALK4_P2 + HO2 = #.963 ROOH + #.037 CROOH + #.963 XC		Same k as rxn S002			
H091	ALK4_P2 + SumRO2 = SumRO2 + #.458 HO2 + #.251 KET2 + #.217 ACET + #.208 RCHO + #.126 OTH3 + #.122 OTH4 + #.087 RO2C + #.039 HCHO + #.035 MEK + #.031 MECHO + #.019 ETCHO + #.016 ETO2 + #.016 MECO3 + #.009 RO2XC + #.006 zRHNO3 + #.002 zRCNO3 + #.002 TBUO + #.001 OTH1 + #.001 OTH2 + #.001 zR1NO3 + #.001 OH + #.847 XC + #.112 SumRO2 + #.016 SumRCO3		Same k as rxn S004			
H092	ALK4_P2 + SumRCO3 = SumRCO3 + #.469 HO2 + #.33 RCHO + #.286 KET2 + #.285 ACET + #.089 RO2C + #.053 MEK + #.039 HCHO + #.033 MECHO + #.026 ETCHO + #.021 ETO2 + #.016 MECO3 + #.009 RO2XC + #.006 zRHNO3 + #.003 TBUO + #.002 zRCNO3 + #.001 OTH2 + #.001 zR1NO3 + #.001 OH + #.864 XC + #.119 SumRO2 + #.016 SumRCO3		Same k as rxn S009			
H093	ALK5 + OH = ALK5_P1 + SumRO2	8.34e-12				

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H094	ALK5_P1 + NO = #.796 NO2 + #.587 ALK5_P2 + #.16 OTH3 + #.136 R2NO3 + #.108 OH + #.088 HO2 + #.068 R1NO3 + #.03 OTH4 + #.026 KET2 + #.018 RCHO + #.012 ETO2 + #.01 MECHO + #.006 ACET + #.004 ETCHO + #.001 HCHO + #.001 MEK + #.835 XC + #.599 SumRO2		Same k as rxn S001			
H095	ALK5_P1 + NO3 = NO2 + #.748 ALK5_P2 + #.192 OTH3 + #.131 OH + #.106 HO2 + #.037 OTH4 + #.033 KET2 + #.022 RCHO + #.014 ETO2 + #.012 MECHO + #.008 ACET + #.006 ETCHO + #.001 HCHO + #.001 MEK + #.748 XC + #.762 SumRO2		Same k as rxn S003			
H096	ALK5_P1 + HO2 = ROOH + #4 XC		Same k as rxn S002			
H097	ALK5_P1 + SumRO2 = SumRO2 + #.374 ALK5_P2 + #.239 OTH4 + #.227 OTH3 + #.155 KET2 + #.066 OH + #.053 HO2 + #.02 RCHO + #.007 ETO2 + #.006 MECHO + #.004 ACET + #.003 ETCHO + #.001 HCHO + #2.241 XC + #.381 SumRO2		Same k as rxn S004			
H098	ALK5_P1 + SumRCO3 = SumRCO3 + #.573 KET2 + #.479 RO2C + #.394 HO2 + #.184 OTH3 + #.115 RO2XC + #.097 RCHO + #.07 zRHNO3 + #.068 OH + #.049 OTH4 + #.031 ACET + #.031 MECHO + #.021 zRCNO3 + #.02 HCHO + #.017 ETO2 + #.009 ETCHO + #.009 MECO3 + #.006 MEK + #.005 ETCO3 + #.003 zR1NO3 + #.001 ACETO2 + #.001 OTH2 + #3.018 XC + #.612 SumRO2 + #.014 SumRCO3		Same k as rxn S009			
H099	ALK5_P2 + NO = #.836 NO2 + #.633 HO2 + #.565 KET2 + #.191 ALK5_P3 + #.138 RHNO3 + #.035 ACET + #.031 RCHO + #.019 RCNO3 + #.011 MECHO + #.008 ETO2 + #.007 MEK + #.006 ETCHO + #.006 R1NO3 + #.004 OH + #.003 OTH3 + #.002 OTH2 + #.001 OTH4 + #.001 R2NO3 + #2.58 XC + #.199 SumRO2		Same k as rxn S001			
H100	ALK5_P2 + NO3 = NO2 + #.753 HO2 + #.677 KET2 + #.233 ALK5_P3 + #.037 ACET + #.036 RCHO + #.013 MECHO + #.008 ETO2 + #.007 MEK + #.007 ETCHO + #.005 OH + #.004 OTH3 + #.002 OTH2 + #.001 OTH4 + #2.612 XC + #.241 SumRO2		Same k as rxn S003			
H101	ALK5_P2 + HO2 = #.902 ROOH + #.098 CROOH + #3.902 XC		Same k as rxn S002			
H102	ALK5_P2 + SumRO2 = SumRO2 + #.534 KET2 + #.377 HO2 + #.213 OTH4 + #.117 ALK5_P3 + #.066 RCHO + #.035 OTH3 + #.026 ACET + #.006 MECHO + #.006 MEK + #.004 ETO2 + #.004 ETCHO + #.003 OH + #.002 OTH2 + #3.115 XC + #.121 SumRO2		Same k as rxn S004			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H103	ALK5_P2 + SumRCO3 = SumRCO3 + #.757 KET2 + #.497 HO2 + #.167 RCHO + #.127 RO2C + #.043 ACET + #.03 HCHO + #.025 MECHO + #.022 RO2XC + #.013 zRHNO3 + #.011 MEK + #.007 MECO3 + #.007 ETCHO + #.007 zRCNO3 + #.005 ETO2 + #.004 ETCO3 + #.004 OTH3 + #.003 OH + #.002 OTH2 + #.001 OTH4 + #.001 ACETO2 + #.001 zRNNO3 + #3.099 XC + #.155 SumRO2 + #.011 SumRCO3		Same k as rxn S009			
H104	ALK5_P3 + NO = #.857 NO2 + #.746 HO2 + #.417 KET2 + #.411 RCHO + #.146 MECHO + #.139 HCHO + #.081 RHNO3 + #.063 MECO3 + #.055 RCNO3 + #.047 RO2C + #.042 ACET + #.036 ETCO3 + #.023 ETCHO + #.013 MEK + #.007 ACETO2 + #.006 RNNO3 + #.005 RO2XC + #.004 zRHNO3 + #.001 R1NO3 + #.001 OTHN + #1.586 XC + #.059 SumRO2 + #.099 SumRCO3		Same k as rxn S001			
H105	ALK5_P3 + NO3 = NO2 + #.872 HO2 + #.495 KET2 + #.476 RCHO + #.176 MECHO + #.165 HCHO + #.072 MECO3 + #.052 RO2C + #.045 ACET + #.042 ETCO3 + #.027 ETCHO + #.017 MEK + #.009 ACETO2 + #.005 RO2XC + #.005 zRHNO3 + #.001 OTHN + #1.481 XC + #.066 SumRO2 + #.114 SumRCO3		Same k as rxn S003			
H106	ALK5_P3 + HO2 = #.549 ROOH + #.41 CROOH + #.041 OTHN + #2.262 XC		Same k as rxn S002			
H107	ALK5_P3 + SumRO2 = SumRO2 + #.499 KET2 + #.436 HO2 + #.295 RCHO + #.133 OTH4 + #.088 MECHO + #.083 HCHO + #.036 MECO3 + #.03 ACET + #.028 BACL + #.026 RO2C + #.021 ETCO3 + #.015 OTH3 + #.014 ETCHO + #.008 MEK + #.006 OTHN + #.004 ACETO2 + #.003 RO2XC + #.002 zRHNO3 + #1.967 XC + #.033 SumRO2 + #.057 SumRCO3		Same k as rxn S004			
H108	ALK5_P3 + SumRCO3 = SumRCO3 + #.544 KET2 + #.463 HO2 + #.368 RCHO + #.09 MECHO + #.089 HCHO + #.057 BACL + #.039 ACET + #.036 MECO3 + #.027 RO2C + #.021 ETCO3 + #.015 ETCHO + #.009 MEK + #.007 ACETO2 + #.003 RO2XC + #.002 zRHNO3 + #.001 OTHN + #1.933 XC + #.037 SumRO2 + #.057 SumRCO3		Same k as rxn S009			
H109	OLE1 + OH = #.973 OLE1_P1 + #.021 OH + #.02 RO2C + #.011 HPALD + #.006 OLEP + #.005 HO2 + #.005 OLEA2 + #.002 RO2XC + #.002 RUOOH + #.001 zRHNO3 + #.001 HCHO + #.001 MACR + #.001 OLEA1 + #-0.001 XC + #.995 SumRO2	3.16e-11				
H110	OLE1 + O3 = #.5 HCHO + #.43 RCHO + #.425 RCHO2 + #.302 CO + #.185 HCHO2 + #.143 HO2 + #.128 OH + #.088 CO2 + #.081 ETCHO + #.053 RO2C + #.037 ACET + #.009 PROP + #.009 ETO2 + #.003 RO2XC + #.002 zR1NO3 + #.002 TBUO + #.002 ETHAN + #.001 NC4 + #.505 XC + #.065 SumRO2	8.66e-18				

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H111	OLE1 + NO3 = #.998 OLE1_P2 + #.004 HNO3 + #.002 RO2C + #.002 OH + #.001 HPALD + #.001 OLEA2 + #-0.002 XN + SumRO2	1.48e-14				
H112	OLE1 + O3P = #.449 OTH2 + #.25 RCHO + #.214 KET2 + #.036 MEK + #.031 OTH3 + #.02 OTH1 + #1.255 XC	4.32e-12				
H113	OLE1_P1 + NO = #.944 NO2 + #.533 HO2 + #.528 HCHO + #.393 RCHO + #.391 OLE1_P3 + #.291 GLCHO + #.133 ETCHO + #.052 RHNO3 + #.019 MVK + #.016 MEO2 + #.005 KET2 + #.005 MECHO + #.004 R2NO3 + #.003 RO2C + #.002 HPALD + #.002 ETO2 + #.001 OH + #.001 ACRO + #.001 LVKS + #.001 OLEP + #-0.142 XC + #.412 SumRO2	Same k as rxn S001				
H114	OLE1_P1 + NO3 = NO2 + #.561 HO2 + #.556 HCHO + #.417 OLE1_P3 + #.416 RCHO + #.309 GLCHO + #.137 ETCHO + #.021 MVK + #.018 MEO2 + #.005 MECHO + #.005 KET2 + #.003 RO2C + #.002 HPALD + #.002 OH + #.002 ETO2 + #.002 ACRO + #.001 LVKS + #.001 OLEP + #-0.083 XC + #.44 SumRO2	Same k as rxn S003				
H115	OLE1_P1 + HO2 = #.962 ROOH + #.038 RUOOH + #.962 XC	Same k as rxn S002				
H116	OLE1_P1 + SumRO2 = SumRO2 + #.293 RCHO + #.281 HO2 + #.278 HCHO + #.24 OTH4 + #.208 OLE1_P3 + #.158 KET2 + #.154 GLCHO + #.069 ETCHO + #.017 OLEP + #.011 MVK + #.009 MEO2 + #.003 MECHO + #.002 OLEA2 + #.001 RO2C + #.001 LVKS + #.001 HPALD + #.001 OH + #.001 ETO2 + #.001 ACRO + #.285 XC + #.219 SumRO2	Same k as rxn S004				
H117	OLE1_P1 + SumRCO3 = SumRCO3 + #.377 RCHO + #.314 KET2 + #.281 HO2 + #.278 HCHO + #.208 OLE1_P3 + #.154 GLCHO + #.069 ETCHO + #.021 MVK + #.018 MEO2 + #.004 OLEP + #.003 OLEA2 + #.003 MECHO + #.002 LVKS + #.001 RO2C + #.001 ETO2 + #.001 HPALD + #.001 OH + #.001 ACRO + #.136 XC + #.228 SumRO2	Same k as rxn S009				
H118	OLE1_P2 + NO = #1.001 NO2 + #.755 OLE1_P4 + #.728 RCNO3 + #.123 HO2 + #.056 HCHO + #.055 RDNO3 + #.041 ETCHO + #.015 RCHO + #.009 ETO2 + #.002 MVK + #.002 MEO2 + #-0.801 XC + #.161 XN + #.766 SumRO2	Same k as rxn S001				
H119	OLE1_P2 + NO3 = #1.058 NO2 + #.803 OLE1_P4 + #.768 RCNO3 + #.128 HO2 + #.058 HCHO + #.042 ETCHO + #.016 RCHO + #.01 ETO2 + #.002 MVK + #.002 MEO2 + #-0.794 XC + #.174 XN + #.815 SumRO2	Same k as rxn S003				
H120	OLE1_P2 + HO2 = #.998 RHNO3 + #.002 RUOOH + #-0.998 XC + #.002 XN	Same k as rxn S002				

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H121	OLE1_P2 + SumRO2 = SumRO2 + #.633 RCNO3 + #.401 OLE1_P4 + #.249 RHNO3 + #.064 HO2 + #.029 HCHO + #.118 NO2 + #.021 ETCHO + #.008 RCHO + #.005 ETO2 + #.001 OLEP + #.001 MVK + #.001 MEO2 + #-0.141 XC + #.407 SumRO2		Same k as rxn S004			
H122	OLE1_P2 + SumRCO3 = SumRCO3 + #.883 RCNO3 + #.401 OLE1_P4 + #.064 HO2 + #.029 HCHO + #.117 NO2 + #.021 ETCHO + #.008 RCHO + #.005 ETO2 + #.002 MVK + #.002 MEO2 + #.603 XC + #.408 SumRO2		Same k as rxn S009			
H123	OLE1_P3 + NO = #.951 NO2 + #.891 HO2 + #.653 ACET + #.149 RCHO + #.061 KET2 + #.056 TBUO + #.032 R1NO3 + #.018 ACRO + #.016 RHNO3 + #.006 MVK + #.004 RO2C + #.003 MEK + #.003 GLCHO + #.003 MECHO + #.003 HCHO + #.002 ETO2 + #.001 R2NO3 + #.001 OTHN + #.001 MEO2 + #.53 XC + #.007 SumRO2		Same k as rxn S001			
H124	OLE1_P3 + NO3 = NO2 + #.936 HO2 + #.681 ACET + #.158 RCHO + #.067 KET2 + #.06 TBUO + #.018 ACRO + #.007 MVK + #.005 RO2C + #.003 MEK + #.003 GLCHO + #.003 MECHO + #.003 HCHO + #.002 ETO2 + #.001 OTHN + #.001 MEO2 + #.624 XC + #.008 SumRO2		Same k as rxn S003			
H125	OLE1_P3 + HO2 = #.966 ROOH + #.025 RUOOH + #.009 OTHN + #-0.097 XC		Same k as rxn S002			
H126	OLE1_P3 + SumRO2 = SumRO2 + #.51 ACET + #.468 HO2 + #.171 OTH3 + #.102 RCHO + #.068 KET2 + #.058 OTH4 + #.03 OTH1 + #.03 TBUO + #.014 ACRO + #.007 OLEP + #.005 MVK + #.003 MEK + #.002 RO2C + #.002 GLCHO + #.002 MECHO + #.001 HCHO + #.001 ETO2 + #.001 OTHN + #.464 XC + #.003 SumRO2		Same k as rxn S004			
H127	OLE1_P3 + SumRCO3 = SumRCO3 + #.68 ACET + #.468 HO2 + #.124 RCHO + #.103 KET2 + #.06 TBUO + #.018 ACRO + #.007 MVK + #.005 MEK + #.002 RO2C + #.002 GLCHO + #.002 MECHO + #.001 HCHO + #.001 ETO2 + #.001 MEO2 + #.001 OTHN + #.583 XC + #.004 SumRO2		Same k as rxn S009			
H128	OLE1_P4 + NO = #.951 NO2 + #.904 HO2 + #.703 ACET + #.197 RCNO3 + #.045 TBUO + #.034 R1NO3 + #.015 RDNO3 + #.003 MEK + #.002 MECHO + #.002 ETO2 + #.001 ETCHO + #.837 XC + #-0.212 XN + #.002 SumRO2		Same k as rxn S001			
H129	OLE1_P4 + NO3 = NO2 + #.949 HO2 + #.733 ACET + #.211 RCNO3 + #.048 TBUO + #.004 MEK + #.002 MECHO + #.002 ETO2 + #.001 ETCHO + #.001 RO2C + #.949 XC + #-0.211 XN + #.003 SumRO2		Same k as rxn S003			
H130	OLE1_P4 + HO2 = #.788 ROOH + #.203 RHNO3 + #.009 RNNO3 + #-0.46 XC + #-0.212 XN		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H131	OLE1_P4 + SumRO2 = SumRO2 + #.55 ACET + #.475 HO2 + #.185 OTH3 + #.121 RCNO3 + #.09 RHNO3 + #.024 OTH1 + #.024 TBUO + #.003 MEK + #.001 MECHO + #.001 ETO2 + #.001 ETCHO + #.52 XC + #-0.211 XN + #.001 SumRO2		Same k as rxn S004			
H132	OLE1_P4 + SumRCO3 = SumRCO3 + #.733 ACET + #.475 HO2 + #.137 RCNO3 + #.074 RHNO3 + #.048 TBUO + #.005 MEK + #.001 ETCHO + #.001 MECHO + #.001 ETO2 + #.727 XC + #-0.211 XN + #.001 SumRO2		Same k as rxn S009			
H133	OLE2 + OH = #.988 OLE2_P1 + #.008 RO2C + #.008 OH + #.005 HPALD + #.003 HO2 + #.003 ACRO + #.002 MECHO + #.002 OLEP + #.001 RO2XC + #.001 RUOOH + #.001 LVKS + #.003 XC + #.997 SumRO2	6.37e-11				
H134	OLE2 + O3 = #.645 MECHO + #.458 MEO2 + #.382 CO + #.382 OH + #.31 ETCHO + #.302 RCHO2 + #.219 CO2 + #.126 HO2 + #.097 MECHO2 + #.09 CH4 + #.049 RCHO + #.038 ETO2 + #.008 ETHAN + #.007 RO2C + #.002 ACET + #.001 PROP + #.234 XC + #.503 SumRO2	1.56e-16				
H135	OLE2 + NO3 = OLE2_P2 + SumRO2	4.62e-13				
H136	OLE2 + O3P = #.325 KET2 + #.309 OTH2 + #.175 OTH1 + #.175 MEK + #.012 OTH3 + #.004 OTH4 + #1.159 XC	1.93e-11				
H137	OLE2_P1 + NO = #1.24 MECHO + #.949 NO2 + #.948 HO2 + #.575 ETCHO + #.078 RCHO + #.051 RHNO3 + #.002 RO2C + #.001 KET2 + #.172 XC + #.002 SumRO2		Same k as rxn S001			
H138	OLE2_P1 + NO3 = #1.295 MECHO + NO2 + #.999 HO2 + #.611 ETCHO + #.089 RCHO + #.002 RO2C + #.001 KET2 + #.216 XC + #.002 SumRO2		Same k as rxn S003			
H139	OLE2_P1 + HO2 = #.999 ROOH + #.001 RUOOH + #.999 XC		Same k as rxn S002			
H140	OLE2_P1 + SumRO2 = SumRO2 + #.648 MECHO + #.5 HO2 + #.306 ETCHO + #.25 KET2 + #.25 OTH4 + #.045 RCHO + #.001 RO2C + #.356 XC + #.001 SumRO2		Same k as rxn S004			
H141	OLE2_P1 + SumRCO3 = SumRCO3 + #.648 MECHO + #.5 KET2 + #.5 HO2 + #.306 ETCHO + #.045 RCHO + #.001 RO2C + #.106 XC + #.001 SumRO2		Same k as rxn S009			
H142	OLE2_P2 + NO = #1.847 NO2 + #1.198 MECHO + #.542 ETCHO + #.057 RCHO + #.052 RDNO3 + #.046 HO2 + #.046 RCNO3 + #.044 RO2C + #.005 RO2XC + #.003 zRDNO3 + #.001 zRNNO3 + #.001 ACET + #.269 XC + #.049 SumRO2		Same k as rxn S001			
H143	OLE2_P2 + NO3 = #1.946 NO2 + #1.25 MECHO + #.575 ETCHO + #.063 RCHO + #.051 HO2 + #.05 RCNO3 + #.049 RO2C + #.005 RO2XC + #.004 zRDNO3 + #.001 zRNNO3 + #.001 ACET + #.336 XC + #.054 SumRO2		Same k as rxn S003			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H144	OLE2_P2 + HO2 = RHNO3 + #-1 XC		Same k as rxn S002			
H145	OLE2_P2 + SumRO2 = SumRO2 + #.625 MECHO + #.473 NO2 + #.287 ETCHO + #.275 RCNO3 + #.25 RHNO3 + #.032 RCHO + #.025 HO2 + #.025 RO2C + #.003 RO2XC + #.002 zRDNO3 + #.001 zRNNO3 + #.001 ACET + #.411 XC + #.028 SumRO2		Same k as rxn S004			
H146	OLE2_P2 + SumRCO3 = SumRCO3 + #.625 MECHO + #.525 RCNO3 + #.473 NO2 + #.287 ETCHO + #.032 RCHO + #.025 HO2 + #.025 RO2C + #.003 RO2XC + #.002 zRDNO3 + #.001 zRNNO3 + #.001 ACET + #1.161 XC + #.028 SumRO2		Same k as rxn S009			
H147	OLE3 + OH = #.994 OLE3_P1 + #.004 OH + #.003 HPALD + #.003 RO2C + #.001 HO2 + #.001 OLEP + #.001 HCHO + #.001 MVK + #.001 RO2XC + #.005 XC + #.998 SumRO2	5.69e-11				
H148	OLE3 + O3 = #.723 OH + #.67 HCHO + #.396 OLE3_P2 + #.274 ACETO2 + #.176 MEK + #.168 CO + #.135 ACET + #.122 HCHO2 + #.053 HO2 + #.04 CO2 + #.02 KET2 + #.385 XC + #.67 SumRO2	1.36e-17				
H149	OLE3 + NO3 = OLE3_P3 + SumRO2	3.72e-13				
H150	OLE3 + O3P = #.5 RCHO + #.296 OTH2 + #.204 OTH1 + #1.5 XC	1.75e-11				
H151	OLE3_P1 + NO = #.924 NO2 + #.922 HO2 + #.917 HCHO + #.496 MEK + #.37 ACET + #.075 RHNO3 + #.054 KET2 + #.004 LVKS + #.003 ETO2 + #.001 RO2C + #.001 R2NO3 + #.239 XC + #.004 SumRO2		Same k as rxn S001			
H152	OLE3_P1 + NO3 = NO2 + #.997 HO2 + #.992 HCHO + #.524 MEK + #.411 ACET + #.06 KET2 + #.004 LVKS + #.003 ETO2 + #.001 RO2C + #.001 RCHO + #.353 XC + #.004 SumRO2		Same k as rxn S003			
H153	OLE3_P1 + HO2 = #.995 ROOH + #.005 RUOOH + #.995 XC		Same k as rxn S002			
H154	OLE3_P1 + SumRO2 = SumRO2 + #.498 HO2 + #.498 OTH3 + #.496 HCHO + #.262 MEK + #.206 ACET + #.03 KET2 + #.003 LVKS + #.002 ETO2 + #.001 OLEP + #.675 XC + #.002 SumRO2		Same k as rxn S004			
H155	OLE3_P1 + SumRCO3 = SumRCO3 + #.994 HO2 + #.992 HCHO + #.524 MEK + #.411 ACET + #.06 KET2 + #.005 LVKS + #.003 ETO2 + #.001 RO2C + #.001 RCHO + #.349 XC + #.004 SumRO2		Same k as rxn S009			
H156	OLE3_P2 + NO = #.928 NO2 + #.81 MECO3 + #.73 MECHO + #.118 HCHO + #.109 ETCO3 + #.072 RCNO3 + #.071 ETCHO + #.009 R2CO3 + #.009 RCHO + #-0.017 XC + #.928 SumRCO3		Same k as rxn S001			
H157	OLE3_P2 + NO3 = NO2 + #.873 MECO3 + #.783 MECHO + #.127 HCHO + #.117 ETCO3 + #.079 ETCHO + #.011 RCHO + #.01 R2CO3 + #-0.101 XC + SumRCO3		Same k as rxn S003			
H158	OLE3_P2 + HO2 = CROOH + #-1 XC		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H159	OLE3_P2 + SumRO2 = SumRO2 + #.436 MECO3 + #.391 MECHO + #.25 KET2 + #.218 BACL + #.064 HCHO + #.059 ETCO3 + #.04 ETCHO + #.032 MGLY + #.005 RCHO + #.005 R2CO3 + #-0.268 XC + #.5 SumRCO3		Same k as rxn S004			
H160	OLE3_P2 + SumRCO3 = SumRCO3 + #.436 BACL + #.436 MECO3 + #.391 MECHO + #.064 MGLY + #.064 HCHO + #.059 ETCO3 + #.04 ETCHO + #.005 RCHO + #.005 R2CO3 + #.014 XC + #.5 SumRCO3		Same k as rxn S009			
H161	OLE3_P3 + NO = #1.804 NO2 + #.862 HCHO + #.428 MEK + #.397 ACET + #.092 RCNO3 + #.076 ETO2 + #.046 RDNO3 + #.046 RO2C + #.022 HO2 + #.022 KET2 + #.007 RO2XC + #.006 RHNO3 + #.005 RCHO + #.005 zRDNO3 + #.003 ETCHO + #.001 RNNO3 + #.316 XC + #.129 SumRO2		Same k as rxn S001			
H162	OLE3_P3 + NO3 = #1.89 NO2 + #.903 HCHO + #.452 MEK + #.409 ACET + #.098 RCNO3 + #.08 ETO2 + #.051 RO2C + #.025 HO2 + #.024 KET2 + #.008 RO2XC + #.006 RHNO3 + #.005 RCHO + #.005 zRDNO3 + #.003 ETCHO + #.001 RNNO3 + #.383 XC + #.139 SumRO2		Same k as rxn S003			
H163	OLE3_P3 + HO2 = RHNO3 + #-1 XC		Same k as rxn S002			
H164	OLE3_P3 + SumRO2 = SumRO2 + #.503 RHNO3 + #.451 HCHO + #.445 NO2 + #.226 MEK + #.205 ACET + #.049 RCNO3 + #.04 ETO2 + #.025 RO2C + #.012 HO2 + #.012 KET2 + #.004 RO2XC + #.003 RCHO + #.003 zRDNO3 + #.002 ETCHO + #-0.311 XC + #.069 SumRO2		Same k as rxn S004			
H165	OLE3_P3 + SumRCO3 = SumRCO3 + #.903 HCHO + #.89 NO2 + #.452 MEK + #.409 ACET + #.098 RCNO3 + #.08 ETO2 + #.051 RO2C + #.025 HO2 + #.024 KET2 + #.008 RO2XC + #.006 RHNO3 + #.005 RCHO + #.005 zRDNO3 + #.003 ETCHO + #.001 RNNO3 + #.383 XC + #.139 SumRO2		Same k as rxn S009			
H166	OLE4 + OH = #.998 OLE4_P1 + #.001 OH + #.001 HPALD + #.005 XC + #.998 SumRO2	8.66e-11				
H167	OLE4 + O3 = #.849 OH + #.66 MECHO + #.655 ACETO2 + #.282 ACET + #.19 MEO2 + #.147 CO + #.085 CO2 + #.067 ETCHO + #.047 HO2 + #.044 RO2C + #.04 MECHO2 + #.038 MECO3 + #.037 CH4 + #.026 RCHO2 + #.02 MEK + #.008 RCHO + #.006 HCHO + #.005 ETCO3 + #.003 ETO2 + #.003 RO2XC + #.003 zRCNO3 + #.002 KET2 + #.001 ETHAN + #-0.185 XC + #.895 SumRO2 + #.043 SumRCO3	4.16e-16				
H168	OLE4 + NO3 = OLE4_P2 + SumRO2	9.62e-12				
H169	OLE4 + O3P = #.498 KET2 + #.415 OTH1 + #.085 OTH2 + #.003 OTH3 + #.998 XC	5.09e-11				

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H170	OLE4_P1 + NO = #.941 HO2 + #.941 NO2 + #.884 ACET + #.843 MECHO + #.084 ETCHO + #.059 RHNO3 + #.057 MEK + #.009 RCHO + #.004 KET2 + #-0.228 XC		Same k as rxn S001			
H171	OLE4_P1 + NO3 = HO2 + NO2 + #.937 ACET + #.893 MECHO + #.091 ETCHO + #.062 MEK + #.011 RCHO + #.005 KET2 + #-0.187 XC		Same k as rxn S003			
H172	OLE4_P1 + HO2 = ROOH + XC		Same k as rxn S002			
H173	OLE4_P1 + SumRO2 = SumRO2 + #.5 HO2 + #.469 ACET + #.447 MECHO + #.435 OTH4 + #.065 KET2 + #.046 ETCHO + #.031 MEK + #.005 RCHO + #.002 OTH2 + #.346 XC		Same k as rxn S004			
H174	OLE4_P1 + SumRCO3 = SumRCO3 + #.875 HO2 + #.821 ACET + #.781 MECHO + #.129 KET2 + #.08 ETCHO + #.055 MEK + #.009 RCHO + #-0.166 XC		Same k as rxn S009			
H175	OLE4_P2 + NO = #1.881 NO2 + #.882 ACET + #.842 MECHO + #.083 ETCHO + #.059 RDNO3 + #.057 MEK + #.009 RCHO + #.004 KET2 + #.002 RO2C + #.001 HO2 + #.001 RCNO3 + #.001 HCHO + #-0.221 XC + #.002 SumRO2		Same k as rxn S001			
H176	OLE4_P2 + NO3 = #1.999 NO2 + #.936 ACET + #.892 MECHO + #.091 ETCHO + #.063 MEK + #.011 RCHO + #.005 KET2 + #.002 RO2C + #.001 HO2 + #.001 RCNO3 + #.001 HCHO + #-0.19 XC + #.002 SumRO2		Same k as rxn S003			
H177	OLE4_P2 + HO2 = RHNO3 + #-1 XC		Same k as rxn S002			
H178	OLE4_P2 + SumRO2 = SumRO2 + #.5 RHNO3 + #.5 NO2 + #.468 ACET + #.446 MECHO + #.046 ETCHO + #.031 MEK + #.005 RCHO + #.002 KET2 + #.001 RO2C + #.001 HO2 + #-0.588 XC + #.001 SumRO2		Same k as rxn S004			
H179	OLE4_P2 + SumRCO3 = SumRCO3 + #.999 NO2 + #.936 ACET + #.892 MECHO + #.091 ETCHO + #.063 MEK + #.011 RCHO + #.005 KET2 + #.002 RO2C + #.001 HO2 + #.001 RCNO3 + #.001 HCHO + #-0.19 XC + #.002 SumRO2		Same k as rxn S009			
H180	OLEC + OH = OLEC_P1 + SumRO2	6.73e-11				
H181	OLEC + O3 = #.821 RCHO2 + #.279 OH + #.139 OTH1 + #.092 CO + #.053 CO2 + #.031 HO2 + #.025 RCHO + #.01 OTH2 + #.004 OTH3 + #.002 RO2C + #1.829 XC + #.002 SumRO2	4.11e-16				
H182	OLEC + NO3 = OLEC_P2 + SumRO2	9.16e-13				
H183	OLEC + O3P = #.673 OTH2 + #.327 OTH3 + #1.673 XC	2.17e-11				
H184	OLEC_P1 + NO = #.931 NO2 + #.894 HO2 + #.891 RCHO + #.063 RHNO3 + #.03 OH + #.029 OLEP + #.011 RO2C + #.006 R2NO3 + #.003 MACO3 + #.003 HCHO + #.003 ACRO + #.002 LVKS + #.001 HOCCO3 + #.001 RO2XC + #.001 AFG2A + #.001 MECO3 + #.001 CROOH + #.001 zRCNO3 + #.816 XC + #.012 SumRO2 + #.005 SumRCO3		Same k as rxn S001			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H185	OLEC_P1 + NO3 = NO2 + #.958 HO2 + #.954 RCHO + #.034 OH + #.033 OLEP + #.012 RO2C + #.003 MACO3 + #.003 HCHO + #.003 ACRO + #.002 LVKS + #.002 HOCCO3 + #.001 RO2XC + #.001 AFG2A + #.001 MECO3 + #.001 CROOH + #.001 zRCNO3 + #.968 XC + #.013 SumRO2 + #.006 SumRCO3		Same k as rxn S003			
H186	OLEC_P1 + HO2 = #.954 ROOH + #.046 RUOOH + #.954 XC		Same k as rxn S002			
H187	OLEC_P1 + SumRO2 = SumRO2 + #.479 HO2 + #.477 RCHO + #.267 OTH4 + #.207 OTH3 + #.033 OLEP + #.017 OH + #.008 LVKS + #.006 RO2C + #.003 OTH2 + #.002 MACO3 + #.002 HCHO + #.001 ACRO + #.001 HOCCO3 + #.001 RO2XC + #.001 AFG2A + #.001 MECO3 + #.001 CROOH + #.001 zRCNO3 + #.96 XC + #.007 SumRO2 + #.004 SumRCO3		Same k as rxn S004			
H188	OLEC_P1 + SumRCO3 = SumRCO3 + #.498 HO2 + #.495 RCHO + #.415 OTH3 + #.039 OTH4 + #.025 OLEP + #.017 OH + #.014 LVKS + #.009 RO2C + #.006 OTH2 + #.003 HCHO + #.002 ACRO + #.002 MACO3 + #.001 AFG2A + #.001 MECO3 + #.001 RO2XC + #.001 zRCNO3 + #.001 HOCCO3 + #.001 CROOH + #.971 XC + #.01 SumRO2 + #.004 SumRCO3		Same k as rxn S009			
H189	OLEC_P2 + NO = #1.858 NO2 + #.924 RCHO + #.066 RDNO3 + #.01 RCNO3 + #.01 OH + #.878 XC		Same k as rxn S001			
H190	OLEC_P2 + NO3 = #1.989 NO2 + #.989 RCHO + #.011 RCNO3 + #.011 OH + #1.011 XC		Same k as rxn S003			
H191	OLEC_P2 + HO2 = RHNO3 + #-1 XC		Same k as rxn S002			
H192	OLEC_P2 + SumRO2 = SumRO2 + #.495 RCHO + #.495 NO2 + #.262 RHNO3 + #.243 RCNO3 + #.005 OH + #.719 XC		Same k as rxn S004			
H193	OLEC_P2 + SumRCO3 = SumRCO3 + #.519 RCHO + #.519 NO2 + #.481 RCNO3 + #.005 OH + #1.481 XC		Same k as rxn S009			
H194	OLED + OH = #.314 OLED_A1 + #.314 OLED_A2 + #.208 OLED_P1 + #.163 OLED_A3 + #.005 XC + #.208 SumRO2	6.80e-11				
H195	OLED + O3 = #.5 RCHO + #.263 CO + #.25 OLEA1 + #.25 HCHO + #.25 ACRO + #.25 MECHO + #.178 MEO2 + #.175 OH + #.108 CO2 + #.092 HCHO2 + #.083 HO2 + #.037 MECHO2 + #.035 CH4 + #-0.5 XC + #.178 SumRO2	1.33e-17				
H196	OLED + NO3 = #.482 OLED_A4 + #.482 OLED_A5 + #.034 NO2 + #.019 RO2C + #.017 ACRO + #.017 MECHO + #.016 HPALD + #.001 LVKS + #.001 RO2XC + #.001 zRDNO3 + #.001 RCNO3 + #.001 HO2 + #.002 XC + #.02 SumRO2	1.40e-12				
H197	OLED + O3P = #.5 OLEP + #.25 OLEA2 + #.25 LVKS + #.25 XC	4.75e-11				
H198	OLED_A1 = #.5 OLED_A6 + #.5 OLED_P2 + #.5 SumRO2	3.62e-1	7.40e+10	15.53	0.00	

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H199	OLED_A1 + NO = #.946 NO2 + #.945 HO2 + #.885 OLEA1 + #.885 HCHO + #.054 RHNO3 + #.029 RO2C + #.026 ACRO + #.026 GLCHO + #.024 HPALD + #.01 LVKS + #.002 RO2XC + #.002 zRHNO3 + #-0.936 XC + #.031 SumRO2		Same k as rxn S001			
H200	OLED_A2 = #.5 HPALD + #.5 HO2 + #.5 OLED_P3 + #.5 SumRO2	1.72e+0	4.93e+10	14.36	0.00	
H201	OLED_A2 + NO = #.946 NO2 + #.473 OLEA1 + #.473 HO2 + #.473 OLED_P4 + #.054 RHNO3 + #-0.054 XC + #.473 SumRO2		Same k as rxn S001			
H202	OLED_P1 + NO = #.946 HO2 + #.946 NO2 + #.74 ACRO + #.74 MECHO + #.206 OLEP + #.054 RHNO3 + #-0.054 XC		Same k as rxn S001			
H203	OLED_P1 + NO3 = HO2 + NO2 + #.782 ACRO + #.782 MECHO + #.218 OLEP		Same k as rxn S003			
H204	OLED_P1 + HO2 = RUOOH		Same k as rxn S002			
H205	OLED_P1 + SumRO2 = SumRO2 + #.5 HO2 + #.391 ACRO + #.391 MECHO + #.386 OLEP + #.195 LVKS + #.027 OLEA2 + #.2 XC		Same k as rxn S004			
H206	OLED_P1 + SumRCO3 = SumRCO3 + #.5 HO2 + #.391 LVKS + #.391 ACRO + #.391 MECHO + #.164 OLEP + #.055 OLEA2 + #.386 XC		Same k as rxn S009			
H207	OLED_A3 = #.5 HPALD + #.5 HO2 + #.473 RO2C + #.473 MECO3 + #.473 CROOH + #.027 RO2XC + #.027 zRCNO3 + #-0.892 XC + #.5 SumRO2 + #.473 SumRCO3	8.60e-1	2.47e+10	14.36	0.00	
H208	OLED_A3 + NO = #.946 NO2 + #.473 LVKS + #.473 HO2 + #.448 RO2C + #.448 MECO3 + #.448 CROOH + #.054 RHNO3 + #.025 RO2XC + #.025 zRCNO3 + #-0.427 XC + #.473 SumRO2 + #.448 SumRCO3		Same k as rxn S001			
H209	OLED_A4 = #.5 OLED_A7 + #.5 OLED_P5 + #.5 SumRO2	3.62e-1	7.40e+10	15.53	0.00	
H210	OLED_A4 + NO = #1.023 NO2 + #.385 OLED_A8 + #.385 OLED_P6 + #.099 RCNO3 + #.099 HO2 + #.077 OLEA1 + #.077 HCHO + #.054 RDNO3 + #.067 XC + #.385 SumRO2		Same k as rxn S001			
H211	OLED_A5 = HPALD + NO2	1.72e+0	4.93e+10	14.36	0.00	
H212	OLED_A5 + NO = #1.601 NO2 + #.656 OLEA1 + #.291 RCNO3 + #.291 HO2 + #.054 RDNO3 + #.523 XC		Same k as rxn S001			
H213	OLED_A6 = HPALD + OH	8.60e-1	2.47e+10	14.36	0.00	
H214	OLED_A6 + NO = #.946 NO2 + #.898 LVKS + #.898 OH + #.054 RHNO3 + #.049 CROOH + #.049 HO2 + #.839 XC		Same k as rxn S001			
H215	OLED_P2 + NO = #.946 NO2 + #.559 ACRO + #.559 GLCHO + #.559 OH + #.366 RO2C + #.366 OLEP + #.366 HO2 + #.054 RHNO3 + #.021 RO2XC + #.021 zRHNO3 + #-0.075 XC + #.387 SumRO2		Same k as rxn S001			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H216	OLED_P2 + NO3 = NO2 + #.591 ACRO + #.591 GLCHO + #.591 OH + #.387 RO2C + #.387 OLEP + #.387 HO2 + #.022 RO2XC + #.022 zRHNO3 + #-0.022 XC + #.409 SumRO2		Same k as rxn S003			
H217	OLED_P2 + HO2 = RUOOH		Same k as rxn S002			
H218	OLED_P2 + SumRO2 = SumRO2 + #.295 ACRO + #.295 GLCHO + #.295 OH + #.25 HPALD + #.25 RUOOH + #.194 RO2C + #.194 OLEP + #.194 HO2 + #.011 RO2XC + #.011 zRHNO3 + #-0.011 XC + #.205 SumRO2		Same k as rxn S004			
H219	OLED_P2 + SumRCO3 = SumRCO3 + #.5 HPALD + #.295 ACRO + #.295 GLCHO + #.295 OH + #.194 RO2C + #.194 OLEP + #.194 HO2 + #.011 RO2XC + #.011 zRHNO3 + #-0.011 XC + #.205 SumRO2		Same k as rxn S009			
H220	OLED_P3 + NO = #.946 NO2 + #.709 OLED_P7 + #.237 MECHO + #.237 OLEA1 + #.237 OH + #.054 RHNO3 + #-0.528 XC + #.709 SumRO2		Same k as rxn S001			
H221	OLED_P3 + NO3 = NO2 + #.75 OLED_P7 + #.25 MECHO + #.25 OLEA1 + #.25 OH + #-0.5 XC + #.75 SumRO2		Same k as rxn S003			
H222	OLED_P3 + HO2 = RUOOH		Same k as rxn S002			
H223	OLED_P3 + SumRO2 = SumRO2 + #.375 OLED_P7 + #.25 HPALD + #.25 RUOOH + #.125 MECHO + #.125 OLEA1 + #.125 OH + #-0.25 XC + #.375 SumRO2		Same k as rxn S004			
H224	OLED_P3 + SumRCO3 = SumRCO3 + #.5 HPALD + #.375 OLED_P7 + #.125 MECHO + #.125 OLEA1 + #.125 OH + #-0.25 XC + #.375 SumRO2		Same k as rxn S009			
H225	OLED_P4 + NO = #.946 MECHO + #.946 OLEA1 + #.946 HO2 + #.946 NO2 + #.054 RHNO3 + #-1.946 XC		Same k as rxn S001			
H226	OLED_P4 + NO3 = MECHO + OLEA1 + HO2 + NO2 + #-2 XC		Same k as rxn S003			
H227	OLED_P4 + HO2 = RUOOH		Same k as rxn S002			
H228	OLED_P4 + SumRO2 = SumRO2 + #.5 MECHO + #.5 OLEA1 + #.5 HO2 + #.25 LVKS + #.25 OLEP + #-0.75 XC		Same k as rxn S004			
H229	OLED_P4 + SumRCO3 = SumRCO3 + #.5 LVKS + #.5 MECHO + #.5 OLEA1 + #.5 HO2 + #-0.5 XC		Same k as rxn S009			
H230	OLED_A7 = RCNO3 + OH + #2 XC	8.60e-1	2.47e+10	14.36	0.00	
H231	OLED_A7 + NO = #.946 RCNO3 + #.946 OH + #.946 NO2 + #.054 RDNO3 + #1.838 XC		Same k as rxn S001			
H232	OLED_P5 + NO = #.946 NO2 + #.559 ACRO + #.559 RCNO3 + #.559 OH + #.366 RO2C + #.366 R2NO3 + #.366 HO2 + #.054 RDNO3 + #.021 RO2XC + #.021 zRDNO3 + #-1.732 XC + #.387 SumRO2		Same k as rxn S001			
H233	OLED_P5 + NO3 = NO2 + #.591 ACRO + #.591 RCNO3 + #.591 OH + #.387 RO2C + #.387 R2NO3 + #.387 HO2 + #.022 RO2XC + #.022 zRDNO3 + #-1.774 XC + #.409 SumRO2		Same k as rxn S003			
H234	OLED_P5 + HO2 = RHNO3 + #-1 XC		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H235	OLED_P5 + SumRO2 = SumRO2 + #.545 RCNO3 + #.295 ACRO + #.295 OH + #.25 RHNO3 + #.194 RO2C + #.194 R2NO3 + #.194 HO2 + #.011 RO2XC + #.011 zRDNO3 + #-0.638 XC + #.205 SumRO2		Same k as rxn S004			
H236	OLED_P5 + SumRCO3 = SumRCO3 + #.795 RCNO3 + #.295 ACRO + #.295 OH + #.194 RO2C + #.194 R2NO3 + #.194 HO2 + #.011 RO2XC + #.011 zRDNO3 + #.112 XC + #.205 SumRO2		Same k as rxn S009			
H237	OLED_A8 = #.5 RCNO3 + #.5 HO2 + #.473 RO2C + #.473 CROOH + #.473 R2NCO3 + #.027 RO2XC + #.027 zRNNO3 + #-0.081 XC + #.027 XN + #.5 SumRO2 + #.473 SumRCO3	8.60e-1	2.47e+10	14.36	0.00	
H238	OLED_A8 + NO = #.971 NO2 + #.473 RCNO3 + #.473 HO2 + #.448 RO2C + #.448 CROOH + #.448 R2NCO3 + #.054 RDNO3 + #.025 RO2XC + #.025 zRNNO3 + #-0.129 XC + #.473 SumRO2 + #.448 SumRCO3		Same k as rxn S001			
H239	OLED_P6 + NO = #.946 ACRO + #.946 RCNO3 + #.946 HO2 + #.946 NO2 + #.054 RDNO3 + #-1 XC		Same k as rxn S001			
H240	OLED_P6 + NO3 = ACRO + RCNO3 + HO2 + NO2 + #-1 XC		Same k as rxn S003			
H241	OLED_P6 + HO2 = RHNO3 + #-1 XC		Same k as rxn S002			
H242	OLED_P6 + SumRO2 = SumRO2 + #.75 RCNO3 + #.5 ACRO + #.5 HO2 + #.25 RHNO3 + #-0.25 XC		Same k as rxn S004			
H243	OLED_P6 + SumRCO3 = SumRCO3 + RCNO3 + #.5 ACRO + #.5 HO2 + #.5 XC		Same k as rxn S009			
H244	OLED_P7 + NO = #.946 OLEP + #.946 HO2 + #.946 NO2 + #.054 RHNO3 + #-0.054 XC		Same k as rxn S001			
H245	OLED_P7 + NO3 = OLEP + HO2 + NO2		Same k as rxn S003			
H246	OLED_P7 + HO2 = RUOOH		Same k as rxn S002			
H247	OLED_P7 + SumRO2 = SumRO2 + OLEP + #.5 HO2		Same k as rxn S004			
H248	OLED_P7 + SumRCO3 = SumRCO3 + OLEP + #.5 HO2		Same k as rxn S009			
H249	TERP + OH = #.774 TERP_P1 + #.172 OH + #.074 RO2C + #.07 OLEP + #.057 OTHN + #.03 HO2 + #.025 RO2XC + #.023 LVKS + #.022 RUOOH + #.02 HPALD + #.015 zRNNO3 + #.007 zRHNO3 + #.006 CROOH + #.006 GLCHO + #.006 OLEA1 + #.004 OLEA2 + #.003 ACET + #.001 MEO2 + #.001 HCHO + #.629 XC + #.874 SumRO2	1.02e-10				
H250	TERP + O3 = #.68 OH + #.399 TERP_P2 + #.197 RCHO2 + #.169 OTH3 + #.135 OLEA2 + #.107 CO + #.107 ACETO2 + #.076 HCHO + #.062 OLEP + #.062 HCHO2 + #.047 ACET + #.036 HO2 + #.033 CO2 + #.031 KET2 + #.029 RO2C + #.021 R2CO3 + #.013 MVK + #.009 RO2XC + #.008 zRCNO3 + #.002 HPALD + #.001 BACL + #.001 OLED + #.001 LVKS + #.001 OLEA1 + #2.696 XC + #.544 SumRO2 + #.021 SumRCO3	1.87e-16				

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H251	TERP + NO3 = #.801 TERP_P3 + #.109 TERP_A1 + #.065 OH + #.049 RNNO3 + #.037 RO2C + #.012 RO2XC + #.021 NO2 + #.011 zRNNO3 + #.01 HPALD + #.01 RCNO3 + #.009 R2NO3 + #.003 HO2 + #.002 LVKS + #.001 RHNO3 + #.001 OTHN + #.122 XC + #.85 SumRO2	7.88e-12				
H252	TERP + O3P = #.36 OTH3 + #.262 OLEP + #.227 OTH4 + #.109 RCHO + #.024 OTH2 + #.014 OLEA2 + #.003 LVKS + #5.752 XC	5.67e-11				
H253	TERP_P1 + NO = #.848 NO2 + #.769 HO2 + #.554 RCHO + #.173 RO2C + #.161 OTH3 + #.151 RHNO3 + #.145 HCHO + #.051 OLEA2 + #.037 ACET + #.035 RO2XC + #.023 R2CO3 + #.018 OH + #.017 OTHN + #.016 zRCNO3 + #.014 KET2 + #.014 HOCCO3 + #.007 zRNNO3 + #.003 OLEP + #.001 R2NO3 + #.001 OLEA1 + #.001 zR1NO3 + #5.201 XC + #.208 SumRO2 + #.037 SumRCO3	Same k as rxn S001				
H254	TERP_P1 + NO3 = NO2 + #.908 HO2 + #.648 RCHO + #.203 RO2C + #.189 OTH3 + #.171 HCHO + #.066 OLEA2 + #.044 ACET + #.041 RO2XC + #.027 R2CO3 + #.021 OH + #.02 OTHN + #.019 zRCNO3 + #.017 KET2 + #.016 HOCCO3 + #.008 zRNNO3 + #.004 OLEP + #.001 OLEA1 + #.001 zR1NO3 + #5.414 XC + #.244 SumRO2 + #.043 SumRCO3	Same k as rxn S003				
H255	TERP_P1 + HO2 = #.927 ROOH + #.073 RUOOH + #5.927 XC	Same k as rxn S002				
H256	TERP_P1 + SumRO2 = SumRO2 + #.46 OTH4 + #.454 HO2 + #.324 RCHO + #.101 RO2C + #.098 OTH3 + #.085 HCHO + #.038 OLEP + #.033 OLEA2 + #.022 ACET + #.02 RO2XC + #.013 R2CO3 + #.011 OH + #.01 OTHN + #.009 zRCNO3 + #.008 KET2 + #.008 HOCCO3 + #.004 zRNNO3 + #.001 OLEA1 + #5.679 XC + #.121 SumRO2 + #.021 SumRCO3	Same k as rxn S004				
H257	TERP_P1 + SumRCO3 = SumRCO3 + #.818 HO2 + #.567 RCHO + #.202 RO2C + #.197 OTH3 + #.171 HCHO + #.073 OTH4 + #.058 OLEA2 + #.044 ACET + #.04 RO2XC + #.027 R2CO3 + #.021 OH + #.02 OTHN + #.019 zRCNO3 + #.017 KET2 + #.016 HOCCO3 + #.012 OLEP + #.008 zRNNO3 + #.001 OLEA1 + #.001 zR1NO3 + #5.414 XC + #.242 SumRO2 + #.043 SumRCO3	Same k as rxn S009				
H258	TERP_P2 + NO = #.751 NO2 + #.565 OH + #.547 BACL + #.248 RCNO3 + #.088 R2CO3 + #.078 RCHO + #.059 MECO3 + #.05 RO2C + #.032 HCHO + #.024 HO2 + #.017 ACET + #.016 RO2XC + #.012 OTH1 + #.012 zRCNO3 + #.005 OLEP + #.004 OLEA1 + #.002 MVK + #.002 MEO2 + #.001 R2NO3 + #.001 AFG3 + #.001 CO2 + #.001 CO + #6.148 XC + #.068 SumRO2 + #.147 SumRCO3	Same k as rxn S001				

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H259	TERP_P2 + NO3 = NO2 + #.755 OH + #.733 BACL + #.115 R2CO3 + #.104 RCHO + #.079 MECO3 + #.065 RO2C + #.041 HCHO + #.031 HO2 + #.022 ACET + #.021 RO2XC + #.016 OTH1 + #.016 zRCNO3 + #.006 OLEP + #.005 OLEA1 + #.002 MVK + #.002 MEO2 + #.001 AFG3 + #.001 CO2 + #.001 CO + #.001 zR2NO3 + #5.865 XC + #.088 SumRO2 + #.194 SumRCO3		Same k as rxn S003			
H260	TERP_P2 + HO2 = #.991 CROOH + #.008 RUOOH + #.002 HPALD + #4.995 XC		Same k as rxn S002			
H261	TERP_P2 + SumRO2 = SumRO2 + #.445 RCHO + #.4 BACL + #.378 OH + #.058 OTH3 + #.058 R2CO3 + #.039 MECO3 + #.033 RO2C + #.021 HCHO + #.016 HO2 + #.011 ACET + #.01 RO2XC + #.008 OTH1 + #.008 zRCNO3 + #.007 OLEP + #.007 OTH4 + #.003 MGLY + #.003 OLEA1 + #.001 OLEA2 + #.001 MVK + #.001 MEO2 + #.001 LVKS + #.001 AFG3 + #.001 CO2 + #.001 CO + #5.925 XC + #.044 SumRO2 + #.097 SumRCO3		Same k as rxn S004			
H262	TERP_P2 + SumRCO3 = SumRCO3 + #.799 BACL + #.744 OH + #.083 R2CO3 + #.078 RCHO + #.053 RO2C + #.041 MECO3 + #.022 ACET + #.022 HCHO + #.018 RO2XC + #.016 HO2 + #.014 zRCNO3 + #.008 OTH1 + #.006 MGLY + #.003 OLEP + #.003 OLEA2 + #.002 OLEA1 + #.002 MVK + #.002 MEO2 + #.001 CO2 + #.001 AFG3 + #.001 CO + #5.931 XC + #.073 SumRO2 + #.124 SumRCO3		Same k as rxn S009			
H263	TERP_P3 + NO = #1.296 NO2 + #.451 RCHO + #.242 TERP_P4 + #.231 RDNO3 + #.073 OLEA2 + #.003 OLEP + #.003 ACET + #4.001 XC + #.242 SumRO2		Same k as rxn S001			
H264	TERP_P3 + NO3 = #1.685 NO2 + #.586 RCHO + #.315 TERP_P4 + #.095 OLEA2 + #.003 OLEP + #.003 ACET + #.001 OH + #4.007 XC + #.315 SumRO2		Same k as rxn S003			
H265	TERP_P3 + HO2 = RHNO3 + #4 XC		Same k as rxn S002			
H266	TERP_P3 + SumRO2 = SumRO2 + #.5 RHNO3 + #.342 NO2 + #.293 RCHO + #.158 TERP_P4 + #.048 OLEA2 + #.002 OLEP + #.002 ACET + #3.992 XC + #.158 SumRO2		Same k as rxn S004			
H267	TERP_P3 + SumRCO3 = SumRCO3 + #.685 NO2 + #.586 RCHO + #.315 TERP_P4 + #.095 OLEA2 + #.003 OLEP + #.003 ACET + #.001 OH + #4.007 XC + #.315 SumRO2		Same k as rxn S009			
H268	TERP_A1 = #.451 RO2C + #.375 RNNO3 + #.359 OH + #.351 NO2 + #.275 OTHN + #.185 RO2XC + #.181 HO2 + #.147 zRNNO3 + #.145 RHNO3 + #.04 OLEA1 + #.037 CROOH + #.021 RCNO3 + #.003 HCHO + #.159 XC + #.108 XN + #.636 SumRO2	1.77e+1	9.50e+10	13.36	0.00	
H269	TERP_A1 + NO = #1.538 NO2 + #.769 OLEA2 + #.769 ACET + #.231 RDNO3 + #2.462 XC		Same k as rxn S001			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H270	TERP_P4 + NO = #.772 NO2 + #.654 RCNO3 + #.569 OH + #.301 RO2C + #.231 RDNO3 + #.127 ACET + #.061 R2CO3 + #.058 RO2XC + #.046 HO2 + #.044 zRNNO3 + #.037 HOCCO3 + #.01 zRDNO3 + #.002 HCHO + #.002 zR1NO3 + #.002 MVK + #.001 CO2 + #.001 BACL + #5.489 XC + #.102 XN + #.359 SumRO2 + #.098 SumRCO3		Same k as rxn S001			
H271	TERP_P4 + NO3 = #1.004 NO2 + #.85 RCNO3 + #.739 OH + #.391 RO2C + #.165 ACET + #.079 R2CO3 + #.076 RO2XC + #.06 HO2 + #.057 zRNNO3 + #.049 HOCCO3 + #.013 zRDNO3 + #.003 HCHO + #.002 zR1NO3 + #.002 MVK + #.001 CO2 + #.001 BACL + #5.946 XC + #.133 XN + #.467 SumRO2 + #.128 SumRCO3		Same k as rxn S003			
H272	TERP_P4 + HO2 = RCNO3 + #7 XC		Same k as rxn S002			
H273	TERP_P4 + SumRO2 = SumRO2 + #.925 RCNO3 + #.37 OH + #.195 RO2C + #.083 ACET + #.039 R2CO3 + #.038 RO2XC + #.03 HO2 + #.028 zRNNO3 + #.024 HOCCO3 + #.007 zRDNO3 + #.068 NO2 + #.001 HCHO + #.001 zR1NO3 + #.001 MVK + #.001 CO2 + #.001 BACL + #6.474 XC + #.233 SumRO2 + #.063 SumRCO3		Same k as rxn S004			
H274	TERP_P4 + SumRCO3 = SumRCO3 + #.917 RCNO3 + #.416 OH + #.245 RO2C + #.137 ACET + #.044 RO2XC + #.039 R2CO3 + #.031 HO2 + #.028 zRNNO3 + #.025 HOCCO3 + #.013 zRDNO3 + #.002 MVK + #.07 NO2 + #.001 HCHO + #.001 zR1NO3 + #.001 CO2 + #.001 BACL + #6.294 XC + #.289 SumRO2 + #.064 SumRCO3		Same k as rxn S009			
H297	AMINS + OH = #.81 AMINS_P1 + #.19 HO2 + #.177 IMINE + #.013 RCHO + #.001 HCHO + #-0.027 XC + #.013 XN + #.81 SumRO2	3.57e-11				
H298	AMINS + O3 = AMINS_P2 + OH + SumRO2	3.11e-18				
H299	AMINS_P1 + NO = #1.001 NO2 + #.999 AMINS + #.841 HO2 + #.159 MEO2 + #.072 HCHO + #.004 RO2C + #.001 RCHO + #-0.233 XC + #.163 SumRO2		Same k as rxn S001			
H300	AMINS_P1 + NO3 = #1.001 NO2 + #.999 AMINS + #.841 HO2 + #.159 MEO2 + #.072 HCHO + #.004 RO2C + #.001 RCHO + #-0.233 XC + #.163 SumRO2		Same k as rxn S003			
H301	AMINS_P1 + HO2 = ROOH + #-2 XC + XN		Same k as rxn S002			
H302	AMINS_P1 + SumRO2 = SumRO2 + #.999 AMINS + #.42 HO2 + #.08 MEO2 + #.036 HCHO + #.002 RO2C + #.001 RCHO + #-0.118 XC + #.001 XN + #.082 SumRO2		Same k as rxn S004			
H303	AMINS_P1 + SumRCO3 = SumRCO3 + #.998 AMINS + #.42 HO2 + #.08 MEO2 + #.036 HCHO + #.002 RCHO + #.002 RO2C + #-0.12 XC + #.002 XN + #.082 SumRO2		Same k as rxn S009			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H304	AMINS_P2 + NO = AMINS + NO2 + #.813 HO2 + #.187 MEO2 + #.088 HCHO + #-0.275 XC + #.187 SumRO2		Same k as rxn S001			
H305	AMINS_P2 + NO3 = AMINS + NO2 + #.813 HO2 + #.187 MEO2 + #.088 HCHO + #-0.275 XC + #.187 SumRO2		Same k as rxn S003			
H306	AMINS_P2 + HO2 = ROOH + #-2 XC + XN		Same k as rxn S002			
H307	AMINS_P2 + SumRO2 = SumRO2 + AMINS + #.406 HO2 + #.094 MEO2 + #.044 HCHO + #-0.138 XC + #.094 SumRO2		Same k as rxn S004			
H308	AMINS_P2 + SumRCO3 = SumRCO3 + AMINS + #.406 HO2 + #.094 MEO2 + #.044 HCHO + #-0.138 XC + #.094 SumRO2		Same k as rxn S009			
H315	ARO1 + OH = #.774 ARO1_P1 + #.135 HO2 + #.103 XYNL + #.089 OH + #.087 AFG4 + #.028 BALD + #.008 RO2C + #.005 CROOH + #.002 RO2XC + #.002 zRHNO3 + #.001 AFG3 + #.001 HCHO + #.001 MECHO + #.001 ARO2 + #.35 XC + #.784 SumRO2	8.15e-12				
H316	ARO1_P1 + NO = #.773 NO2 + #.487 HO2 + #.214 ARO1 + #.18 BUDAL + #.178 MGLY + #.178 GLY + #.177 AFG2A + #.175 ARO1_P2 + #.13 RANO3 + #.093 RPNO3 + #.09 MEO2 + #.066 MECHO + #.06 ACET + #.059 BALD + #.015 ETO2 + #.014 CO + #.005 OH + #.005 OTHN + #.005 CO2 + #.004 RNNO3 + #.003 AFG1 + #.002 HCHO + #.001 CROOH + #.001 MACO3 + #.001 RCHO + #.751 XC + #.28 SumRO2 + #.001 SumRCO3		Same k as rxn S001			
H317	ARO1_P1 + NO3 = NO2 + #.622 HO2 + #.282 ARO1 + #.232 ARO1_P2 + #.228 BUDAL + #.226 GLY + #.225 MGLY + #.224 AFG2A + #.119 MEO2 + #.086 MECHO + #.08 ACET + #.079 BALD + #.019 ETO2 + #.017 CO + #.006 OH + #.006 OTHN + #.006 CO2 + #.004 AFG1 + #.003 HCHO + #.002 CROOH + #.001 MACO3 + #.001 RCHO + #.653 XC + #.37 SumRO2 + #.001 SumRCO3		Same k as rxn S003			
H318	ARO1_P1 + HO2 = #.533 ROOH + #.435 RAOOH + #.032 OTHN + #3.439 XC		Same k as rxn S002			
H319	ARO1_P1 + SumRO2 = SumRO2 + #.339 ARO1 + #.311 HO2 + #.229 OLEP + #.116 ARO1_P2 + #.114 BUDAL + #.113 GLY + #.113 MGLY + #.112 AFG2A + #.068 ARO2 + #.06 MEO2 + #.043 MECHO + #.04 ACET + #.039 BALD + #.01 ETO2 + #.008 CO + #.008 OTHN + #.003 OH + #.003 CO2 + #.002 AFG1 + #.001 HCHO + #.001 RCHO + #.001 CROOH + #.001 MACO3 + #1.225 XC + #.186 SumRO2 + #.001 SumRCO3		Same k as rxn S004			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H320	ARO1_P1 + SumRCO3 = SumRCO3 + #.442 HO2 + #.366 ARO1 + #.23 OLEP + #.14 BALD + #.132 RO2C + #.12 MEO2 + #.114 BUDAL + #.114 GLY + #.113 MGLY + #.113 AFG2A + #.109 ACET + #.043 MECHO + #.025 RO2XC + #.023 zRANO3 + #.01 ETO2 + #.008 CO + #.004 OTHN + #.003 OH + #.003 CO2 + #.002 AFG1 + #.002 RCHO + #.001 MACO3 + #.001 zR1NO3 + #.001 HCHO + #.001 TBUO + #.001 ARO2 + #.001 CROOH + #1.146 XC + #.287 SumRO2 + #.001 SumRCO3		Same k as rxn S009			
H321	ARO1_P2 + NO = #.853 NO2 + #.834 HO2 + #.589 BALD + #.245 ACET + #.136 RANO3 + #.011 R1NO3 + #.01 TBUO + #.008 ARO1 + #.008 MEO2 + #-0.121 XC + #.008 SumRO2		Same k as rxn S001			
H322	ARO1_P2 + NO3 = NO2 + #.979 HO2 + #.723 BALD + #.256 ACET + #.011 TBUO + #.01 ARO1 + #.01 MEO2 + #.027 XC + #.01 SumRO2		Same k as rxn S003			
H323	ARO1_P2 + HO2 = ROOH + #2 XC		Same k as rxn S002			
H324	ARO1_P2 + SumRO2 = SumRO2 + #.542 BALD + #.489 HO2 + #.192 ACET + #.181 ARO2 + #.064 OTH3 + #.01 ARO1 + #.006 OTH1 + #.006 TBUO + #.005 MEO2 + #-0.392 XC + #.005 SumRO2		Same k as rxn S004			
H325	ARO1_P2 + SumRCO3 = SumRCO3 + #.723 BALD + #.489 HO2 + #.256 ACET + #.011 TBUO + #.01 ARO1 + #.01 MEO2 + #.027 XC + #.01 SumRO2		Same k as rxn S009			
H326	ARO2 + OH = #.786 ARO2_P1 + #.126 OH + #.126 AFG4 + #.088 HO2 + #.088 XYNL + #.34 XC + #.786 SumRO2	1.83e-11				
H327	ARO2_P1 + NO = #.785 NO2 + #.776 HO2 + #.496 MGLY + #.42 AFG2A + #.177 RPNO3 + #.116 GLY + #.1 AFG1 + #.072 AFG3 + #.054 BACL + #.049 ARO1 + #.044 BUDAL + #.038 RANO3 + #.037 ARO2 + #.031 BALD + #.03 AFG2B + #.008 HCHO + #.008 RO2C + #.007 MEO2 + #.002 RO2XC + #.002 zRANO3 + #.002 MECHO + #.93 XC + #.017 SumRO2		Same k as rxn S001			
H328	ARO2_P1 + NO3 = NO2 + #.987 HO2 + #.627 MGLY + #.531 AFG2A + #.146 GLY + #.126 AFG1 + #.092 AFG3 + #.069 BACL + #.065 ARO1 + #.056 BUDAL + #.049 ARO2 + #.04 BALD + #.038 AFG2B + #.01 HCHO + #.01 RO2C + #.009 MEO2 + #.003 RO2XC + #.003 zRANO3 + #.003 MECHO + #.001 ETO2 + #.905 XC + #.023 SumRO2		Same k as rxn S003			
H329	ARO2_P1 + HO2 = #.842 RAOOH + #.158 ROOH + #2.474 XC		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H330	ARO2_P1 + SumRO2 = SumRO2 + #.494 HO2 + #.421 OLEP + #.314 MGLY + #.265 AFG2A + #.077 ARO2 + #.073 GLY + #.063 AFG1 + #.049 ARO1 + #.046 AFG3 + #.034 BACL + #.028 BALD + #.028 BUDAL + #.019 AFG2B + #.005 HCHO + #.005 RO2C + #.005 MEO2 + #.003 RCHO + #.001 RO2XC + #.001 zRANO3 + #.001 MECHO + #2.167 XC + #.011 SumRO2		Same k as rxn S004			
H331	ARO2_P1 + SumRCO3 = SumRCO3 + #.553 HO2 + #.362 OLEP + #.334 MGLY + #.279 AFG2A + #.112 GLY + #.092 AFG3 + #.066 ARO1 + #.063 AFG1 + #.049 ARO2 + #.036 BALD + #.035 BACL + #.028 BUDAL + #.019 AFG2B + #.009 MEO2 + #.005 RCHO + #.005 HCHO + #.005 RO2C + #.001 RO2XC + #.001 zRANO3 + #.001 MECHO + #2.005 XC + #.015 SumRO2		Same k as rxn S009			
H347	OTH1 + OH = OTH1_P1 + SumRO2	3.33e-13				
H348	OTH1_P1 + NO = #46.992 NROG + #.983 NO2 + #.669 HO2 + #.262 HCHO + #.198 R2CO3 + #.11 OTH1_P2 + #.045 MECHO + #.021 AACID + #.018 RCHO + #.017 RCNO3 + #.014 CO + #.01 MGLY + #.007 MECO3 + #1.391 XC + #.11 SumRO2 + #.205 SumRCO3		Same k as rxn S001			
H349	OTH1_P1 + NO3 = #47.01 NROG + NO2 + #.67 HO2 + #.275 HCHO + #.206 R2CO3 + #.117 OTH1_P2 + #.047 MECHO + #.022 AACID + #.018 RCHO + #.015 CO + #.011 MGLY + #.007 MECO3 + #1.367 XC + #.117 SumRO2 + #.213 SumRCO3		Same k as rxn S003			
H350	OTH1_P1 + HO2 = CROOH + #-2 XC		Same k as rxn S002			
H351	OTH1_P1 + SumRO2 = SumRO2 + #35.589 NROG + #.335 HO2 + #.185 OTH2 + #.137 HCHO + #.103 R2CO3 + #.065 OTH3 + #.058 OTH1_P2 + #.048 MGLY + #.043 RCHO + #.024 MECHO + #.012 BACL + #.011 AACID + #.007 CO + #.004 MECO3 + #1.058 XC + #.058 SumRO2 + #.107 SumRCO3		Same k as rxn S004			
H352	OTH1_P1 + SumRCO3 = SumRCO3 + #47.672 NROG + #.335 HO2 + #.137 HCHO + #.103 R2CO3 + #.091 MGLY + #.076 RCHO + #.058 OTH1_P2 + #.024 MECHO + #.023 BACL + #.011 AACID + #.007 CO + #.004 MECO3 + #1.568 XC + #.058 SumRO2 + #.107 SumRCO3		Same k as rxn S009			
H353	OTH1_P2 + NO = #11.148 NROG + #.965 NO2 + #.815 HO2 + #.809 ACET + #.809 CO2 + #.127 MEO2 + #.035 RCNO3 + #.024 R2CO3 + #.021 HCHO + #.003 RCHO + #.003 MGLY + #.003 MECHO + #.412 XC + #.127 SumRO2 + #.024 SumRCO3		Same k as rxn S001			
H354	OTH1_P2 + NO3 = #11.547 NROG + NO2 + #.844 HO2 + #.838 ACET + #.838 CO2 + #.131 MEO2 + #.024 R2CO3 + #.021 HCHO + #.003 RCHO + #.003 MECHO + #.003 MGLY + #.397 XC + #.131 SumRO2 + #.024 SumRCO3		Same k as rxn S003			
H355	OTH1_P2 + HO2 = CROOH + #-1 XC		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H356	OTH1_P2 + SumRO2 = SumRO2 + #5.774 NROG + #.484 OTH1 + #.422 HO2 + #.419 ACET + #.419 CO2 + #.066 MEO2 + #.012 R2CO3 + #.011 HCHO + #.007 MGLY + #.006 OTH2 + #.003 RCHO + #.002 OTH3 + #.002 MECHO + #.001 BACL + #.692 XC + #.066 SumRO2 + #.012 SumRCO3		Same k as rxn S004			
H357	OTH1_P2 + SumRCO3 = SumRCO3 + #11.547 NROG + #.841 HO2 + #.838 ACET + #.838 CO2 + #.131 MEO2 + #.013 MGLY + #.012 R2CO3 + #.011 HCHO + #.004 RCHO + #.002 BACL + #.002 MECHO + #.403 XC + #.131 SumRO2 + #.012 SumRCO3		Same k as rxn S009			
H358	OTH2 + OH = OTH2_P1 + SumRO2	2.80e-12				
H359	OTH2_P1 + NO = #.986 NO2 + #.98 OTH1 + #.938 HO2 + #.051 RO2C + #.048 HCHO + #.047 MEO2 + #.014 R1NO3 + #.004 OTH3 + #.002 RO2XC + #.002 zR1NO3 + #-0.131 XC + #.1 SumRO2		Same k as rxn S001			
H360	OTH2_P1 + NO3 = NO2 + #.993 OTH1 + #.948 HO2 + #.054 RO2C + #.051 HCHO + #.05 MEO2 + #.005 OTH3 + #.002 RO2XC + #.002 zR1NO3 + #-0.11 XC + #.106 SumRO2		Same k as rxn S003			
H361	OTH2_P1 + HO2 = ROOH + #-1 XC		Same k as rxn S002			
H362	OTH2_P1 + SumRO2 = SumRO2 + #.735 OTH1 + #.474 HO2 + #.192 OTH4 + #.061 OTH3 + #.027 RO2C + #.026 HCHO + #.025 MEO2 + #.012 RCHO + #.001 RO2XC + #.001 zR1NO3 + #-0.321 XC + #.053 SumRO2		Same k as rxn S004			
H363	OTH2_P1 + SumRCO3 = SumRCO3 + #.973 OTH1 + #.474 HO2 + #.027 RO2C + #.026 HCHO + #.025 MEO2 + #.023 RCHO + #.002 OTH3 + #.001 RO2XC + #.001 zR1NO3 + #-0.075 XC + #.053 SumRO2		Same k as rxn S009			
H364	OTH3 + OH = #.666 HO2 + #.594 ACET + #.334 OTH3_P1 + #.025 MEK + #.025 RCHO + #.022 ETCHO + #.282 XC + #.334 SumRO2	4.99e-12				
H365	OTH3_P1 + NO = #8.06 NROG + #.938 NO2 + #.513 HO2 + #.253 AACID + #.25 KET2 + #.215 ETCO3 + #.11 HCHO + #.108 MECHO + #.106 OTH1 + #.103 RO2C + #.087 MEO2 + #.073 ETO2 + #.059 RCNO3 + #.051 ACET + #.051 RCHO + #.039 OTH3 + #.023 R2CO3 + #.018 ETCHO + #.018 CO2 + #.016 CO + #.015 OH + #.006 OTH2 + #.006 MECO3 + #.005 MGLY + #.005 RO2XC + #.005 zRCNO3 + #.004 RCOOH + #.003 RHNO3 + #.001 ETHEO2 + #.783 XC + #.269 SumRO2 + #.244 SumRCO3		Same k as rxn S001			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H366	OTH3_P1 + NO3 = #8.623 NROG + NO2 + #.545 HO2 + #.27 AACID + #.268 KET2 + #.228 ETCO3 + #.113 HCHO + #.112 OTH1 + #.112 RO2C + #.11 MECHO + #.092 MEO2 + #.077 ETO2 + #.055 ACET + #.054 RCHO + #.045 OTH3 + #.025 R2CO3 + #.019 ETCHO + #.019 OH + #.019 CO2 + #.017 CO + #.007 OTH2 + #.006 MECO3 + #.006 MGLY + #.006 RO2XC + #.005 zRCNO3 + #.004 RCOOH + #.001 ETHEO2 + #.712 XC + #.288 SumRO2 + #.259 SumRCO3		Same k as rxn S003			
H367	OTH3_P1 + HO2 = #.874 CROOH + #.126 ROOH + #.126 XC		Same k as rxn S002			
H368	OTH3_P1 + SumRO2 = SumRO2 + #4.311 NROG + #.273 HO2 + #.213 KET2 + #.202 OTH4 + #.186 OTH1 + #.135 AACID + #.114 ETCO3 + #.056 HCHO + #.056 RO2C + #.055 RCHO + #.055 MECHO + #.049 OTH3 + #.046 MEO2 + #.039 ETO2 + #.03 OTH2 + #.028 ACET + #.013 R2CO3 + #.01 ETCHO + #.01 OH + #.009 CO2 + #.009 MGLY + #.008 CO + #.003 MECO3 + #.003 RO2XC + #.003 zRCNO3 + #.002 RCOOH + #.001 BACL + #.001 ETHEO2 + #.937 XC + #.145 SumRO2 + #.13 SumRCO3		Same k as rxn S004			
H369	OTH3_P1 + SumRCO3 = SumRCO3 + #4.536 NROG + #.291 KET2 + #.287 HO2 + #.262 OTH1 + #.138 AACID + #.114 ETCO3 + #.092 MEO2 + #.084 RCHO + #.065 HCHO + #.061 RO2C + #.055 MECHO + #.052 ACET + #.045 OTH2 + #.039 ETO2 + #.023 OTH3 + #.019 CO2 + #.016 MGLY + #.013 R2CO3 + #.011 CO + #.01 ETCHO + #.01 OH + #.003 MECO3 + #.003 RO2XC + #.003 zRCNO3 + #.002 RCOOH + #.001 BACL + #.001 ETHEO2 + #.903 XC + #.196 SumRO2 + #.13 SumRCO3		Same k as rxn S009			
H370	OTH4 + OH = #.652 HO2 + #.348 OTH4_P1 + #.28 GLCHO + #.211 KET2 + #.127 RCHO + #.052 HCHO + #.017 MECHO + #-0.297 XC + #.348 SumRO2	2.36e-11				
H371	OTH4_P1 + NO = #.893 NO2 + #.487 OTH3 + #.449 HO2 + #.358 OTH4_P2 + #.339 HCHO + #.119 OTH1 + #.092 RHNO3 + #.088 NROG + #.085 OTH4 + #.056 MEO2 + #.055 MECHO + #.037 RCHO + #.02 OTH2 + #.014 KET2 + #.014 OH + #.009 ETO2 + #.009 GLCHO + #.009 RCNO3 + #.007 ACET + #.006 R2NO3 + #.005 ETHEO2 + #.002 R2CO3 + #.001 RCOOH + #.001 MECO3 + #.001 AACID + #.433 XC + #.428 SumRO2 + #.003 SumRCO3		Same k as rxn S001			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H372	OTH4_P1 + NO3 = NO2 + #.554 OTH3 + #.504 HO2 + #.404 OTH4_P2 + #.383 HCHO + #.127 OTH1 + #.102 OTH4 + #.097 NROG + #.06 MEO2 + #.058 MECHO + #.042 RCHO + #.022 OTH2 + #.016 KET2 + #.014 OH + #.01 ETO2 + #.009 GLCHO + #.007 ACET + #.005 ETHEO2 + #.002 R2CO3 + #.001 RCOOH + #.001 MECO3 + #.001 AACID + #.424 XC + #.479 SumRO2 + #.003 SumRCO3		Same k as rxn S003			
H373	OTH4_P1 + HO2 = #.915 ROOH + #.085 CROOH + #1.915 XC		Same k as rxn S002			
H374	OTH4_P1 + SumRO2 = SumRO2 + #.413 OTH3 + #.347 OTH4 + #.252 HO2 + #.202 OTH4_P2 + #.192 HCHO + #.096 OTH1 + #.048 NROG + #.03 MEO2 + #.029 MECHO + #.028 OTH2 + #.024 RCHO + #.022 KET2 + #.007 OH + #.005 ETO2 + #.004 GLCHO + #.004 ACET + #.003 ETHEO2 + #.001 R2CO3 + #.001 RCOOH + #.001 MECO3 + #1.25 XC + #.24 SumRO2 + #.002 SumRCO3		Same k as rxn S004			
H375	OTH4_P1 + SumRCO3 = SumRCO3 + #.56 OTH3 + #.442 HO2 + #.31 NROG + #.209 RO2C + #.192 HCHO + #.16 OTH1 + #.15 OTH4 + #.089 RCHO + #.07 ETCHO + #.047 OTH2 + #.038 KET2 + #.036 MEO2 + #.029 MECHO + #.011 AACID + #.009 MECO3 + #.007 RO2XC + #.007 ACET + #.007 OH + #.005 ETO2 + #.005 ETHEO2 + #.004 GLCHO + #.003 CO + #.003 zR1NO3 + #.003 zRCNO3 + #.002 MGLY + #.001 RCOOH + #.001 R2CO3 + #.001 zR2NO3 + #.001 BACL + #.001 zRHNO3 + #1.351 XC + #.262 SumRO2 + #.01 SumRCO3		Same k as rxn S009			
H376	OTH4_P2 + NO = #1.33 NROG + #.966 NO2 + #.922 HO2 + #.335 ETCHO + #.327 RCHO + #.125 OTH3 + #.089 OTH1 + #.055 AACID + #.048 RO2C + #.041 MECO3 + #.016 CO + #.015 R1NO3 + #.014 RCNO3 + #.009 MGLY + #.009 OTH2 + #.007 OTH4 + #.006 KET2 + #.004 ACET + #.003 R2NO3 + #.002 RCOOH + #.002 RHNO3 + #.001 RO2XC + #.001 R2CO3 + #.001 zRCNO3 + #.001 zRHNO3 + #.417 XC + #.049 SumRO2 + #.042 SumRCO3		Same k as rxn S001			
H377	OTH4_P2 + NO3 = #1.354 NROG + NO2 + #.954 HO2 + #.349 ETCHO + #.338 RCHO + #.13 OTH3 + #.09 OTH1 + #.057 AACID + #.051 RO2C + #.043 MECO3 + #.016 CO + #.01 MGLY + #.009 OTH2 + #.007 OTH4 + #.007 KET2 + #.005 ACET + #.003 RCOOH + #.002 RO2XC + #.001 R2CO3 + #.001 zRCNO3 + #.001 zRHNO3 + #.439 XC + #.053 SumRO2 + #.044 SumRCO3		Same k as rxn S003			
H378	OTH4_P2 + HO2 = #.581 ROOH + #.404 CROOH + #.015 OTHN + #-0.524 XC		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H379	OTH4_P2 + SumRO2 = SumRO2 + #1.354 NROG + #.477 HO2 + #.289 OTH3 + #.262 ETCHO + #.242 RCHO + #.076 OTH1 + #.073 OTH4 + #.029 AACID + #.026 RO2C + #.021 MECO3 + #.012 MGLY + #.008 CO + #.005 OTH2 + #.003 ACET + #.003 KET2 + #.001 RCOOH + #.001 RO2XC + #.001 R2CO3 + #.381 XC + #.027 SumRO2 + #.022 SumRCO3		Same k as rxn S004			
H380	OTH4_P2 + SumRCO3 = SumRCO3 + #2.03 NROG + #.48 HO2 + #.349 ETCHO + #.315 RCHO + #.14 OTH3 + #.109 OTH1 + #.029 AACID + #.028 RO2C + #.021 MECO3 + #.018 MGLY + #.012 OTH4 + #.008 CO + #.007 OTH2 + #.005 ACET + #.003 KET2 + #.001 RCOOH + #.001 RO2XC + #.001 R2CO3 + #.539 XC + #.029 SumRO2 + #.022 SumRCO3		Same k as rxn S009			
H381	RCHO + OH = #.837 R2CO3 + #.087 RO2C + #.086 HO2 + #.081 RCHO + #.069 OH + #.042 CO2 + #.025 OTH1 + #.025 ACET + #.007 KET2 + #.007 CO + #.006 MGLY + #.006 ETCHO + #.006 MECHO + #.005 CROOH + #.005 HOCCO3 + #.003 HCHO + #.003 RO2XC + #.003 GLCHO + #.003 zRCNO3 + #.001 NROG + #.83 XC + #.09 SumRO2 + #.842 SumRCO3	2.85e-11				
H382	RCHO + NO3 = HNO3 + #.961 R2CO3 + #.028 OH + #.025 OTH1 + #.011 HO2 + #.008 RCHO + #.004 RO2C + #.003 CO2 + #.003 ACET + #.002 MGLY + #.001 CO + #.001 KET2 + #.001 MECHO + #.984 XC + #.004 SumRO2 + #.961 SumRCO3	1.34e-14				
H383	RCHO + HV = #1.048 HO2 + CO + #.927 RCHO_P1 + #.048 MECHO + #.025 OTH1 + #.025 OH + #.048 XC + #.927 SumRO2		Phot Set= C2CHO			
H384	RCHO_P1 + NO = #.97 NO2 + #.956 HO2 + #.337 RCHO + #.336 ACET + #.161 ETCHO + #.093 RO2C + #.083 HCHO + #.081 KET2 + #.035 MECHO + #.023 R1NO3 + #.011 ETHEO2 + #.007 RHNO3 + #.003 RO2XC + #.002 zRHNO3 + #.001 zR1NO3 + #-0.593 XC + #.107 SumRO2		Same k as rxn S001			
H385	RCHO_P1 + NO3 = NO2 + #.985 HO2 + #.35 ACET + #.341 RCHO + #.168 ETCHO + #.097 RO2C + #.087 HCHO + #.084 KET2 + #.037 MECHO + #.012 ETHEO2 + #.003 RO2XC + #.002 zRHNO3 + #.001 zR1NO3 + #-0.54 XC + #.112 SumRO2		Same k as rxn S003			
H386	RCHO_P1 + HO2 = #.98 ROOH + #.02 CROOH + #-1.02 XC		Same k as rxn S002			
H387	RCHO_P1 + SumRO2 = SumRO2 + #.493 HO2 + #.267 RCHO + #.259 ACET + #.147 OTH3 + #.126 ETCHO + #.103 OTH4 + #.061 KET2 + #.048 RO2C + #.043 HCHO + #.018 MECHO + #.006 ETHEO2 + #.002 RO2XC + #.001 zRHNO3 + #-0.625 XC + #.056 SumRO2		Same k as rxn S004			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H388	RCHO_P1 + SumRCO3 = SumRCO3 + #.493 HO2 + #.364 RCHO + #.343 ACET + #.168 ETCHO + #.08 KET2 + #.048 RO2C + #.043 HCHO + #.018 MECHO + #.006 ETHEO2 + #.002 RO2XC + #.001 zRHNO3 + #-0.486 XC + #.056 SumRO2		Same k as rxn S009			
H389	KET2 + OH = #.631 KET2_P1 + #.348 HO2 + #.188 RCHO + #.1 KET2 + #.06 MGLY + #.016 HCHO + #.014 MECO3 + #.008 ACET + #.007 ACETO2 + #.001 MECHO + #.001 RO2C + #-0.309 XC + #.639 SumRO2 + #.014 SumRCO3	1.07e-11				
H390	KET2 + HV = #.807 R2CO3 + #.621 MEO2 + #.256 ETO2 + #.122 HO2 + #.098 ETCO3 + #.095 MECO3 + #.077 HCHO + #.051 RO2C + #.027 RCHO + #.018 ACET + #.001 RO2XC + #.001 zR1NO3 + #.001 zRHNO3 + #.712 XC + #.929 SumRO2 + SumRCO3		Phot Set= MEK-06, qy= 7.53e-2			
H391	KET2_P1 + NO = #6.023 NROG + #.914 NO2 + #.323 RCHO + #.309 HO2 + #.251 MECHO + #.216 HCHO + #.214 ACETO2 + #.166 MECO3 + #.16 ETCO3 + #.133 GLCHO + #.11 RO2C + #.086 RCNO3 + #.067 ACET + #.059 KET2 + #.051 R2CO3 + #.024 ETCHO + #.011 MGLY + #.009 RO2XC + #.009 zRCNO3 + #.005 HOCCO3 + #.001 OTH2 + #1.218 XC + #.333 SumRO2 + #.382 SumRCO3		Same k as rxn S001			
H392	KET2_P1 + NO3 = #6.428 NROG + NO2 + #.352 RCHO + #.339 HO2 + #.279 MECHO + #.234 HCHO + #.232 ACETO2 + #.18 MECO3 + #.179 ETCO3 + #.142 GLCHO + #.123 RO2C + #.076 ACET + #.065 KET2 + #.056 R2CO3 + #.027 ETCHO + #.012 MGLY + #.01 RO2XC + #.01 zRCNO3 + #.005 HOCCO3 + #.001 OTH2 + #1.042 XC + #.365 SumRO2 + #.42 SumRCO3		Same k as rxn S003			
H393	KET2_P1 + HO2 = CROOH + XC		Same k as rxn S002			
H394	KET2_P1 + SumRO2 = SumRO2 + #3.214 NROG + #.416 KET2 + #.197 RCHO + #.17 HO2 + #.14 MECHO + #.117 HCHO + #.116 ACETO2 + #.09 MECO3 + #.089 ETCO3 + #.08 BACL + #.071 GLCHO + #.062 RO2C + #.038 ACET + #.028 R2CO3 + #.014 ETCHO + #.012 MGLY + #.005 RO2XC + #.005 zRCNO3 + #.002 HOCCO3 + #1.183 XC + #.183 SumRO2 + #.209 SumRCO3		Same k as rxn S004			
H395	KET2_P1 + SumRCO3 = SumRCO3 + #3.213 NROG + #.274 KET2 + #.217 RCHO + #.182 HO2 + #.16 BACL + #.147 ACETO2 + #.14 MECHO + #.133 HCHO + #.1 MECO3 + #.093 ETCO3 + #.071 GLCHO + #.065 RO2C + #.057 ACET + #.028 R2CO3 + #.018 MGLY + #.014 ETCHO + #.005 RO2XC + #.005 zRCNO3 + #.002 HOCCO3 + #1.277 XC + #.217 SumRO2 + #.223 SumRCO3		Same k as rxn S009			
H416	OLEP + OH = #.707 OLEP_P1 + #.293 OLEP + #.293 HO2 + #.707 SumRO2	1.80e-10				

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H417	OLEP + O3 = #.266 KET2 + #.266 OLEA1 + #.136 LVKS + #.132 RCHO2 + #.132 RCHO + #.068 RCOOH + #.668 XC	4.27e-16				
H418	OLEP + NO3 = #.656 OLEP_P2 + #.344 RCNO3 + #.344 HO2 + #.688 XC + #.656 SumRO2	5.36e-12				
H419	OLEP_P1 + NO = #.946 NO2 + #.688 HO2 + #.382 LVKS + #.279 OLEA1 + #.236 OH + #.165 AFG2A + #.071 AFG2B + #.054 RHNO3 + #.027 OLEP + #.022 MECO3 + #.019 RCHO + #.003 RCOOH + #.003 GLY + #.001 KET2 + #.001 CO + #.001 MACO3 + #.222 XC + #.023 SumRCO3		Same k as rxn S001			
H420	OLEP_P1 + NO3 = NO2 + #.727 HO2 + #.403 LVKS + #.295 OLEA1 + #.249 OH + #.175 AFG2A + #.074 AFG2B + #.029 OLEP + #.023 MECO3 + #.02 RCHO + #.003 RCOOH + #.003 GLY + #.001 KET2 + #.001 CO + #.001 MACO3 + #.298 XC + #.024 SumRCO3		Same k as rxn S003			
H421	OLEP_P1 + HO2 = RUOOH		Same k as rxn S002			
H422	OLEP_P1 + SumRO2 = SumRO2 + #.441 OLEP + #.364 HO2 + #.275 LVKS + #.147 OLEA1 + #.125 OH + #.087 AFG2A + #.037 AFG2B + #.011 MECO3 + #.01 RCHO + #.002 RCOOH + #.002 GLY + #.231 XC + #.011 SumRCO3		Same k as rxn S004			
H423	OLEP_P1 + SumRCO3 = SumRCO3 + #.562 HO2 + #.546 LVKS + #.17 OLEP + #.147 OLEA1 + #.125 OH + #.087 AFG2A + #.037 AFG2B + #.011 MECO3 + #.01 RCHO + #.002 RCOOH + #.002 GLY + #.502 XC + #.011 SumRCO3		Same k as rxn S009			
H424	OLEP_P2 + NO = #1.668 NO2 + #.497 LVKS + #.225 OLEA1 + #.197 NO3 + #.115 AFG2A + #.082 AFG2B + #.054 RDNO3 + #.015 RCNO3 + #.015 HO2 + #.013 MECO3 + #.013 RHNO3 + #.001 CO + #.346 XC + #-0.001 XN + #.013 SumRCO3		Same k as rxn S001			
H425	OLEP_P2 + NO3 = #1.762 NO2 + #.525 LVKS + #.238 OLEA1 + #.208 NO3 + #.122 AFG2A + #.086 AFG2B + #.016 HO2 + #.016 RCNO3 + #.014 MECO3 + #.014 RHNO3 + #.001 CO + #.423 XC + #.014 SumRCO3		Same k as rxn S003			
H426	OLEP_P2 + HO2 = RHNO3 + #-1 XC		Same k as rxn S002			
H427	OLEP_P2 + SumRO2 = SumRO2 + #.388 RHNO3 + #.381 NO2 + #.262 LVKS + #.127 RCNO3 + #.119 OLEA1 + #.104 NO3 + #.061 AFG2A + #.043 AFG2B + #.008 HO2 + #.007 MECO3 + #.071 XC + #.007 SumRCO3		Same k as rxn S004			
H428	OLEP_P2 + SumRCO3 = SumRCO3 + #.644 NO2 + #.525 LVKS + #.245 RCNO3 + #.119 OLEA1 + #.104 NO3 + #.061 AFG2A + #.043 AFG2B + #.008 HO2 + #.007 MECO3 + #.007 RHNO3 + #.951 XC + #.007 SumRCO3		Same k as rxn S009			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H429	OLEA1 + OH = #.345 MACO3 + #.189 OLEA1_A3 + #.123 OLEA1_P1 + #.107 OLEA1_A2 + #.104 OLEA1_A1 + #.092 HO2 + #.053 RO2C + #.037 RCHO + #.031 AFG1 + #.027 OH + #.021 CO2 + #.02 KET2 + #.017 MGLY + #.013 LVKS + #.006 R2CO3 + #.005 OTHN + #.004 CO + #.004 GLY + #.004 OLEA1 + #.003 RO2XC + #.001 zRNNO3 + #.001 zRCNO3 + #.001 CROOH + #.001 HPALD + #.641 XC + #.179 SumRO2 + #.351 SumRCO3	6.03e-11				
H430	OLEA1 + O3 = #.756 OH + #.634 CO + #.492 OLEA1_P2 + #.416 MGLY + #.362 HO2 + #.251 GLCHO + #.235 HCOOH + #.214 GLY + #.192 RCHO2 + #.092 KET2 + #.052 CO2 + #.013 HCHO + #.003 MEOH + #-0.135 XC + #.492 SumRO2	1.08e-17				
H431	OLEA1 + NO3 = #.354 OLEA1_A4 + #.332 OLEA1_A5 + #.302 OLEA1_P3 + #.012 HNO3 + #.008 MACO3 + #.004 OLEA1_A3 + #.344 XC + #.302 SumRO2 + #.008 SumRCO3	9.51e-14				
H432	OLEA1 + HV = HO2 + #.664 MACO3 + #.336 OLEA1_A3 + XC + #.664 SumRCO3		Phot Set= MACR-06			
H433	OLEA1_P1 + NO = #.946 HO2 + #.946 NO2 + #.681 KET2 + #.681 MGLY + #.266 BACL + #.266 GLCHO + #.054 RNNO3 + #-2.584 XC		Same k as rxn S001			
H434	OLEA1_P1 + NO3 = HO2 + NO2 + #.719 KET2 + #.719 MGLY + #.281 BACL + #.281 GLCHO + #-2.438 XC		Same k as rxn S003			
H435	OLEA1_P1 + HO2 = OTHN + #-7 XC		Same k as rxn S002			
H436	OLEA1_P1 + SumRO2 = SumRO2 + #.5 HO2 + #.43 OTHN + #.359 KET2 + #.359 MGLY + #.141 BACL + #.141 GLCHO + #.07 CROOH + #-4.228 XC		Same k as rxn S004			
H437	OLEA1_P1 + SumRCO3 = SumRCO3 + #.859 HO2 + #.719 KET2 + #.719 MGLY + #.141 CROOH + #.141 BACL + #.141 GLCHO + #-2.303 XC		Same k as rxn S009			
H438	OLEA1_A1 = OLEA1_P4 + SumRO2	7.15e-1	1.64e+11	15.60	0.00	
H439	OLEA1_A1 + NO = #.946 HO2 + #.946 NO2 + #.82 MGLY + #.82 GLCHO + #.127 KET2 + #.127 CO + #.054 RHNO3 + #-0.186 XC		Same k as rxn S001			
H440	OLEA1_A2 = OLEA1_P5 + SumRO2	7.15e-1	1.64e+11	15.60	0.00	
H441	OLEA1_A2 + NO = #.969 HO2 + #.969 NO2 + #.869 KET2 + #.869 CO + #.101 MGLY + #.101 HCOOH + #.031 RHNO3 + #-1.804 XC		Same k as rxn S001			
H442	OLEA1_A3 = OLEA1_P6 + SumRO2	7.15e-1	1.64e+11	15.60	0.00	
H443	OLEA1_A3 + NO = #.969 NO2 + #.766 MGLY + #.766 OH + #.766 CO2 + #.178 R2CO3 + #.031 RCNO3 + #.025 BACL + #.025 CO + #.025 HO2 + #.184 XC + #.178 SumRCO3		Same k as rxn S001			
H444	OLEA1_P2 + NO = HOCCO3 + NO2 + #.013 HCHO + #-0.013 XC + SumRCO3		Same k as rxn S001			
H445	OLEA1_P2 + NO3 = HOCCO3 + NO2 + #.013 HCHO + #-0.013 XC + SumRCO3		Same k as rxn S003			
H446	OLEA1_P2 + HO2 = CROOH + #-3 XC		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H447	OLEA1_P2 + SumRO2 = SumRO2 + #.5 HOCCO3 + #.25 MGLY + #.247 CROOH + #.006 HCHO + #.003 KET2 + #-1.006 XC + #.5 SumRCO3		Same k as rxn S004			
H448	OLEA1_P2 + SumRCO3 = SumRCO3 + #.5 MGLY + #.5 HOCCO3 + #.006 HCHO + #-0.506 XC + #.5 SumRCO3		Same k as rxn S009			
H449	OLEA1_A4 = OLEA1_P7 + SumRO2	7.15e-1	1.64e+11	15.60	0.00	
H450	OLEA1_A4 + NO = #1.109 NO2 + #.783 RCNO3 + #.783 CO + #.783 HO2 + #.163 MGLY + #.163 GLCHO + #.054 RDNO3 + #.729 XC		Same k as rxn S001			
H451	OLEA1_A5 = OLEA1_P8 + SumRO2	7.15e-1	1.64e+11	15.60	0.00	
H452	OLEA1_A5 + NO = #1.172 NO2 + #.766 RCNO3 + #.766 CO + #.766 HO2 + #.203 MGLY + #.203 HCOOH + #.031 RDNO3 + #-0.062 XC		Same k as rxn S001			
H453	OLEA1_P3 + NO = #1.879 NO2 + #.873 KET2 + #.873 MGLY + #.067 RCNO3 + #.067 HCHO + #.067 HO2 + #.054 RNNO3 + #.007 R2CO3 + #-2.813 XC + #.007 SumRCO3		Same k as rxn S001			
H454	OLEA1_P3 + NO3 = #1.93 NO2 + #.922 KET2 + #.922 MGLY + #.07 RCNO3 + #.07 HCHO + #.07 HO2 + #.008 R2CO3 + #-2.68 XC + #.008 SumRCO3		Same k as rxn S003			
H455	OLEA1_P3 + HO2 = RNNO3 + #-5 XC		Same k as rxn S002			
H456	OLEA1_P3 + SumRO2 = SumRO2 + #.5 RNNO3 + #.461 KET2 + #.461 MGLY + #.465 NO2 + #.035 RCNO3 + #.035 HCHO + #.035 HO2 + #.004 R2CO3 + #-3.84 XC + #.004 SumRCO3		Same k as rxn S004			
H457	OLEA1_P3 + SumRCO3 = SumRCO3 + #.922 KET2 + #.922 MGLY + #.93 NO2 + #.07 RCNO3 + #.07 HCHO + #.07 HO2 + #.008 R2CO3 + #-2.68 XC + #.008 SumRCO3		Same k as rxn S009			
H458	OLEA1_P4 + NO = #.946 NO2 + #.766 KET2 + #.766 OH + #.766 CO2 + #.164 BACL + #.164 GLCHO + #.164 HO2 + #.054 RNNO3 + #.016 R2CO3 + #-1.168 XC + #.016 SumRCO3		Same k as rxn S001			
H459	OLEA1_P4 + NO3 = NO2 + #.81 KET2 + #.81 OH + #.81 CO2 + #.174 BACL + #.174 GLCHO + #.174 HO2 + #.017 R2CO3 + #-0.955 XC + #.017 SumRCO3		Same k as rxn S003			
H460	OLEA1_P4 + HO2 = OTHN + #-7 XC		Same k as rxn S002			
H461	OLEA1_P4 + SumRO2 = SumRO2 + #.5 OTHN + #.405 KET2 + #.405 OH + #.405 CO2 + #.087 BACL + #.087 GLCHO + #.087 HO2 + #.008 R2CO3 + #-3.976 XC + #.008 SumRCO3		Same k as rxn S004			
H462	OLEA1_P4 + SumRCO3 = SumRCO3 + #.81 KET2 + #.81 OH + #.81 CO2 + #.174 BACL + #.174 GLCHO + #.174 HO2 + #.017 R2CO3 + #-0.955 XC + #.017 SumRCO3		Same k as rxn S009			
H463	OLEA1_P5 + NO = #.969 KET2 + #.969 OH + #.969 CO2 + #.969 NO2 + #.031 RNNO3 + #-2.124 XC		Same k as rxn S001			
H464	OLEA1_P5 + NO3 = KET2 + OH + CO2 + NO2 + #-2 XC		Same k as rxn S003			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H465	OLEA1_P5 + HO2 = OTHN + #-8 XC		Same k as rxn S002			
H466	OLEA1_P5 + SumRO2 = SumRO2 + #.5 CROOH + #.5 KET2 + #.5 OH + #.5 CO2 + #-1.5 XC		Same k as rxn S004			
H467	OLEA1_P5 + SumRCO3 = SumRCO3 + KET2 + OH + CO2 + #-2 XC		Same k as rxn S009			
H468	OLEA1_P6 + NO = #.969 NO2 + #.548 BACL + #.548 OH + #.548 CO2 + #.421 R2CO3 + #.031 RNNO3 + #-0.313 XC + #.421 SumRCO3		Same k as rxn S001			
H469	OLEA1_P6 + NO3 = NO2 + #.566 BACL + #.566 OH + #.566 CO2 + #.434 R2CO3 + #-0.132 XC + #.434 SumRCO3		Same k as rxn S003			
H470	OLEA1_P6 + HO2 = OTHN + #-8 XC		Same k as rxn S002			
H471	OLEA1_P6 + SumRO2 = SumRO2 + #.5 CROOH + #.283 BACL + #.283 OH + #.283 CO2 + #.217 R2CO3 + #-0.566 XC + #.217 SumRCO3		Same k as rxn S004			
H472	OLEA1_P6 + SumRCO3 = SumRCO3 + #.566 BACL + #.566 OH + #.566 CO2 + #.434 R2CO3 + #-0.132 XC + #.434 SumRCO3		Same k as rxn S009			
H473	OLEA1_P7 + NO = #1.025 NO2 + #.921 RCNO3 + #.921 OH + #.921 CO2 + #.054 RNNO3 + #.019 R2CO3 + #.006 BACL + #.006 GLCHO + #.683 XC + #.019 SumRCO3		Same k as rxn S001			
H474	OLEA1_P7 + NO3 = #1.027 NO2 + #.973 RCNO3 + #.973 OH + #.973 CO2 + #.02 R2CO3 + #.007 BACL + #.007 GLCHO + #1.006 XC + #.02 SumRCO3		Same k as rxn S003			
H475	OLEA1_P7 + HO2 = RNNO3 + #-5 XC		Same k as rxn S002			
H476	OLEA1_P7 + SumRO2 = SumRO2 + #.5 RNNO3 + #.487 RCNO3 + #.487 OH + #.487 CO2 + #.01 R2CO3 + #.003 BACL + #.003 GLCHO + #.013 NO2 + #-1.996 XC + #.01 SumRCO3		Same k as rxn S004			
H477	OLEA1_P7 + SumRCO3 = SumRCO3 + #.973 RCNO3 + #.973 OH + #.973 CO2 + #.02 R2CO3 + #.007 BACL + #.007 GLCHO + #.027 NO2 + #1.006 XC + #.02 SumRCO3		Same k as rxn S009			
H478	OLEA1_P8 + NO = #1.008 NO2 + #.961 RCNO3 + #.961 OH + #.961 CO2 + #.031 RNNO3 + #.008 BACL + #.008 HCOOH + #-0.194 XC		Same k as rxn S001			
H479	OLEA1_P8 + NO3 = #1.009 NO2 + #.991 RCNO3 + #.991 OH + #.991 CO2 + #.009 BACL + #.009 HCOOH + #-0.009 XC		Same k as rxn S003			
H480	OLEA1_P8 + HO2 = RNNO3 + #-6 XC		Same k as rxn S002			
H481	OLEA1_P8 + SumRO2 = SumRO2 + #.996 RCNO3 + #.496 OH + #.496 CO2 + #.004 BACL + #.004 HCOOH + #.004 NO2 + #.496 XC		Same k as rxn S004			
H482	OLEA1_P8 + SumRCO3 = SumRCO3 + #.991 RCNO3 + #.991 OH + #.991 CO2 + #.009 BACL + #.009 HCOOH + #.009 NO2 + #-0.009 XC		Same k as rxn S009			
H502	RCOOH + OH = #.57 RCOOH_P1 + #.43 ETO2 + #.43 CO2 + SumRO2	1.20e-12				

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H503	RCOOH_P1 + NO = HO2 + NO2 + #.706 CO2 + #.596 MECHO + #.265 HCHO + #.249 RCHO + #.155 RO2C + #.045 MGLY + #-0.294 XC + #.155 SumRO2		Same k as rxn S001			
H504	RCOOH_P1 + NO3 = HO2 + NO2 + #.706 CO2 + #.596 MECHO + #.265 HCHO + #.249 RCHO + #.155 RO2C + #.045 MGLY + #-0.294 XC + #.155 SumRO2		Same k as rxn S003			
H505	RCOOH_P1 + HO2 = CROOH + #-2 XC		Same k as rxn S002			
H506	RCOOH_P1 + SumRO2 = SumRO2 + #.5 HO2 + #.353 CO2 + #.298 MECHO + #.25 RCOOH + #.225 RCHO + #.149 BACL + #.133 HCHO + #.078 RO2C + #.023 MGLY + #-0.397 XC + #.078 SumRO2		Same k as rxn S004			
H507	RCOOH_P1 + SumRCO3 = SumRCO3 + #.5 HO2 + #.353 CO2 + #.326 RCHO + #.298 BACL + #.298 MECHO + #.133 HCHO + #.078 RO2C + #.023 MGLY + #-0.647 XC + #.078 SumRO2		Same k as rxn S009			
H508	RANO3 + OH = #.635 RANO3_P1 + #.337 RHNO3 + #.186 HO2 + #.151 OH + #.028 NO2 + #.019 BALD + #.008 ARO1 + #.001 CROOH + #.688 XC + #.635 SumRO2	8.35e-12				
H509	RANO3 + HV = NO2 + #.996 HO2 + #.543 BALD + #.426 ARO1 + #.032 ARO2 + #.004 ETO2 + #.069 XC + #.004 SumRO2		Phot Set= IC3ONO2			
H510	RANO3_P1 + NO = #.868 NO2 + #.825 RCNO3 + #.825 HO2 + #.367 GLY + #.32 BUDAL + #.1 RNNO3 + #.064 MGLY + #.056 AFG2A + #.053 RDNO3 + #.022 AFG1 + #.016 MECHO + #.007 BALD + #.005 HCHO + #.001 OLEP + #.001 ETCHO + #1.517 XC + #.101 XN		Same k as rxn S001			
H511	RANO3_P1 + NO3 = #1.026 NO2 + #.974 HO2 + #.974 RCNO3 + #.431 GLY + #.375 BUDAL + #.078 MGLY + #.068 AFG2A + #.026 AFG1 + #.019 MECHO + #.009 BALD + #.006 HCHO + #.001 OLEP + #.001 ETCHO + #.001 AFG3 + #1.891 XC		Same k as rxn S003			
H512	RANO3_P1 + HO2 = #.98 RNNO3 + #.02 RHNO3 + #-1.92 XC		Same k as rxn S002			
H513	RANO3_P1 + SumRO2 = SumRO2 + #.721 RCNO3 + #.487 HO2 + #.225 RPNO3 + #.216 GLY + #.187 BUDAL + #.039 MGLY + #.036 RNNO3 + #.034 AFG2A + #.013 NO2 + #.013 AFG1 + #.01 MECHO + #.005 RHNO3 + #.005 BALD + #.003 HCHO + #.001 OLEP + #.001 ETCHO + #2.049 XC		Same k as rxn S004			
H514	RANO3_P1 + SumRCO3 = SumRCO3 + #.986 RCNO3 + #.518 HO2 + #.242 GLY + #.187 BUDAL + #.041 MGLY + #.036 AFG2A + #.014 NO2 + #.013 AFG1 + #.011 MECHO + #.005 BALD + #.003 HCHO + #.001 OLEP + #.001 ETCHO + #.001 AFG3 + #3.368 XC		Same k as rxn S009			
H515	RCNO3 + OH = #.386 NO2 + #.382 MGLY + #.315 R2NCO3 + #.249 RCNO3_P1 + #.05 RCNO3 + #.043 HO2 + #.007 OH + #.004 GLY + #.07 XC + #.249 SumRO2 + #.315 SumRCO3	9.31e-12				

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H516	RCNO3 + HV = NO2 + #.965 HCHO + #.489 MECO3 + #.324 HO2 + #.289 CO + #.124 R2CO3 + #.047 ETCO3 + #.03 GLY + #.014 ACO3 + #.003 RCHO + #.002 KET2 + #.002 RO2C + #.001 HOCCO3 + #.129 XC + #.002 SumRO2 + #.675 SumRCO3		Phot Set= CRBNIT			
H517	RCNO3_P1 + NO = #.983 NO2 + #.805 R2NCO3 + #.646 HCHO + #.159 RCNO3 + #.159 HO2 + #.147 MECHO + #.09 RO2C + #.089 GLCHO + #.04 BUDAL + #.04 AFG2A + #.026 ACET + #.02 RCHO + #.018 RDNO3 + #.017 RNNO3 + #.004 ETCHO + #.003 GLY + #.001 OLEP + #.001 MGLY + #-0.027 XC + #.09 SumRO2 + #.805 SumRCO3		Same k as rxn S001			
H518	RCNO3_P1 + NO3 = #1.001 NO2 + #.825 R2NCO3 + #.654 HCHO + #.174 RCNO3 + #.174 HO2 + #.153 MECHO + #.095 RO2C + #.093 GLCHO + #.048 BUDAL + #.048 AFG2A + #.028 ACET + #.022 RCHO + #.004 ETCHO + #.003 GLY + #.001 OLEP + #.001 MGLY + #.052 XC + #.095 SumRO2 + #.825 SumRCO3		Same k as rxn S003			
H519	RCNO3_P1 + HO2 = #.899 RCNO3 + #.101 RNNO3 + #.293 XC		Same k as rxn S002			
H520	RCNO3_P1 + SumRO2 = SumRO2 + #.561 RCNO3 + #.413 R2NCO3 + #.327 HCHO + #.087 HO2 + #.076 MECHO + #.048 RO2C + #.047 GLCHO + #.025 RNNO3 + #.024 BUDAL + #.024 AFG2A + #.014 ACET + #.011 RCHO + #.002 ETCHO + #.001 GLY + #.001 OLEP + #.353 XC + #.001 XN + #.048 SumRO2 + #.413 SumRCO3		Same k as rxn S004			
H521	RCNO3_P1 + SumRCO3 = SumRCO3 + #.572 RCNO3 + #.427 R2NCO3 + #.327 HCHO + #.087 HO2 + #.076 MECHO + #.048 RO2C + #.047 GLCHO + #.028 ACET + #.024 BUDAL + #.024 AFG2A + #.011 RCHO + #.002 ETCHO + #.001 OLEP + #.001 GLY + #.001 RNNO3 + #.49 XC + #.048 SumRO2 + #.427 SumRCO3		Same k as rxn S009			
H522	RHNO3 + OH = #.576 HO2 + #.516 RCNO3 + #.366 RHNO3_P1 + #.06 RHNO3 + #.058 NO2 + #.04 RCHO + #.02 ACET + #.013 HCHO + #.007 KET2 + #1.262 XC + #.366 SumRO2	8.28e-12				
H523	RHNO3 + HV = NO2 + #.647 HO2 + #.466 KET2 + #.353 RHNO3_P2 + #.348 HCHO + #.118 ACET + #.094 GLCHO + #.063 RCHO + #.41 XC + #.353 SumRO2		Phot Set= IC3ONO2			
H524	RHNO3_P1 + NO = #.966 NO2 + #.799 HO2 + #.726 RCNO3 + #.394 ACET + #.277 HCHO + #.179 RO2C + #.108 RDNO3 + #.096 MECHO + #.071 RHNO3 + #.057 RCHO + #.034 GLCHO + #.027 RO2XC + #.021 ETCHO + #.018 KET2 + #.018 zRDNO3 + #.004 zRNNO3 + #.003 RNNO3 + #1.47 XC + #.206 SumRO2		Same k as rxn S001			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H525	RHNO3_P1 + NO3 = #1.082 NO2 + #.898 HO2 + #.818 RCNO3 + #.449 ACET + #.317 HCHO + #.203 RO2C + #.103 MECHO + #.077 RHNO3 + #.063 RCHO + #.036 GLCHO + #.03 RO2XC + #.023 ETCHO + #.02 zRDNO3 + #.02 KET2 + #.004 zRNNO3 + #.003 RNNO3 + #1.531 XC + #.233 SumRO2		Same k as rxn S003			
H526	RHNO3_P1 + HO2 = #.903 RHNO3 + #.097 RNNO3 + #.612 XC		Same k as rxn S002			
H527	RHNO3_P1 + SumRO2 = SumRO2 + #.59 RCNO3 + #.449 HO2 + #.355 RHNO3 + #.225 ACET + #.158 HCHO + #.102 RO2C + #.052 MECHO + #.04 NO2 + #.031 RCHO + #.018 GLCHO + #.015 RO2XC + #.012 ETCHO + #.01 zRDNO3 + #.01 KET2 + #.005 RNNO3 + #.002 zRNNO3 + #1.787 XC + #.117 SumRO2		Same k as rxn S004			
H528	RHNO3_P1 + SumRCO3 = SumRCO3 + #.77 RCNO3 + #.449 HO2 + #.243 ACET + #.159 RHNO3 + #.158 HCHO + #.102 RO2C + #.059 NO2 + #.052 MECHO + #.036 GLCHO + #.031 RCHO + #.015 RO2XC + #.012 ETCHO + #.01 zRDNO3 + #.01 KET2 + #.002 zRNNO3 + #.002 RNNO3 + #2.363 XC + #.117 SumRO2		Same k as rxn S009			
H529	RHNO3_P2 + NO = #.908 NO2 + #.607 HO2 + #.301 RHNO3_P3 + #.29 HCHO + #.289 KET2 + #.277 ACET + #.081 RHNO3 + #.063 RCHO + #.011 R1NO3 + #.534 XC + #.301 SumRO2		Same k as rxn S001			
H530	RHNO3_P2 + NO3 = NO2 + #.658 HO2 + #.342 RHNO3_P3 + #.322 HCHO + #.321 KET2 + #.291 ACET + #.07 RCHO + #.526 XC + #.342 SumRO2		Same k as rxn S003			
H531	RHNO3_P2 + HO2 = #.986 ROOH + #.014 OTHN + #1.888 XC		Same k as rxn S002			
H532	RHNO3_P2 + SumRO2 = SumRO2 + #.329 HO2 + #.212 ACET + #.171 RHNO3_P3 + #.164 KET2 + #.164 OTH2 + #.161 HCHO + #.133 RCHO + #.101 OTH4 + #.067 OTH3 + #1.49 XC + #.171 SumRO2		Same k as rxn S004			
H533	RHNO3_P2 + SumRCO3 = SumRCO3 + #.334 RHNO3_P3 + #.329 HO2 + #.291 ACET + #.231 RCHO + #.167 KET2 + #.161 HCHO + #.869 XC + #.334 SumRO2		Same k as rxn S009			
H534	RHNO3_P3 + NO = #.882 HO2 + #.882 NO2 + #.843 HCHO + #.777 KET2 + #.118 RHNO3 + #.063 ACET + #.042 RCHO + #.005 RO2C + #1.207 XC + #.005 SumRO2		Same k as rxn S001			
H535	RHNO3_P3 + NO3 = #.999 HO2 + #.999 NO2 + #.956 HCHO + #.884 KET2 + #.069 ACET + #.046 RCHO + #.006 RO2C + #.001 RHNO3 + #1.227 XC + #.006 SumRO2		Same k as rxn S003			
H536	RHNO3_P3 + HO2 = #.955 ROOH + #.045 OTHN + #2.64 XC		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H537	RHNO3_P3 + SumRO2 = SumRO2 + #.5 HO2 + #.478 HCHO + #.453 KET2 + #.262 RCHO + #.239 OTH3 + #.035 ACET + #.011 OTH4 + #.003 RO2C + #2.104 XC + #.003 SumRO2		Same k as rxn S004			
H538	RHNO3_P3 + SumRCO3 = SumRCO3 + #.5 RCHO + #.5 HO2 + #.478 HCHO + #.465 KET2 + #.035 ACET + #.003 RO2C + #2.092 XC + #.003 SumRO2		Same k as rxn S009			
H539	RPNO3 + OH = #.503 HO2 + #.468 RPNO3_P1 + #.377 RCNO3 + #.126 RHNO3 + #.029 NO2 + #.029 RCHO + #.001 HPALD + #2.716 XC + #.468 SumRO2	7.75e-11				
H540	RPNO3 + HV = #8 XC + XN		Phot Set= COOH			
H541	RPNO3_P1 + NO = #.967 NO2 + #.744 HO2 + #.623 RPNO3 + #.132 RNNO3 + #.125 RCNO3 + #.052 RCHO + #.052 OLEA1 + #.01 RDNO3 + #.006 RO2C + #.004 AFG2A + #.004 OH + #.003 MGLY + #.002 BACL + #.001 RO2XC + #.001 MECHO + #.001 zRNNO3 + #-0.256 XC + #.133 XN + #.007 SumRO2		Same k as rxn S001			
H542	RPNO3_P1 + NO3 = #1.128 NO2 + #.868 HO2 + #.722 RPNO3 + #.15 RCNO3 + #.062 RCHO + #.059 OLEA1 + #.007 RO2C + #.005 AFG2A + #.004 OH + #.003 MGLY + #.002 BACL + #.001 RO2XC + #.001 MECHO + #.001 zRNNO3 + #.177 XC + #.008 SumRO2		Same k as rxn S003			
H543	RPNO3_P1 + HO2 = #.991 RNNO3 + #.009 RPNO3 + #-2.982 XC		Same k as rxn S002			
H544	RPNO3_P1 + SumRO2 = SumRO2 + #.437 RNNO3 + #.434 HO2 + #.408 RPNO3 + #.091 RCNO3 + #.064 NO2 + #.031 RCHO + #.03 OLEA1 + #.004 RO2C + #.003 AFG2A + #.002 OH + #.002 MGLY + #.001 BACL + #.001 RO2XC + #.001 MECHO + #-1.208 XC + #.005 SumRO2		Same k as rxn S004			
H545	RPNO3_P1 + SumRCO3 = SumRCO3 + #.49 HO2 + #.408 RNNO3 + #.361 RPNO3 + #.163 RCNO3 + #.068 NO2 + #.032 RCHO + #.03 OLEA1 + #.007 RO2C + #.005 AFG2A + #.003 MGLY + #.002 OH + #.002 BACL + #.001 RO2XC + #.001 zRNNO3 + #.001 MECHO + #-0.789 XC + #.008 SumRO2		Same k as rxn S009			
H546	RDNO3 + OH = #.676 RDNO3_P1 + #.23 NO2 + #.225 RCNO3 + #.094 RDNO3 + #.069 HO2 + #.026 OH + #.003 RHNO3 + #.002 RO2C + #.002 RNNO3 + #.001 RO2XC + #.001 zRNNO3 + #.657 XC + #.679 SumRO2	8.22e-12				
H547	RDNO3 + HV = #1.615 NO2 + #.295 MECHO + #.273 RDNO3_P2 + #.272 HCHO + #.23 RCNO3 + #.139 ACET + #.109 ETCHO + #.108 BALD + #.105 HO2 + #.099 OLEA2 + #.08 MEK + #.036 RCHO + #.007 ETO2 + #.883 XC + #.155 XN + #.28 SumRO2		Phot Set= DIONO2			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H548	RDNO3_P1 + NO = #1.404 NO2 + #.477 RCNO3 + #.257 RDNO3 + #.228 HO2 + #.206 ACET + #.176 RDNO3_P3 + #.147 HCHO + #.132 MECHO + #.075 KET2 + #.061 RNNO3 + #.06 GLY + #.059 BUDAL + #.036 RHNO3 + #.018 ETCHO + #.005 AFG2A + #.003 OH + #.003 RO2C + #.001 RO2XC + #.001 zRNNO3 + #-0.704 XC + #.156 XN + #.18 SumRO2		Same k as rxn S001			
H549	RDNO3_P1 + NO3 = #1.595 NO2 + #.545 RCNO3 + #.399 RDNO3 + #.369 HO2 + #.218 ACET + #.192 RO2C + #.176 HCHO + #.168 MECHO + #.097 KET2 + #.072 GLY + #.071 BUDAL + #.043 OH + #.041 RHNO3 + #.019 ETCHO + #.018 RO2XC + #.015 zRDNO3 + #.006 RNNO3 + #.005 AFG2A + #.003 zRNNO3 + #-0.616 XC + #.21 SumRO2		Same k as rxn S003			
H550	RDNO3_P1 + HO2 = #.697 RDNO3 + #.303 RNNO3 + #-1.212 XC + #.303 XN		Same k as rxn S002			
H551	RDNO3_P1 + SumRO2 = SumRO2 + #.557 RDNO3 + #.285 NO2 + #.272 RCNO3 + #.184 HO2 + #.145 RNNO3 + #.109 ACET + #.096 RO2C + #.088 HCHO + #.084 MECHO + #.049 KET2 + #.036 GLY + #.036 BUDAL + #.022 OH + #.021 RHNO3 + #.009 ETCHO + #.009 RO2XC + #.007 zRDNO3 + #.003 AFG2A + #.001 zRNNO3 + #-0.872 XC + #.156 XN + #.105 SumRO2		Same k as rxn S004			
H552	RDNO3_P1 + SumRCO3 = SumRCO3 + #.509 RDNO3 + #.489 NO2 + #.382 RCNO3 + #.228 HO2 + #.218 ACET + #.141 RO2C + #.107 HCHO + #.097 KET2 + #.084 MECHO + #.077 RNNO3 + #.041 OH + #.037 GLY + #.036 BUDAL + #.021 RHNO3 + #.016 RO2XC + #.013 zRDNO3 + #.009 ETCHO + #.003 AFG2A + #.002 zRNNO3 + #-0.868 XC + #.157 SumRO2		Same k as rxn S009			
H553	RDNO3_P2 + NO = #.954 NO2 + #.95 HO2 + #.436 RHNO3 + #.413 ACET + #.1 RCNO3 + #.03 RDNO3 + #.018 R1NO3 + #.002 HCHO + #.002 RO2C + #.002 MECHO + #.002 GLCHO + #.001 ETCHO + #-0.438 XC + #-0.568 XN + #.002 SumRO2		Same k as rxn S001			
H554	RDNO3_P2 + NO3 = #1.002 NO2 + #.998 HO2 + #.461 RHNO3 + #.43 ACET + #.106 RCNO3 + #.002 HCHO + #.002 RO2C + #.002 MECHO + #.002 GLCHO + #.001 ETCHO + #-0.387 XC + #-0.569 XN + #.002 SumRO2		Same k as rxn S003			
H555	RDNO3_P2 + HO2 = #.516 RHNO3 + #.431 ROOH + #.053 RNNO3 + #-1.35 XC + #-0.569 XN		Same k as rxn S002			
H556	RDNO3_P2 + SumRO2 = SumRO2 + #.499 HO2 + #.478 RHNO3 + #.323 ACET + #.108 OTH3 + #.09 RCNO3 + #.001 NO2 + #.001 HCHO + #.001 RO2C + #.001 MECHO + #.001 GLCHO + #.001 ETCHO + #-0.547 XC + #-0.569 XN + #.001 SumRO2		Same k as rxn S004			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H557	RDNO3_P2 + SumRCO3 = SumRCO3 + #.499 HO2 + #.44 RHNO3 + #.43 ACET + #.127 RCNO3 + #.001 NO2 + #.001 HCHO + #.001 RO2C + #.001 MECHO + #.001 GLCHO + #.001 ETCHO + #-0.319 XC + #-0.568 XN + #.001 SumRO2		Same k as rxn S009			
H558	RDNO3_P3 + NO = #1.246 NO2 + #.753 RDNO3 + #.517 HO2 + #.221 RCNO3 + #.17 OH + #.155 MECHO + #.081 HCHO + #.016 RHNO3 + #.011 RNNO3 + #.003 RO2C + #.001 GLCHO + #.22 XC + #.003 SumRO2		Same k as rxn S001			
H559	RDNO3_P3 + NO3 = #1.249 NO2 + #.752 RDNO3 + #.562 HO2 + #.229 RCNO3 + #.193 OH + #.16 MECHO + #.084 HCHO + #.016 RHNO3 + #.003 RO2C + #.002 RNNO3 + #.001 GLCHO + #.279 XC + #.003 SumRO2		Same k as rxn S003			
H560	RDNO3_P3 + HO2 = #.596 RDNO3 + #.403 RNNO3 + #.001 RHNO3 + #-1.612 XC + #.404 XN		Same k as rxn S002			
H561	RDNO3_P3 + SumRO2 = SumRO2 + #.8 RDNO3 + #.281 HO2 + #.2 NO2 + #.114 RCNO3 + #.097 OH + #.08 MECHO + #.077 RNNO3 + #.042 HCHO + #.009 RHNO3 + #.002 RO2C + #.001 GLCHO + #-0.17 XC + #.002 SumRO2		Same k as rxn S004			
H562	RDNO3_P3 + SumRCO3 = SumRCO3 + #.876 RDNO3 + #.281 HO2 + #.124 NO2 + #.114 RCNO3 + #.097 OH + #.08 MECHO + #.042 HCHO + #.009 RHNO3 + #.002 RO2C + #.001 RNNO3 + #.001 GLCHO + #.134 XC + #.002 SumRO2		Same k as rxn S009			
H563	R1NO3 + OH = #.84 R1NO3_P1 + #.16 NO2 + #.074 ACET + #.054 MEK + #.031 KET2 + #.207 XC + #.84 SumRO2	9.97e-13				
H564	R1NO3 + HV = NO2 + #.322 ETO2 + #.309 ACET + #.302 HO2 + #.29 R1NO3_P2 + #.191 MEK + #.162 MECHO + #.074 TBUO + #.044 KET2 + #.021 ETCHO + #.013 MEO2 + #.001 RCHO + #.295 XC + #.625 SumRO2		Phot Set= IC3ONO2			
H565	R1NO3_P1 + NO = #1.546 NO2 + #.542 MECHO + #.292 ACET + #.277 R1NO3_P3 + #.201 HCHO + #.085 ETCHO + #.066 MEK + #.065 RCNO3 + #.064 HO2 + #.056 RDNO3 + #.026 RCHO + #.013 KET2 + #.235 XC + #.277 SumRO2		Same k as rxn S001			
H566	R1NO3_P1 + NO3 = #1.634 NO2 + #.566 MECHO + #.31 ACET + #.298 R1NO3_P3 + #.21 HCHO + #.09 ETCHO + #.071 MEK + #.068 RCNO3 + #.067 HO2 + #.031 RCHO + #.014 KET2 + #.286 XC + #.298 SumRO2		Same k as rxn S003			
H567	R1NO3_P1 + HO2 = RHNO3 + #-1 XC		Same k as rxn S002			
H568	R1NO3_P1 + SumRO2 = SumRO2 + #.317 NO2 + #.283 MECHO + #.27 RCNO3 + #.264 RHNO3 + #.155 ACET + #.149 R1NO3_P3 + #.105 HCHO + #.045 ETCHO + #.036 MEK + #.034 HO2 + #.015 RCHO + #.007 KET2 + #.351 XC + #.149 SumRO2		Same k as rxn S004			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H569	R1NO3_P1 + SumRCO3 = SumRCO3 + #.506 RCNO3 + #.345 NO2 + #.311 MECHO + #.183 ACET + #.149 R1NO3_P3 + #.105 HCHO + #.045 ETCHO + #.036 MEK + #.034 HO2 + #.015 RCHO + #.007 KET2 + #1.087 XC + #.149 SumRO2		Same k as rxn S009			
H570	R1NO3_P2 + NO = #.92 NO2 + #.876 HO2 + #.533 KET2 + #.325 RO2C + #.306 HCHO + #.258 ACET + #.077 RHNO3 + #.048 ETCHO + #.044 RCHO + #.038 RO2XC + #.027 zRHNO3 + #.007 TBUO + #.003 R1NO3 + #.268 XC + #.363 SumRO2		Same k as rxn S001			
H571	R1NO3_P2 + NO3 = #.985 NO2 + #.947 HO2 + #.584 KET2 + #.372 RO2C + #.356 HCHO + #.271 ACET + #.05 RCHO + #.05 ETCHO + #.044 RO2XC + #.03 zRHNO3 + #.015 RHNO3 + #.008 TBUO + #.259 XC + #.416 SumRO2		Same k as rxn S003			
H572	R1NO3_P2 + HO2 = ROOH + XC		Same k as rxn S002			
H573	R1NO3_P2 + SumRO2 = SumRO2 + #.473 HO2 + #.292 KET2 + #.199 ACET + #.198 RCHO + #.186 RO2C + #.178 HCHO + #.158 OTH3 + #.092 OTH4 + #.037 ETCHO + #.022 RO2XC + #.015 zRHNO3 + #.007 RHNO3 + #.004 TBUO + #-0.007 NO2 + #.714 XC + #.208 SumRO2		Same k as rxn S004			
H574	R1NO3_P2 + SumRCO3 = SumRCO3 + #.473 HO2 + #.372 RCHO + #.292 KET2 + #.263 ACET + #.186 RO2C + #.178 HCHO + #.05 ETCHO + #.022 RO2XC + #.015 zRHNO3 + #.007 RHNO3 + #.004 TBUO + #-0.007 NO2 + #.787 XC + #.208 SumRO2		Same k as rxn S009			
H575	R1NO3_P3 + NO = #1.088 NO2 + #.774 HO2 + #.457 RHNO3 + #.318 RCNO3 + #.115 KET2 + #.092 HCHO + #.085 MECHO + #.065 RDNO3 + #.061 RO2C + #.009 RCHO + #.009 ACET + #.008 RO2XC + #.007 zRDNO3 + #.002 TBUO + #.001 zRNNO3 + #-0.046 XC + #.069 SumRO2		Same k as rxn S001			
H576	R1NO3_P3 + NO3 = #1.167 NO2 + #.825 HO2 + #.482 RHNO3 + #.343 RCNO3 + #.126 KET2 + #.101 HCHO + #.091 MECHO + #.068 RO2C + #.01 ACET + #.009 RCHO + #.009 RO2XC + #.008 zRDNO3 + #.002 TBUO + #.001 zRNNO3 + #.001 ETCHO + #.001 GLCHO + #.029 XC + #.077 SumRO2		Same k as rxn S003			
H577	R1NO3_P3 + HO2 = #.998 RHNO3 + #.002 ROOH + #-0.996 XC + #.002 XN		Same k as rxn S002			
H578	R1NO3_P3 + SumRO2 = SumRO2 + #.68 RHNO3 + #.413 HO2 + #.232 RCNO3 + #.084 NO2 + #.063 KET2 + #.05 HCHO + #.045 MECHO + #.034 RO2C + #.005 ACET + #.005 RCHO + #.005 RO2XC + #.004 zRDNO3 + #.001 OTH1 + #.001 TBUO + #-0.297 XC + #.039 SumRO2		Same k as rxn S004			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H579	R1NO3_P3 + SumRCO3 = SumRCO3 + #.588 RHNO3 + #.415 HO2 + #.294 RCNO3 + #.11 NO2 + #.086 KET2 + #.077 HCHO + #.064 RO2C + #.045 MECHO + #.009 ACET + #.009 RO2XC + #.008 zRDNO3 + #.005 RCHO + #.002 TBUO + #-0.11 XC + #.073 SumRO2		Same k as rxn S009			
H580	R2NO3 + OH = #.965 R2NO3_P1 + #.035 NO2 + #.018 KET2 + #.013 OTH3 + #.004 OTH4 + #.122 XC + #.965 SumRO2	6.15e-12				
H581	R2NO3 + HV = NO2 + #.58 R2NO3_P2 + #.361 OTH3 + #.231 OH + #.189 HO2 + #.056 OTH4 + #.003 KET2 + #1.677 XC + #.58 SumRO2		Phot Set= IC3ONO2			
H582	R2NO3_P1 + NO = #.984 NO2 + #.385 R2NO3_P3 + #.341 RCNO3 + #.175 OH + #.165 HO2 + #.145 RDNO3 + #.113 RCHO + #.02 KET2 + #.009 ETCHO + #.005 MECHO + #.004 HCHO + #.001 OTH3 + #.001 ETO2 + #2.428 XC + #.386 SumRO2		Same k as rxn S001			
H583	R2NO3_P1 + NO3 = #1.149 NO2 + #.467 R2NO3_P3 + #.384 RCNO3 + #.197 OH + #.185 HO2 + #.13 RCHO + #.025 KET2 + #.01 ETCHO + #.006 MECHO + #.004 HCHO + #.001 OTH3 + #.001 ETO2 + #2.415 XC + #.468 SumRO2		Same k as rxn S003			
H584	R2NO3_P1 + HO2 = RHNO3 + #2 XC		Same k as rxn S002			
H585	R2NO3_P1 + SumRO2 = SumRO2 + #.416 RCNO3 + #.276 RHNO3 + #.234 R2NO3_P3 + #.099 OH + #.093 HO2 + #.074 NO2 + #.065 RCHO + #.013 KET2 + #.005 ETCHO + #.003 MECHO + #.002 HCHO + #.001 OTH3 + #2.872 XC + #.234 SumRO2		Same k as rxn S004			
H586	R2NO3_P1 + SumRCO3 = SumRCO3 + #.808 RCNO3 + #.281 RO2C + #.27 HO2 + #.097 NO2 + #.099 OH + #.078 RCHO + #.065 RO2XC + #.054 zRDNO3 + #.039 RHNO3 + #.029 MECO3 + #.021 KET2 + #.007 ETCHO + #.006 HCHO + #.005 MECHO + #.002 RNNO3 + #.002 zRNNO3 + #.001 ACETO2 + #.001 OTH3 + #4.459 XC + #.347 SumRO2 + #.029 SumRCO3		Same k as rxn S009			
H587	R2NO3_P2 + NO = #.811 NO2 + #.607 HO2 + #.605 KET2 + #.204 R2NO3_P4 + #.141 RHNO3 + #.048 RCNO3 + #.002 RCHO + #2.549 XC + #.204 SumRO2		Same k as rxn S001			
H588	R2NO3_P2 + NO3 = NO2 + #.747 HO2 + #.744 KET2 + #.253 R2NO3_P4 + #.002 RCHO + #2.501 XC + #.253 SumRO2		Same k as rxn S003			
H589	R2NO3_P2 + HO2 = #.754 ROOH + #.246 CROOH + #3.754 XC		Same k as rxn S002			
H590	R2NO3_P2 + SumRO2 = SumRO2 + #.616 KET2 + #.373 HO2 + #.188 OTH4 + #.127 R2NO3_P4 + #.069 RCHO + #3.003 XC + #.127 SumRO2		Same k as rxn S004			
H591	R2NO3_P2 + SumRCO3 = SumRCO3 + #.736 KET2 + #.373 HO2 + #.137 RCHO + #.127 R2NO3_P4 + #2.883 XC + #.127 SumRO2		Same k as rxn S009			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H592	R2NO3_P3 + NO = #.87 NO2 + #.691 HO2 + #.652 RCNO3 + #.173 RDNO3 + #.142 RO2C + #.106 RHNO3 + #.07 MECO3 + #.025 RCHO + #.022 RO2XC + #.02 KET2 + #.018 zRDNO3 + #.008 HCHO + #.008 RNNO3 + #.008 ETCHO + #.007 MECHO + #.004 zRNNO3 + #.002 OH + #.002 ACETO2 + #3.75 XC + #.166 SumRO2 + #.07 SumRCO3		Same k as rxn S001			
H593	R2NO3_P3 + NO3 = #1.052 NO2 + #.844 HO2 + #.796 RCNO3 + #.164 RO2C + #.125 RHNO3 + #.081 MECO3 + #.03 RCHO + #.026 RO2XC + #.023 KET2 + #.02 zRDNO3 + #.009 HCHO + #.009 ETCHO + #.008 MECHO + #.007 RNNO3 + #.005 zRNNO3 + #.002 OH + #.002 ACETO2 + #.001 MGLY + #4.164 XC + #.192 SumRO2 + #.081 SumRCO3		Same k as rxn S003			
H594	R2NO3_P3 + HO2 = #.572 RHNO3 + #.228 RNNO3 + #.199 RCNO3 + #.001 ROOH + #1.687 XC + #.001 XN		Same k as rxn S002			
H595	R2NO3_P3 + SumRO2 = SumRO2 + #.681 RCNO3 + #.422 HO2 + #.274 RHNO3 + #.082 RO2C + #.041 MECO3 + #.027 NO2 + #.015 RCHO + #.013 RO2XC + #.012 KET2 + #.01 zRDNO3 + #.008 RNNO3 + #.005 ETCHO + #.005 HCHO + #.004 MECHO + #.003 zRNNO3 + #.001 OH + #.001 ACETO2 + #3.91 XC + #.096 SumRO2 + #.041 SumRCO3		Same k as rxn S004			
H596	R2NO3_P3 + SumRCO3 = SumRCO3 + #.865 RCNO3 + #.422 HO2 + #.095 RHNO3 + #.082 RO2C + #.041 MECO3 + #.027 NO2 + #.015 RCHO + #.013 RO2XC + #.012 KET2 + #.01 zRDNO3 + #.005 ETCHO + #.005 HCHO + #.004 MECHO + #.003 RNNO3 + #.003 zRNNO3 + #.001 OH + #.001 ACETO2 + #4.482 XC + #.096 SumRO2 + #.041 SumRCO3		Same k as rxn S009			
H597	R2NO3_P4 + NO = #.866 NO2 + #.839 RCHO + #.664 HO2 + #.178 MECO3 + #.127 RCNO3 + #.031 KET2 + #.023 ACETO2 + #.007 RHNO3 + #.006 ETCHO + #.003 MECHO + #.001 RO2C + #2.617 XC + #.024 SumRO2 + #.178 SumRCO3		Same k as rxn S001			
H598	R2NO3_P4 + NO3 = NO2 + #.967 RCHO + #.768 HO2 + #.204 MECO3 + #.038 KET2 + #.027 ACETO2 + #.007 ETCHO + #.003 MECHO + #.002 RO2C + #2.426 XC + #.029 SumRO2 + #.204 SumRCO3		Same k as rxn S003			
H599	R2NO3_P4 + HO2 = #.964 CROOH + #.02 ROOH + #.016 OTHN + #1.908 XC		Same k as rxn S002			
H600	R2NO3_P4 + SumRO2 = SumRO2 + #.484 RCHO + #.459 KET2 + #.384 HO2 + #.102 MECO3 + #.051 BACL + #.014 ACETO2 + #.009 OTH4 + #.004 ETCHO + #.002 MECHO + #.001 RO2C + #2.267 XC + #.015 SumRO2 + #.102 SumRCO3		Same k as rxn S004			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H601	R2NO3_P4 + SumRCO3 = SumRCO3 + #.533 RCHO + #.433 HO2 + #.367 KET2 + #.102 MECO3 + #.102 BACL + #.022 ACETO2 + #.004 ETCHO + #.002 MECHO + #.001 RO2C + #2.339 XC + #.023 SumRO2 + #.102 SumRCO3		Same k as rxn S009			
H602	RUOOH + OH = #.706 OH + #.429 IEPOX + #.209 RUOOH_P1 + #.168 ROOH + #.091 CROOH + #.084 HO2 + #.039 OTH4 + #.034 LVKS + #.014 HPALD + #.009 OLEA2 + #.007 HCHO + #.005 MVK + #.002 RO2C + #.002 MACR + #.001 OLEA1 + #.236 XC + #.211 SumRO2	6.02e-11				
H603	RUOOH + O3 = #.65 OH + #.44 CROOH + #.435 HCHO + #.354 RCHO2 + #.268 BACL + #.194 CO + #.142 HCOOH + #.12 HCHO2 + #.08 HO2 + #.059 CO2 + #.026 KET2 + #.008 RO2C + #.007 ROOH + #.005 MGLY + #.003 GLCHO + #-0.463 XC + #.008 SumRO2	6.97e-17				
H604	RUOOH + HV = #1.118 OH + #.877 HO2 + #.787 HCHO + #.412 MVK + #.282 MACR + #.144 OLEP + #.065 RO2C + #.048 OLEA1 + #.048 LVKS + #.029 OLEA2 + #.019 HPALD + #.013 RUOOH + #.005 RO2XC + #.004 zRHNO3 + #.001 zRNNO3 + #-0.054 XC + #.07 SumRO2		Phot Set= COOH			
H605	RUOOH_P1 + NO = #.943 NO2 + #.909 HO2 + #.66 CROOH + #.195 HCHO + #.132 RCHO + #.13 GLCHO + #.116 MVK + #.083 RO2C + #.055 KET2 + #.043 MACR + #.036 RNNO3 + #.036 OLEP + #.022 OH + #.021 RHNO3 + #.014 LVKS + #.007 OLEA2 + #.007 HOCCO3 + #.005 RO2XC + #.004 HPALD + #.004 zRHNO3 + #.001 OTHN + #.001 RCOOH + #.001 zRNNO3 + #-1.034 XC + #.088 SumRO2 + #.007 SumRCO3		Same k as rxn S001			
H606	RUOOH_P1 + NO3 = NO2 + #.965 HO2 + #.697 CROOH + #.209 HCHO + #.139 RCHO + #.138 GLCHO + #.125 MVK + #.088 RO2C + #.058 KET2 + #.047 MACR + #.038 OLEP + #.023 OH + #.015 LVKS + #.008 OLEA2 + #.007 HOCCO3 + #.005 RO2XC + #.004 HPALD + #.004 zRHNO3 + #.001 OTHN + #.001 RCOOH + #.001 zRNNO3 + #-0.877 XC + #.093 SumRO2 + #.007 SumRCO3		Same k as rxn S003			
H607	RUOOH_P1 + HO2 = #.761 OTHN + #.013 RUOOH + #-4.197 XC		Same k as rxn S002			
H608	RUOOH_P1 + SumRO2 = SumRO2 + #.54 CROOH + #.482 HO2 + #.172 OTHN + #.104 HCHO + #.1 OLEP + #.07 RCHO + #.069 GLCHO + #.063 MVK + #.044 RO2C + #.029 KET2 + #.023 MACR + #.02 ROOH + #.019 LVKS + #.014 RUOOH + #.012 OH + #.01 OLEA2 + #.006 HPALD + #.004 HOCCO3 + #.003 RO2XC + #.002 zRHNO3 + #.001 RCOOH + #-1.604 XC + #.047 SumRO2 + #.004 SumRCO3		Same k as rxn S004			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H609	RUOOH_P1 + SumRCO3 = SumRCO3 + #.736 CROOH + #.55 HO2 + #.168 HCHO + #.125 MVK + #.07 RCHO + #.069 GLCHO + #.053 RO2C + #.032 LVKS + #.029 KET2 + #.025 OLEP + #.023 MACR + #.016 OLEA2 + #.012 OH + #.01 HPALD + #.007 HOCCO3 + #.003 RO2XC + #.002 zRHNO3 + #.001 OTHN + #.001 RCOOH + #-0.427 XC + #.056 SumRO2 + #.007 SumRCO3	Same k as rxn S009				
H610	RAOOH + OH = #.801 OH + #.521 IEPOX + #.188 HO2 + #.168 RCHO + #.086 OLEP + #.078 CROOH + #.075 RO2C + #.067 MGLY + #.032 HPALD + #.025 OLEA1 + #.012 AFG2A + #.011 RO2XC + #.011 GLY + #.01 BUDAL + #.007 zRNNO3 + #.004 zRPNO3 + #.001 BACL + #.001 AFG3 + #.001 AFG1 + #2.178 XC + #.086 SumRO2	9.12e-11				
H611	RAOOH + HV = #7 XC	Phot Set= COOH				
H612	HPALD + OH = #.853 OH + #.541 OLEP + #.152 RCHO + #.113 HPALD_A1 + #.06 AFG1 + #.055 CROOH + #.042 OTHN + #.031 HO2 + #.021 HPALD + #.015 RO2C + #.012 OLEA1 + #.007 MGLY + #.005 GLY + #.002 HOCCO3 + #.001 CO + #.001 RO2XC + #-0.158 XC + #.016 SumRO2 + #.002 SumRCO3	4.76e-11				
H613	HPALD + HV = #1.042 OH + #.697 MACO3 + #.259 HO2 + #.183 OLEA1 + #.062 HPALD + #.053 AFG1 + #.043 RO2C + #.023 HCHO + #.002 RO2XC + #.002 zRCNO3 + #.002 OLEP + #.683 XC + #.045 SumRO2 + #.697 SumRCO3	Phot Set= HPALDS, qy= 1.00e-1				
H614	HPALD_A1 = CROOH + OH	7.15e-1	1.64e+11	15.60	0.00	
H615	HPALD_A1 + NO = #.946 CROOH + #.946 HO2 + #.946 NO2 + #.82 MGLY + #.127 CO + #.054 RHNO3 + #-2.641 XC	Same k as rxn S001				
H616	CROOH + OH = #1.545 NROG + #.535 OH + #.465 CROOH_P1 + #.209 OTH1 + #.131 KET2 + #.063 RCHO + #.051 OTH4 + #.036 BACL + #.026 OTH2 + #.001 OTH3 + #.711 XC + #.465 SumRO2	1.30e-11				
H617	CROOH + HV = #6.07 NROG + OH + #.292 HO2 + #.24 AACID + #.2 CROOH_P2 + #.169 RCHO + #.158 ETCO3 + #.153 KET2 + #.148 MECO3 + #.088 OTH1 + #.083 ACET + #.07 ACETO2 + #.063 MEO2 + #.053 ETO2 + #.016 CO + #.016 R2CO3 + #.013 CO2 + #.009 MECHO + #.002 OTH2 + #.001 ETCHO + #.113 XC + #.386 SumRO2 + #.322 SumRCO3	Phot Set= HPALDS, qy= 1.00e-1				

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H618	CROOH_P1 + NO = #5.349 NROG + #.922 NO2 + #.34 CROOH_P3 + #.133 HO2 + #.112 AACID + #.11 OTH1 + #.108 MEO2 + #.102 ACET + #.099 MECO3 + #.083 ACETO2 + #.076 RCNO3 + #.072 RCHO + #.067 OH + #.065 ETCO3 + #.063 CROOH + #.06 KET2 + #.027 MGLY + #.026 MECHO + #.022 CO2 + #.022 ETO2 + #.02 HCHO + #.014 CO + #.006 R2CO3 + #.004 ETCHO + #.003 OTH2 + #.001 OTH4 + #.001 RNNO3 + #.001 RHNO3 + #-0.073 XC + #.553 SumRO2 + #.17 SumRCO3		Same k as rxn S001			
H619	CROOH_P1 + NO3 = #5.633 NROG + NO2 + #.373 CROOH_P3 + #.14 HO2 + #.118 AACID + #.116 ACET + #.116 OTH1 + #.113 MEO2 + #.107 MECO3 + #.097 ACETO2 + #.077 RCHO + #.072 OH + #.069 CROOH + #.069 ETCO3 + #.064 KET2 + #.029 MGLY + #.028 MECHO + #.023 CO2 + #.023 ETO2 + #.022 HCHO + #.014 CO + #.006 R2CO3 + #.005 ETCHO + #.003 OTH2 + #.002 OTH4 + #-0.266 XC + #.606 SumRO2 + #.182 SumRCO3		Same k as rxn S003			
H620	CROOH_P1 + HO2 = #.426 CROOH + #.073 OTHN + #1.994 XC		Same k as rxn S002			
H621	CROOH_P1 + SumRO2 = SumRO2 + #3.411 NROG + #.236 CROOH + #.186 CROOH_P3 + #.149 OTH1 + #.117 KET2 + #.07 HO2 + #.059 AACID + #.058 ACET + #.057 RCHO + #.057 MEO2 + #.053 MECO3 + #.048 ACETO2 + #.047 OTH4 + #.036 OH + #.034 ETCO3 + #.021 BACL + #.02 OTH3 + #.019 MGLY + #.014 MECHO + #.012 CO2 + #.012 ETO2 + #.011 HCHO + #.007 CO + #.006 OTH2 + #.003 R2CO3 + #.002 ETCHO + #.002 OTHN + #.195 XC + #.303 SumRO2 + #.09 SumRCO3		Same k as rxn S004			
H622	CROOH_P1 + SumRCO3 = SumRCO3 + #4.005 NROG + #.219 CROOH + #.186 CROOH_P3 + #.172 OTH1 + #.115 ACET + #.113 MEO2 + #.094 ACETO2 + #.076 RCHO + #.07 HO2 + #.069 KET2 + #.059 AACID + #.053 MECO3 + #.041 BACL + #.036 OH + #.034 ETCO3 + #.023 CO2 + #.022 MGLY + #.014 MECHO + #.012 ETO2 + #.011 HCHO + #.01 OTH2 + #.007 CO + #.003 R2CO3 + #.002 ETCHO + #.001 OTH4 + #.186 XC + #.405 SumRO2 + #.09 SumRCO3		Same k as rxn S009			
H623	CROOH_P2 + NO = #2.162 NROG + #.911 NO2 + #.747 RCHO + #.576 MECO3 + #.333 HO2 + #.09 OTH3 + #.088 RCNO3 + #.027 AACID + #.027 CO + #.017 ETCHO + #.005 KET2 + #.002 ACETO2 + #.001 R1NO3 + #1.068 XC + #.002 SumRO2 + #.576 SumRCO3		Same k as rxn S001			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H624	CROOH_P2 + NO3 = #2.195 NROG + NO2 + #.826 RCHO + #.631 MECO3 + #.366 HO2 + #.098 OTH3 + #.027 AACID + #.027 CO + #.018 ETCHO + #.006 KET2 + #.002 ACETO2 + #.871 XC + #.002 SumRO2 + #.631 SumRCO3		Same k as rxn S003			
H625	CROOH_P2 + HO2 = #.982 CROOH + #.018 ROOH + #1.018 XC		Same k as rxn S002			
H626	CROOH_P2 + SumRO2 = SumRO2 + #2.25 NROG + #.437 RCHO + #.316 MECO3 + #.258 KET2 + #.183 HO2 + #.158 BACL + #.067 OTH3 + #.026 OTH4 + #.014 AACID + #.014 CO + #.014 ETCHO + #.001 MGLY + #.001 ACETO2 + #1.236 XC + #.001 SumRO2 + #.316 SumRCO3		Same k as rxn S004			
H627	CROOH_P2 + SumRCO3 = SumRCO3 + #3.402 NROG + #.462 RCHO + #.316 BACL + #.316 MECO3 + #.183 HO2 + #.1 KET2 + #.049 OTH3 + #.018 ETCHO + #.014 AACID + #.014 CO + #.003 MGLY + #.001 ACETO2 + #1.452 XC + #.001 SumRO2 + #.316 SumRCO3		Same k as rxn S009			
H628	CROOH_P3 + NO = #14.486 NROG + #.924 NO2 + #.585 RCHO + #.424 HO2 + #.412 MECO3 + #.278 RO2C + #.141 MECHO + #.119 HCHO + #.074 RCNO3 + #.03 AACID + #.029 KET2 + #.028 R2CO3 + #.028 ETCHO + #.026 OTH1 + #.026 RO2XC + #.026 zRCNO3 + #.022 OTH3 + #.019 ACETO2 + #.019 OTH2 + #.009 ACET + #.007 CROOH + #.007 CO + #.006 MGLY + #.005 OH + #.004 HOCCO3 + #.003 ETHEO2 + #.003 OTH4 + #.002 RHNO3 + #.002 MEO2 + #.001 ETCO3 + #1.352 XC + #.328 SumRO2 + #.445 SumRCO3		Same k as rxn S001			
H629	CROOH_P3 + NO3 = #15.353 NROG + NO2 + #.638 RCHO + #.455 HO2 + #.45 MECO3 + #.305 RO2C + #.15 MECHO + #.127 HCHO + #.032 KET2 + #.031 AACID + #.031 ETCHO + #.03 R2CO3 + #.028 RO2XC + #.028 zRCNO3 + #.028 OTH1 + #.024 OTH3 + #.021 ACETO2 + #.02 OTH2 + #.009 ACET + #.007 CROOH + #.007 CO + #.007 MGLY + #.005 OH + #.004 HOCCO3 + #.003 ETHEO2 + #.003 OTH4 + #.002 MEO2 + #.001 ETCO3 + #1.208 XC + #.359 SumRO2 + #.485 SumRCO3		Same k as rxn S003			
H630	CROOH_P3 + HO2 = #.963 CROOH + #.033 OTHN + #.004 ROOH + #.773 XC		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H631	CROOH_P3 + SumRO2 = SumRO2 + #7.934 NROG + #.426 RCHO + #.227 HO2 + #.225 MECO3 + #.205 KET2 + #.152 RO2C + #.076 OTH4 + #.075 MECHO + #.069 OTH3 + #.063 HCHO + #.049 BACL + #.022 CROOH + #.016 ETCHO + #.016 AACID + #.015 R2CO3 + #.014 RO2XC + #.014 zRCNO3 + #.014 OTH1 + #.012 OTH2 + #.01 ACETO2 + #.005 ACET + #.004 MGLY + #.004 CO + #.003 OH + #.002 HOCCO3 + #.002 ETHEO2 + #.001 MEO2 + #.001 OTHN + #1.395 XC + #.179 SumRO2 + #.242 SumRCO3		Same k as rxn S004			
H632	CROOH_P3 + SumRCO3 = SumRCO3 + #8.191 NROG + #.535 RCHO + #.249 HO2 + #.227 MECO3 + #.154 RO2C + #.097 BACL + #.09 OTH3 + #.082 HCHO + #.079 KET2 + #.075 MECHO + #.028 OTH1 + #.02 ACETO2 + #.018 CROOH + #.017 R2CO3 + #.017 ETCHO + #.016 AACID + #.014 RO2XC + #.014 zRCNO3 + #.013 OTH2 + #.009 ACET + #.006 MGLY + #.004 CO + #.003 OH + #.002 HOCCO3 + #.002 ETHEO2 + #.002 OTH4 + #.002 MEO2 + #1.515 XC + #.192 SumRO2 + #.246 SumRCO3		Same k as rxn S009			
G928	ROOH + OH = #.491 OH + #.44 ROOH_P1 + #.157 MEK + #.155 ACET + #.131 KET2 + #.068 CROOH + #.068 HO2 + #.028 ETCHO + #.02 RCHO + #.001 OTH4 + #-0.016 XC + #.44 SumRO2	1.05e-11				
G929	ROOH + HV = OH + #.692 HO2 + #.384 ACET + #.267 MECHO + #.219 ETO2 + #.144 MEK + #.126 HCHO + #.109 KET2 + #.093 RO2C + #.076 TBUO + #.067 ETCHO + #.009 MEO2 + #.005 RO2XC + #.002 zRHNO3 + #.002 zR1NO3 + #.093 XC + #.326 SumRO2		Phot Set= COOH			
G930	ROOH_P1 + NO = #.941 NO2 + #.492 HO2 + #.42 ACET + #.336 MECHO + #.216 RO2C + #.18 ETO2 + #.145 HCHO + #.132 TBUO + #.107 OH + #.091 MEK + #.06 ETCHO + #.057 KET2 + #.046 R1NO3 + #.013 RHNO3 + #.011 MEO2 + #.01 RO2XC + #.009 ETHEO2 + #.009 zRHNO3 + #.007 CROOH + #.004 RCHO + #.003 GLCHO + #.001 zR1NO3 + #-0.247 XC + #.426 SumRO2		Same k as rxn S001			
G931	ROOH_P1 + NO3 = NO2 + #.515 HO2 + #.449 ACET + #.353 MECHO + #.227 RO2C + #.199 ETO2 + #.149 HCHO + #.141 TBUO + #.113 OH + #.098 MEK + #.063 ETCHO + #.061 KET2 + #.012 MEO2 + #.011 RO2XC + #.01 ETHEO2 + #.009 zRHNO3 + #.007 CROOH + #.005 RCHO + #.003 GLCHO + #.001 zR1NO3 + #-0.202 XC + #.459 SumRO2		Same k as rxn S003			
G932	ROOH_P1 + HO2 = #.4 ROOH + #2.4 XC		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
G933	ROOH_P1 + SumRO2 = SumRO2 + #.257 HO2 + #.257 ACET + #.177 MECHO + #.113 RO2C + #.1 ETO2 + #.082 OTH2 + #.08 ROOH + #.075 HCHO + #.075 MEK + #.074 CROOH + #.074 OTH3 + #.071 OTH1 + #.071 TBUO + #.056 OH + #.054 KET2 + #.04 ETCHO + #.024 OTH4 + #.01 RCHO + #.006 MEO2 + #.005 RO2XC + #.005 ETHEO2 + #.005 zRHNO3 + #.002 GLCHO + #.001 zR1NO3 + #-0.01 XC + #.229 SumRO2	Same k as rxn S004				
G934	ROOH_P1 + SumRCO3 = SumRCO3 + #.377 ACET + #.26 HO2 + #.185 MECHO + #.176 ETO2 + #.144 CROOH + #.141 TBUO + #.116 RO2C + #.106 MEK + #.077 KET2 + #.074 HCHO + #.063 OH + #.049 ETCHO + #.017 RCHO + #.012 MEO2 + #.006 RO2XC + #.005 zRHNO3 + #.005 ETHEO2 + #.002 GLCHO + #.001 zR1NO3 + #-0.296 XC + #.315 SumRO2	Same k as rxn S009				
H633	AFG1 + OH = #.563 OH + #.371 AFG3 + #.329 AFG1_A1 + #.19 CROOH + #.108 AFG1_A2 + #.001 HPALD + #.001 RO2C + #.001 HO2 + #.001 MGLY + #-0.369 XC + #.001 SumRO2	9.17e-11				
H634	AFG1 + HV = AFG3 + OH + HO2 + #-1 XC	Phot Set= AFGS, qy= 3.50e-1				
H635	AFG1_A1 = CROOH + OH	7.15e-1	1.64e+11	15.60	0.00	
H636	AFG1_A1 + NO = #1.352 MGLY + #.946 HO2 + #.946 NO2 + #.27 CROOH + #.27 CO + #.054 RCNO3 + #-0.838 XC	Same k as rxn S001				
H637	AFG1_A2 = CROOH + OH	7.15e-1	1.64e+11	15.60	0.00	
H638	AFG1_A2 + NO = #.946 HO2 + #.946 NO2 + #.901 BACL + #.901 GLY + #.054 RCNO3 + #.045 CROOH + #.045 CO + #-0.838 XC	Same k as rxn S001				
H639	AFG2A + OH = #.339 AFG2A_P1 + #.31 AFG2A_A1 + #.279 MACO3 + #.063 RO2C + #.053 OH + #.049 CO2 + #.044 KET2 + #.015 MGLY + #.012 HO2 + #.008 RCHO + #.006 RO2XC + #.006 zRCNO3 + #.003 AFG3 + #.003 BACL + #.003 CO + #.002 R2CO3 + #.001 CROOH + #.001 GLY + #.229 XC + #.408 SumRO2 + #.281 SumRCO3	5.69e-11				
H640	AFG2A + HV = AFG3 + OH + #.914 MEO2 + #.076 ETO2 + #.01 RO2C + #.01 ACET + #.01 HO2 + #-2.096 XC + SumRO2	Phot Set= AFGS, qy= 2.50e-1				
H641	AFG2A_A1 = AFG2A_P2 + SumRO2	7.15e-1	1.64e+11	15.60	0.00	
H642	AFG2A_A1 + NO = #.946 HO2 + #.946 NO2 + #.487 MGLY + #.487 GLY + #.459 RCHO + #.459 CO + #.054 RCNO3 + #.108 XC	Same k as rxn S001				
H643	AFG2A_P1 + NO = #.944 NO2 + #.942 CROOH + #.916 MECO3 + #.056 RCNO3 + #.026 ETCO3 + #.002 MGLY + #.002 BACL + #.002 HO2 + #-1.802 XC + #.942 SumRCO3	Same k as rxn S001				
H644	AFG2A_P1 + NO3 = NO2 + #.998 CROOH + #.969 MECO3 + #.028 ETCO3 + #.002 MGLY + #.002 BACL + #.002 HO2 + #-2.026 XC + #.997 SumRCO3	Same k as rxn S003				

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H645	AFG2A_P1 + HO2 = #.943 OTHN + #.057 CROOH + #-6.601 XC		Same k as rxn S002			
H646	AFG2A_P1 + SumRO2 = SumRO2 + #.749 CROOH + #.485 MECO3 + #.251 BACL + #.014 ETCO3 + #.001 MGLY + #.001 HO2 + #-0.764 XC + #.499 SumRCO3		Same k as rxn S004			
H647	AFG2A_P1 + SumRCO3 = SumRCO3 + #.501 BACL + #.499 CROOH + #.485 MECO3 + #.014 ETCO3 + #.001 MGLY + #.001 HO2 + #-0.514 XC + #.499 SumRCO3		Same k as rxn S009			
H648	AFG2A_P2 + NO = #.946 NO2 + #.847 RCHO + #.847 OH + #.847 CO2 + #.07 R2CO3 + #.059 MGLY + #.054 RCNO3 + #.03 HO2 + #.216 XC + #.07 SumRCO3		Same k as rxn S001			
H649	AFG2A_P2 + NO3 = NO2 + #.895 RCHO + #.895 OH + #.895 CO2 + #.073 R2CO3 + #.062 MGLY + #.031 HO2 + #.12 XC + #.073 SumRCO3		Same k as rxn S003			
H650	AFG2A_P2 + HO2 = OTHN + #-7 XC		Same k as rxn S002			
H651	AFG2A_P2 + SumRO2 = SumRO2 + #.448 RCHO + #.448 OH + #.448 CO2 + #.25 BACL + #.25 CROOH + #.037 R2CO3 + #.031 MGLY + #.016 HO2 + #.306 XC + #.037 SumRCO3		Same k as rxn S004			
H652	AFG2A_P2 + SumRCO3 = SumRCO3 + #.5 BACL + #.448 RCHO + #.448 OH + #.448 CO2 + #.037 R2CO3 + #.031 MGLY + #.016 HO2 + #.556 XC + #.037 SumRCO3		Same k as rxn S009			
H653	AFG2B + OH = #.661 MACO3 + #.251 AFG2B_P1 + #.079 RO2C + #.04 OH + #.039 CO2 + #.038 BACL + #.038 RCHO + #.037 HO2 + #.025 MGLY + #.01 GLY + #.008 RO2XC + #.008 zRCNO3 + #.003 R2CO3 + #.001 AFG3 + #.001 KET2 + #1.368 XC + #.338 SumRO2 + #.664 SumRCO3	3.52e-11				
H654	AFG2B + HV = AFG3 + OH + #.969 MEO2 + #.031 ETO2 + #-1.031 XC + SumRO2		Phot Set= AFGS, qy= 1.50e-1			
H655	AFG2B_P1 + NO = #.913 NO2 + #.912 CROOH + #.885 MECO3 + #.079 RCNO3 + #.027 ETCO3 + #.008 RNNO3 + #.002 BACL + #.001 HO2 + #-0.736 XC + #.912 SumRCO3		Same k as rxn S001			
H656	AFG2B_P1 + NO3 = NO2 + #.999 CROOH + #.968 MECO3 + #.031 ETCO3 + #.003 BACL + #.001 HO2 + #-1.036 XC + #.999 SumRCO3		Same k as rxn S003			
H657	AFG2B_P1 + HO2 = OTHN + #-6 XC		Same k as rxn S002			
H658	AFG2B_P1 + SumRO2 = SumRO2 + #.999 CROOH + #.484 MECO3 + #.015 ETCO3 + #.001 BACL + #.001 HO2 + #-0.012 XC + #.499 SumRCO3		Same k as rxn S004			
H659	AFG2B_P1 + SumRCO3 = SumRCO3 + #.999 CROOH + #.968 MECO3 + #.031 ETCO3 + #.003 BACL + #.001 HO2 + #-1.036 XC + #.999 SumRCO3		Same k as rxn S009			
H660	AFG3 + OH = AFG3_P1 + SumRO2	5.69e-11				

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H661	AFG3_P1 + NO = #.908 NO2 + #.861 RCHO + #.837 MECO3 + #.092 RCNO3 + #.055 ETCO3 + #.036 KET2 + #.009 MACO3 + #.006 HCHO + #.004 R2CO3 + #.004 MECHO + #.002 HO2 + #.001 RO2C + #.001 AFG3 + #.001 MGLY + #.001 BACL + #.186 XC + #.001 SumRO2 + #.905 SumRCO3		Same k as rxn S001			
H662	AFG3_P1 + NO3 = NO2 + #.946 RCHO + #.919 MECO3 + #.063 ETCO3 + #.041 KET2 + #.011 MACO3 + #.007 HCHO + #.005 MECHO + #.005 R2CO3 + #.002 HO2 + #.002 RO2C + #.001 AFG3 + #.001 MGLY + #.001 BACL + #-0.105 XC + #.002 SumRO2 + #.998 SumRCO3		Same k as rxn S003			
H663	AFG3_P1 + HO2 = #.988 CROOH + #.012 HPALD + XC		Same k as rxn S002			
H664	AFG3_P1 + SumRO2 = SumRO2 + #.473 RCHO + #.459 MECO3 + #.278 KET2 + #.237 BACL + #.032 ETCO3 + #.006 AFG3 + #.005 MACO3 + #.004 HCHO + #.003 MECHO + #.003 R2CO3 + #.002 MGLY + #.001 HO2 + #.001 RO2C + #.675 XC + #.001 SumRO2 + #.499 SumRCO3		Same k as rxn S004			
H665	AFG3_P1 + SumRCO3 = SumRCO3 + #.48 MECO3 + #.474 BACL + #.473 RCHO + #.041 KET2 + #.032 ETCO3 + #.005 MACO3 + #.004 AFG3 + #.004 HCHO + #.003 MGLY + #.003 MECHO + #.003 R2CO3 + #.001 HO2 + #.001 RO2C + #.879 XC + #.001 SumRO2 + #.52 SumRCO3		Same k as rxn S009			
H666	AFG4 + OH = #.734 AFG4_P1 + #.266 OLEP + #.266 HO2 + #.532 XC + #.734 SumRO2	3.86e-10				
H667	AFG4_P1 + NO = #.877 NO2 + #.571 HO2 + #.533 OLEA1 + #.228 OH + #.183 LVKS + #.107 RHNO3 + #.067 OLEP + #.067 RO2C + #.054 MEO2 + #.042 OLEA2 + #.029 OTHN + #.016 RNNO3 + #.012 BACL + #.01 RO2XC + #.009 MECO3 + #.008 zRNNO3 + #.006 AFG2A + #.004 CROOH + #.004 MGLY + #.003 ETO2 + #.002 R2CO3 + #.002 RCOOH + #.002 BUDAL + #.001 zRCNO3 + #.001 HPALD + #1.612 XC + #.134 SumRO2 + #.011 SumRCO3		Same k as rxn S001			
H668	AFG4_P1 + NO3 = NO2 + #.652 HO2 + #.604 OLEA1 + #.258 OH + #.211 LVKS + #.078 OLEP + #.078 RO2C + #.063 MEO2 + #.047 OLEA2 + #.034 OTHN + #.014 BACL + #.012 RO2XC + #.011 MECO3 + #.01 zRNNO3 + #.007 AFG2A + #.004 CROOH + #.004 MGLY + #.003 ETO2 + #.002 R2CO3 + #.002 RCOOH + #.002 BUDAL + #.001 zRCNO3 + #.001 HPALD + #1.761 XC + #.156 SumRO2 + #.013 SumRCO3		Same k as rxn S003			
H669	AFG4_P1 + HO2 = #.61 OTHN + #.39 RUOOH + #-2.27 XC		Same k as rxn S002			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
H670	AFG4_P1 + SumRO2 = SumRO2 + #.377 OLEP + #.326 HO2 + #.302 OLEA1 + #.25 LVKS + #.129 OH + #.039 RO2C + #.034 OTHN + #.031 MEO2 + #.024 OLEA2 + #.007 BACL + #.006 RO2XC + #.005 MECO3 + #.005 zRNNO3 + #.003 AFG2A + #.002 CROOH + #.002 MGLY + #.002 ETO2 + #.001 R2CO3 + #.001 RCOOH + #.001 BUDAL + #.001 zRCNO3 + #1.91 XC + #.078 SumRO2 + #.006 SumRCO3		Same k as rxn S004			
H671	AFG4_P1 + SumRCO3 = SumRCO3 + #.464 LVKS + #.401 HO2 + #.309 OLEA1 + #.165 OLEP + #.134 OH + #.073 RO2C + #.063 MEO2 + #.024 OLEA2 + #.018 OTHN + #.014 BACL + #.011 RO2XC + #.009 zRNNO3 + #.009 MECO3 + #.007 AFG2A + #.003 ETO2 + #.002 CROOH + #.002 MGLY + #.001 zRCNO3 + #.001 R2CO3 + #.001 RCOOH + #.001 BUDAL + #2.141 XC + #.15 SumRO2 + #.01 SumRCO3		Same k as rxn S009			
G935	APAN = ACO3 + NO2 + SumRCO3	4.63e-4	8.56e+16	27.82	-0.20	
G936	APAN + OH = #.519 NO3 + #.481 APAN_P1 + #.389 OTH3 + #.13 RCOOH + #-0.389 XC + #.481 SumRO2	1.81e-11				
G937	APAN + O3 = #.755 CO + #.58 OH + #.56 CO2 + #.5 NO2 + #.5 PAN2 + #.5 HCHO + #.185 HCHO2 + #.08 HO2 + #-0.5 XC	1.32e-18				81
G938	APAN + HV = #.6 ACO3 + #.6 NO2 + #.4 HCHO + #.4 CO2 + #.4 CO + #.4 HO2 + #.4 NO3 + #.6 SumRCO3		Phot Set= PPN-11			
G939	APAN_P1 + NO = #1.727 NO2 + #.996 CO2 + #.73 HO2 + #.727 HCHO + #.727 CO + #.727 OH + #.27 GLCHO + #.27 NO3 + #.004 PAN2 + #-0.002 XC + #-0.001 XN		Same k as rxn S001			
G940	APAN_P1 + NO3 = #1.727 NO2 + #.996 CO2 + #.73 HO2 + #.727 HCHO + #.727 CO + #.727 OH + #.27 GLCHO + #.27 NO3 + #.004 PAN2 + #-0.002 XC + #-0.001 XN		Same k as rxn S003			
G941	APAN_P1 + HO2 = PAN2		Same k as rxn S002			
G942	APAN_P1 + SumRO2 = SumRO2 + #.502 PAN2 + #.498 CO2 + #.365 HO2 + #.363 NO2 + #.363 HCHO + #.363 CO + #.363 OH + #.135 GLCHO + #.135 NO3		Same k as rxn S004			
G943	APAN_P1 + SumRCO3 = SumRCO3 + #.502 PAN2 + #.498 CO2 + #.365 HO2 + #.363 NO2 + #.363 HCHO + #.363 CO + #.363 OH + #.135 GLCHO + #.135 NO3		Same k as rxn S009			
G944	MAPAN = MACO3 + NO2 + SumRCO3	4.63e-4	8.56e+16	27.82	-0.20	
G945	MAPAN + OH = #.8 NO3 + #.6 OTH3 + #.2 MAPAN_P1 + #.2 RCOOH + #.2 XC + #.2 SumRO2	2.90e-11				2
G946	MAPAN + O3 = #.723 OH + #.67 MAPAN_P2 + #.67 HCHO + #.33 PAN2 + #.168 CO + #.122 HCHO2 + #.053 HO2 + #.04 CO2 + #.67 SumRO2	8.20e-18				2
G947	MAPAN + HV = #.6 MACO3 + #.6 NO2 + #.4 MECO3 + #.4 CO2 + #.4 HCHO + #.4 NO3 + SumRCO3		Phot Set= PPN-11			
G948	MAPAN_P1 + NO = #.969 KET2 + #.969 CO2 + #.969 NO3 + #.969 NO2 + #.031 PAN2 + #-1.907 XC + #.031 XN		Same k as rxn S001			

Table A-3 (continued)

Label	Reaction and Products [a]	Rate Parameters [b] k(300)	A	Ea	B	Notes [c]
G949	MAPAN_P1 + NO3 = KET2 + CO2 + NO3 + NO2 + #-2 XC		Same k as rxn S003			
G950	MAPAN_P1 + HO2 = PAN2 + XC		Same k as rxn S002			
G951	MAPAN_P1 + SumRO2 = SumRO2 + #.5 PAN2 + #.5 KET2 + #.5 CO2 + #.5 NO3 + #-0.5 XC		Same k as rxn S004			
G952	MAPAN_P1 + SumRCO3 = SumRCO3 + KET2 + CO2 + NO3 + #-2 XC		Same k as rxn S009			
G953	MAPAN_P2 + NO = CO2 + HCHO + CO + NO3 + NO2		Same k as rxn S001			
G954	MAPAN_P2 + NO3 = CO2 + HCHO + CO + NO3 + NO2		Same k as rxn S003			
G955	MAPAN_P2 + HO2 = PAN2		Same k as rxn S002			
G956	MAPAN_P2 + SumRO2 = SumRO2 + #.5 CO2 + #.5 HCHO + #.5 CO + #.5 NO3 + #.5 PAN2		Same k as rxn S004			
G957	MAPAN_P2 + SumRCO3 = SumRCO3 + #.5 PAN2 + #.5 CO2 + #.5 HCHO + #.5 CO + #.5 NO3		Same k as rxn S009			

Notes

[a] Format of reaction listing: "=" separates reactants from products; "#*number*" indicates stoichiometric coefficient, "#*coefficient* {*product list*}" means that the stoichiometric coefficient is applied to all the products listed.

[b] Except as indicated, the rate constants are given by $k(T) = A \cdot (T/300)^B \cdot e^{-Ea/RT}$, where the units of k and A are cm^3 $molec^{-1}$ s^{-1}, Ea are kcal mol^{-1}, T is ^oK, and R=0.0019872 kcal mol^{-1} deg^{-1}. The following special rate constant expressions are used:

Phot Set = *name*: The absorption cross sections and (if applicable) wavelength-dependent quantum yields for the photolysis reaction, where "*name*" indicates the photolysis set used. These data are given in ASCII .PHF files with the same name and are available upon request. If a "qy=*number*" notation is given, the number given is the overall quantum yield, which is assumed to be wavelength independent.

Falloff: The rate constant as a function of temperature and pressure is calculated using $k(T,M) = \{k0(T)\cdot[M]/[1 + k0(T)\cdot[M]/kinf(T)]\}\cdot F^Z$, where $Z = \{1 + [\log10\{k0(T)\cdot[M])/kinf(T)\}/N]^2\}^{-1}$, [M] is the total pressure in molecules cm^{-3}, F and N are as indicated on the table, and the temperature dependences of k and kinf are as indicated on the table.

k = k0+k3M(1+k3M/k2): The rate constant as a function of temperature and pressure is calculated using $k(T,M) = k0(T) + k3(T)\cdot[M] \cdot(1 + k3(T)\cdot[M]/k2(T))$, where [M] is the total bath gas (air) concentration in molecules cm-3, and the temperature dependences for k0, k2 and k3 are as indicated on the table.

k = k1 + k2 [M]: The rate constant as a function of temperature and pressure is calculated using $k(T,M) = k1(T) + k2(T)\cdot[M]$, where [M] is the total bath gas (air) concentration in molecules cm-3, and the temperature dependences for k1, and k2 are as indicated on the table.

Same K as for (reaction): Uses the same rate constant as the reaction indicated.

[c] Documentation notes are as follows:

1 Based on the NASA (2015) evaluation.

2 Based on the current (as of July, 2016) IUPAC (2016) evaluation.

3 IUPAC (2015) does not recommend incorporation of this reaction in models of the atmosphere but sets an upper limit of 1×10^{-22} cm^3 $molec^{-1}$ s^{-1} for the bimolecular process only. NASA (2011) gives an upper limit of 2.0×10^{-21} cm^3 $molec^{-1}$ s^{-1}. It is recommended that this reaction not be included in gas-phase mechanisms, but that models include this as a heterogeneous process if appropriate.

4 Derived from the recommendations of the NASA (2015) evaluation for O_2 and N_2 and their mole fractions in air.

5 The temperature and pressure-dependence parameters were adjusted to fit the rate constants for the HNO_3

Table A-3 (continued)

forming reaction calculated using the temperature-dependent rate expression of NASA (2015) for the total HO_2 + NO reaction and the temperature- and pressure-dependent expression for the ratio of the rate constant for the HNO_3-forming reaction relative to the total rate constant as given by Butkovska et al (2007), which is recommended by IUPAC (2015). The data were fit for a standard atmosphere for 0 - 5 KM altitude, and atmospheres for 0 - 5 KM with the temperature increased or decreased by 10K.

6 Temperature-dependence parameters adjusted to fit the rate constant for a water concentration corresponding to 50% RH at 300K as a function of temperature at 1 atmosphere, using the parameters given by Stavrakou et al (2013). The reaction is assumed not to be pressure-dependent. This formula somewhat overpredicts the reaction at 100%RH, but probably not by more than the likely uncertainty.

7 SumRO2 or SumRCO3 is added as a product to all reactions that form peroxy or acyl peroxy radicals that react with other peroxy radicals. See discussion of SumRO2 and SumRCO3 in footnotes to Table 1.

8 Absorption cross-sections and quantum yields at 298K and 1 atmosphere are from the IUPAC (2015) recommendation. IUPAC gives recommendation for effect of temperature on the absorption cross-sections, but the effect is negligible (<1% change in action spectrum) for tropospheric modeling applications. The recommendation indicates no significant temperature or pressure effects on quantum yields for radical formation, but that the quantum yield for H_2 + CO formation increases with decreasing pressure. The pressure effect is expected to increase the overall rate constant by about 15% at 15 KM, which is probably a small effect compared to the other uncertainties in modeling reaction rates at such altitudes.

9 Rate constant expression from Calvert et al (2000).

10 Rate constant and mechanism derived using the estimation methods in the current version of the SAPRC mechanism generation system.

11 Absorption cross sections and quantum yields based on current IUPAC (2015) recommendation. Relative product yields based on calculation using IUPAC (2015) wavelength-dependent quantum yields for both processes and solar Z=0 relative spectral distribution.

12 Abstraction from methyl or ethyl groups, estimated to occur ~4% of the time, is ignored.

13 Assume this reacts with same rate constant as analogous reaction of acetaldehyde.

14 NASA (2011) recommendation used for absorption cross sections and overall quantum yields for the three initial reactions, which were HCO + $HOCH_2$(.) (83%); CO + CH_3OH (10%); and OH + $HCOCH_2$(.) (7%).

15 Absorption cross sections of Orlando and Tyndall (2003) for peroxyacetic acid used with unit quantum yields assumed.

16 Assumed to have the same photolysis rate as methyl hydroperoxide

17 ACETO2 is $CH_3C(O)CH_2OO$. The Arrhenius parameters were derived to get same rate constants in the 270-330K temperature range as those derived using the current IUPAC (2015) recommended temperature-dependence parameters.

18 Absorption cross sections and quantum yields based on IUPAC (2015) recommendations. The absorption cross sections are for T=298K. Total quantum yields are calculated for 1 atm and T=298K using the complex expression recommended by IUPAC. For atmospheric conditions the recommendation is to assume most of the reaction occurrs via formation of CH_3CO. and CH_3. However, it is necessary to reduce the acetone photolysis rate by a factor of 0.5 in order for the mechanism to correctly simulate effects of acetone on NO oxidation and ozone formation in incremental reactivity environmental chamber experiments.

19 Absorption cross-sections from IUPAC (2015). Pressure-dependent quantum yields derived using the pressure-dependence recommendation given by IUPAC, but for 425 torr N_2. This "pressure" adjustment was made so the calculated photolysis rates, relative to NO_2, are consistent with the data of Plum et al (1983) and Klotz et al (2000).

20 Rate constant at 296 from Talukdar et al (2011). Temperature dependence estimated by assuming that the A factor per -CHO group is the same as used for acetaldehyde.

21 Absorption cross sections of IUPAC (2015) used. IUPAC gives no recommendation of quantum yields, and no new data seem to be available since SAPRC-07 was developed. Quantum yields derived in the same way as for SAPRC-07, based on recommendation of pressure-dependence of quantum yields for methyl glyoxal from IUPAC, with pressure dependence adjusted to get same photolysis rates relative to NO2 as measured

Table A-3 (continued)

by Plum et al (1983) and Klotz et al (2000).

22 Absorption cross sections recommended by Calvert et al (2011). Based on the discussion there, photolysis under atmospheric conditions forms primarily non-radical products, with benzene + CO formation being important at wavelengths that are too low to be important at ground-level conditions. However, using their recommended quantum yields for the higher wavelengths significantly overpredicts rates of consumption of benzaldehyde measured in chamber experiments, which were used as the basis for the photolysis rate used in previous version of this mechanism. Therefore, for this mechanism the overall quantum yield was derived to give the same atmospheric photolysis rate as used in SAPRC-07. The overall quantum yield derived (0.09) is higher than used in SAPRC-07 because the updated absorption cross sections give lower photolysis rates for the same quantum yields at higher wavelengths. Calvert et al (2011) gives no recommendation as to the major products formed at higher wavelengths, but indicates that they are "unidentified products leading to polymer". Currently they are represented as lost carbon, but it may be more appropriate to represent them using a non-volatile model species such as OTHN.

23 Rate constant expression from review of Calvert et al (2015).

24 The current mechanism generation system does not reliably predict mechanisms for phenolic compounds, predicting much higher rates of ozone formation and NO oxidation in chamber experiments than observed experimentally. Therefore, for this version of the mechanism we retain the simplified and parameterized representation of the reactions of these compounds used in SAPRC-07 and SAPRC-11, with phenolic product model species changed to be consistent with those used in the current mechanism and parameters adjusted to give best fits to the chamber data. Note that the rate constants and mechanisms for CRES and XYNL are based on measured rate constants and chamber data for o-cresol and 2,4-dimethyl phenol, respectively, which are taken as representative. These mechanisms are highly uncertain.

25 Rate constant expression from review of Calvert et al (2011).

26 The SVPHE model species is used to represent unspecified semi-volatile, non-nitrogen-containing products of the reactions of OH and NO_3 with phenolic compounds. A highly simplified parameterized mechanism is used based roughly on the simplified representations used for the phenolic compounds themselves. This is highly uncertain.

27 NPHE is used to represent various nitrogen-containing aromatic products formed primarily in the reactions of phenolic compounds or naphthalenes, and its mechanism is based that estimated for nitrophenols. The rate constant used is from SAPRC-07, and is in the range cited by Barnes (2006) for various nitrocresols. The reaction is assumed to occur via abstraction of H from OH, analogous to pathway in the phenol and cresol + OH reactions that occur with similar rates.

28 Rates of photolysis of nitrophenols forming HONO, relative to the photolysis rate of NO_2, based on the data of Bejan et al (2006) for 2-nitrophenol and various methyl substituted 2-nitrophenols. The co-products are unknown, and are assumed to go mainly into the particle phase and its gas-phase reactivity is assumed not to be significant. Loss by other photolysis processes might be significant, but are ignored. Nitrophenols were found to have lifetimes relative to photolysis in the Euphore chamber of 1-2 hours (Barnes, private communication, 2007). A photolysis rate relative to NO_2 of 0.015 corresponds approximately to this range. The products formed are unknown, but based on the data of Bejan et al (2006) it is apparent that NO_2 formation is not important and that HONO formation represents only about 10% of this process. We assume that the co-product forming HONO has similar reactivity of phenol and that the product for the other routes can be represented by the NPHE model species, so this reaction has no effect on the model and is ignored.

29 The "NAPS" model species is used to represent all naphthalenes but its mechanism is based on that derived for naphthalene. The current mechanism generation system is not yet capable of predicting mechanisms for naphthalene, so the highly simplified and parameterized representation used in SAPRC-07 is retained, with the product model species changed to be consistent with the model species used in this version of the mechanism, and the parameters adjusted to fit results of naphthalene - NO_x chamber experiments.

30 The NAPPRD model species is used to represent unspecified non-nitrogen-containing products of the reactions of OH with phenolic naphthalenes. A highly simplified mechanism is used, with the same rate constants as used in the simplified mechanism for NVPHE, used for unspecified products in the reactions of the phenols.

Table A-3 (continued)

31 The model species "PHOT" is used to represent highly photoreactive model species such as nitrites, which are not important enough in emissions to be represented by separate model species, but is not well represented by other model species. A highly simplified mechanism is used for such compounds, using photolysis rates calculated for biacetyl. This model species should not be used for assessing impacts of specific compounds, only for representing compounds in as minor components in mixtures.

32 The main compound represented by IMINE is $CH_3CH=NH$, which is assumed to rapidly hydrolyze to form acetaldehyde and ammonia. Therefore it is treated as in steady state and replaced by the formation of MECHO and XN. "Lost nitrogen" is used for ammonia because it is not included in the gas-phase mechanism. The rate constant is arbitrarily set at 1 sec^{-1}, but is irrelevant if the steady state approximation is used.

33 The rate constants used for the reactions of peroxy radicals other than methyl peroxy with NO, HO2, and NO3 are the IUPAC (2016) recommendations for the corresponding reactions of ethyl peroxy.

34 The SumRO2 counter species is the sum of concentrations of all explicitly represented peroxy radical (RO_2) species and of the operators RO2C and RO2XC that are used for peroxy radicals not represented explicitly. The products formed would depend on the peroxy radical that this peroxy radical is reacting with, but it is assumed that most have alpha hydrogens and can form disproportionation products. For the current mechanism and mechanism generation system, it is assumed that half react to form O_2 + the corresponding alkoxy radicals and half disproportionate, with the two disproportionation reactions assumed to be equally probable if the peroxy radical has an alpha hydrogen. If the radical does not have an alpha hydrogen, the H is assumed to be abstracted from the other radical. Note that the current peroxy lumping approach requires that the same rate constant be used for the reaction of a given peroxy radical with any other peroxy radical if the latter is represented by SumRO2. SumRO2 is shown as a product in its reactions with individual peroxy or acyl peroxy species since its loss by these reactions are represented separately by its reactions with SumRO2 or SumRCO3.

35 The rate constant expression used for acyl peroxy + NO_2 reactions other than acetyl and $CH_3CH_2C(O)OO$ is based on the IUPAC (2016) for the high pressure limit for $CH_3CH_2C(O)OO + NO_2$.

36 The rate constant expression used for all acyl peroxy + NO reactions other than acetyl peroxy is based on the IUPAC (2016) recommendation for $CH_3CH_2C(O)OO$ + NO.

37 The rate constant expression used for all acyl peroxy + HO_2 reactions is based on the NASA (2015) recommendation for acetyl peroxy + HO_2.

38 The rate constant expression used for all acyl peroxy + NO_3 reactions is based on the IUPAC (2016) recommendation for acetyl peroxy + NO_3.

39 The rate constant and product yields used are the IUPAC (2016) recommendation for ethyl peroxy + acetyl peroxy. No information could be found about reactions of other peroxy or acyl peroxy combinations.

40 The rate constant used is the IUPAC (2016) recommendation for self-reactions of $CH_3CH_2C(O)OO$ radicals. Because of lack of information, this is assumed to apply to all acyl peroxy + acyl peroxy reactions except for acetyl peroxy.

41 The peroxy + peroxy rate constants are highly variable depending on the radical, but the peroxy lumping approach does not allow use of separate rate constants for each pair of rate constants. Except for methyl and ethyl peroxy, the rate constant used is the same as used for general peroxy + peroxy rate constants in the SAPRC-07 mechanism, and given the uncertainties and the approximations involved we see no reason to change this for this update. Note that these reactions are generally not important under atmospheric conditions, but not always negligible.

42 The SumRCO3 counter species is the sum of concentrations of all lumped or explicitly represented acyl peroxy radical (RCO_3) species that react with other peroxy radicals. Except when reacting with methyl peroxy radicals, the major reaction of these species with RO_2 or other RCO_3 radials is formation of the corresponding alkoxy radical, which rapidly decomposes to CO_2 and the corresponding alkyl radical. SumRCO3 is shown as a product in its reactions with individual peroxy or acyl peroxy species since its loss by these reactions are represented separately by its reactions with SumRO2 or SumRCO3.

43 The rate constant used for all methyl peroxy + other peroxy reactions is the average of IUPAC (2015) recommendations for methyl peroxy + methyl peroxy and methyl peroxy + ethyl peroxy rate reactions (3.5

Table A-3 (continued)

and 2 x 10^{-13} cm^3 $molec^{-1}$ s^{-1}, respectively). This may overpredict rates of these reactions for other radicals, though other primary + primary peroxy reactions have higher rate constants than this (IUPAC, 2015).

44 The rate constant and product yields used are the IUPAC (2016) recommendation for methyl peroxy + acetyl peroxy.

45 The rate constant used for all ethyl peroxy + other peroxy reactions is the IUPAC (2015) recommendation for the ethyl peroxy self reaction. This is higher than its rate constant for reaction with methyl peroxy, but lower than other primary + primary peroxy reactions (IUPAC, 2015).

46 The branching ratios and overall product yields are estimated using the procedures in the mechanism generation system.

47 This represents the isomerization of $HC(O)CH_2OO$ to form $HOOCH_2C(O)$ radicals, which undergoes O2 addition and additional isomerization to form $HOOC(O)CH_2OO$., which reacts primarily with NO and isomerizes to form $HOCH_2C(O)OO$, represented by HOCO3. The conversion of NO to NO_2 in these reactions is represented by RO2C and the reactions of the intermediate peroxy radicals with NO_3 or other peroxy radicals are ignored because of the relatively low yield of this radical. This is based on the procedure used processing reactions in the mechanism generation system for inclusion in the mechanism.

48 The chemical operator RO2C is used to represent NO to NO_2 conversions in reactions of peroxy radicals that are formed in relatively low yields (less than 10% yields in the photooxidations of organics processed using the mechanism generation system). This is similar to the approach used in SAPRC-99 for all peroxy radicals, and is based on the approximation that the products can be approximated by those that are formed when reactions with NO dominate. The rate constants used are the same as used for the corresponding reactions of SumRO2, which are based primarily on rate constants used for ethyl peroxy radicals.

49 The chemical operator RO2XC is used to represent NO consumption in the nitrate formation reactions of peroxy radicals that are formed in relatively low yields (less than 10% yields in the photooxidations of organics processed using the mechanism generation system). The zNitrate chemical operators are used to determine which nitrate is formed in these reactions, with a zNitrate species being used for each nitrate model species in the mechanism. The zNitrate species are used rather than the nitrate itself to properly account for nitrogen balance when the peroxy radicals react. These are also used to represent the formation of hydroperoxides when these radicals react with HO2 and the formation of other products when they react with NO_3, RO_2 or RCO_3 radicals. This is similar to the approach used in SAPRC-07 for all peroxy radicals. The rate constants used are the same as used for the corresponding reactions of SumRO2, which are based primarily on rate constants used for ethyl peroxy radicals.

50 The rate constant used is the IUPAC (2016) recommendation for acetyl peroxy self-reactions.

51 Assumed to have the same rate constant as the decomposition of PAN.

52 Same photolysis rates, rate constants and analogous mechanism as used for MECO3 and PAN.

53 Computed using the NASA (2015) recommended rate constant for the reverse reaction and the NASA(2015) recommended equilibrium constant for the zero or infinite pressure limits, assuming the same type of pressure dependence for both forward and reverse.

54 The absorption cross-sections used are those recommended by NASA (2015). They also recommend NO_3 quantum yield of 0.39 at 308 nm. This is assumed for all wavelengths of relevance, with total quantum yield of 1.

55 Unless indicated otherwise, the rate constant expression used for the decomposition of PAN analogue model species is that for the high pressure limit assigned for PPN. This is also used for PAN analogues whose reactions are derived using the mechanism generation system.

56 Absorption cross sections, quantum yields, and reactions based on those used for PPN. PAN2 is the lumped higher saturated PAN excluding PAN and PPN. ETO2 is replaced by NC3OO, the set of peroxy radicals formed from OH + propane.

57 Absorption cross sections, quantum yields, and reactions based on those used for PPN. PAN2N is assumed to be primarily $O_2NOCH_2C(O)OONO_2$, so the products are derived based on this.

58 Rate constants expressions based on the data of Caralp et al (1999).

59 Absorption cross sections, quantum yields, and reactions based on those used for PPN.

Table A-3 (continued)

60 Rate constant from Lotz and Zellner (2000). The reaction with NO is ignored because nitrite formation expected to be rapidly reversed by photolysis.

61 Rate constant expression from Blitz et al (1999).

62 Rate constant from Platz et al (1998).

63 Assumed to have the same rate constant as used for ethyl peroxy + HO2.

64 This is added to avoid problems in the (generally unlikely) conditions where these radicals are formed when concentrations of both NO_2 and HO_2 are low. The rate constant used is that used in the SAPRC-99 mechanism, which is arbitrary and is such that this process becomes significant only if $[NO_2] < \sim 3 \times 10^{-6}$ ppm and $[HO_2] < 1 \times 10^{-5}$ ppm. The likely process is reaction with some VOC forming compounds similar to those formed when the radicals react with HO2.

65 The NPRAD model species represents unknown naphthalene intermediates that react with NO2 forming nitrogen-containing products. In the absence of NO_2 the reaction with HO_2 is assumed to be the major fate, with the reaction with NO_2 forming a compound represented by NPHE and the reaction with HO_2 forming compounds represented by NAPPRD, the unspecified non-nitrogen-containing product of reactions of naphthalenes. The rate constants are unknown but are estimated to be similar to those for the reactions of acyl peroxy radicals.

66 The xNAMIN model species represents nitrogen-centered radicals that do not have alpha hydrogens and can only react with NO_2 or other radicals. In the absence of NO_2 the reaction with HO_2 is assumed to be the major fate, with the reaction with NO_2 forming a nitramine and the reaction with HO_2 forming an amine. The rate constants are unknown but are estimated to be similar to those for the reactions of acyl peroxy radicals.

67 Previous versions of SAPRC assumed that reaction with H_2O, forming the acid, was the major fate of stabilized Criegee biradicals, and represented their formation by the formation of the acid. These are now represented separately in order to account for effects of their reactions with SO_2 and NO_2 as well as H_2O. The rate constants probably depend on the radical, but for now the same rate constants are used for all reactions. See Sarwar et al (2013) for a discussion of stabilized Criegee biradical reactions and rate constants.

68 Rate constant from Welz et al (2012).

69 This reaction is predicted to be the major fate of Criegee biradicals under most atmospheric conditions, even if it has a rate constant lower than the upper limit of Welz et al (2012). The rate constant estimate used here is based on the estimate used by Sarwar et al (2013), which in turn is based on the rate constant ratio relative to reaction with SO_2 given by Calvert et al (1978). This is highly uncertain.

74 Rate constant as recommended or tabulated by Atkinson and Arey (2003).

80 Rate constant from Bierbach et al (1994).

81 Rate constant estimated based on the rate constants for MPAN (IUPAC, 2016) and the ratio of rate constants for methacrylic acid and acrylic acid (Calvert et al, 2011).

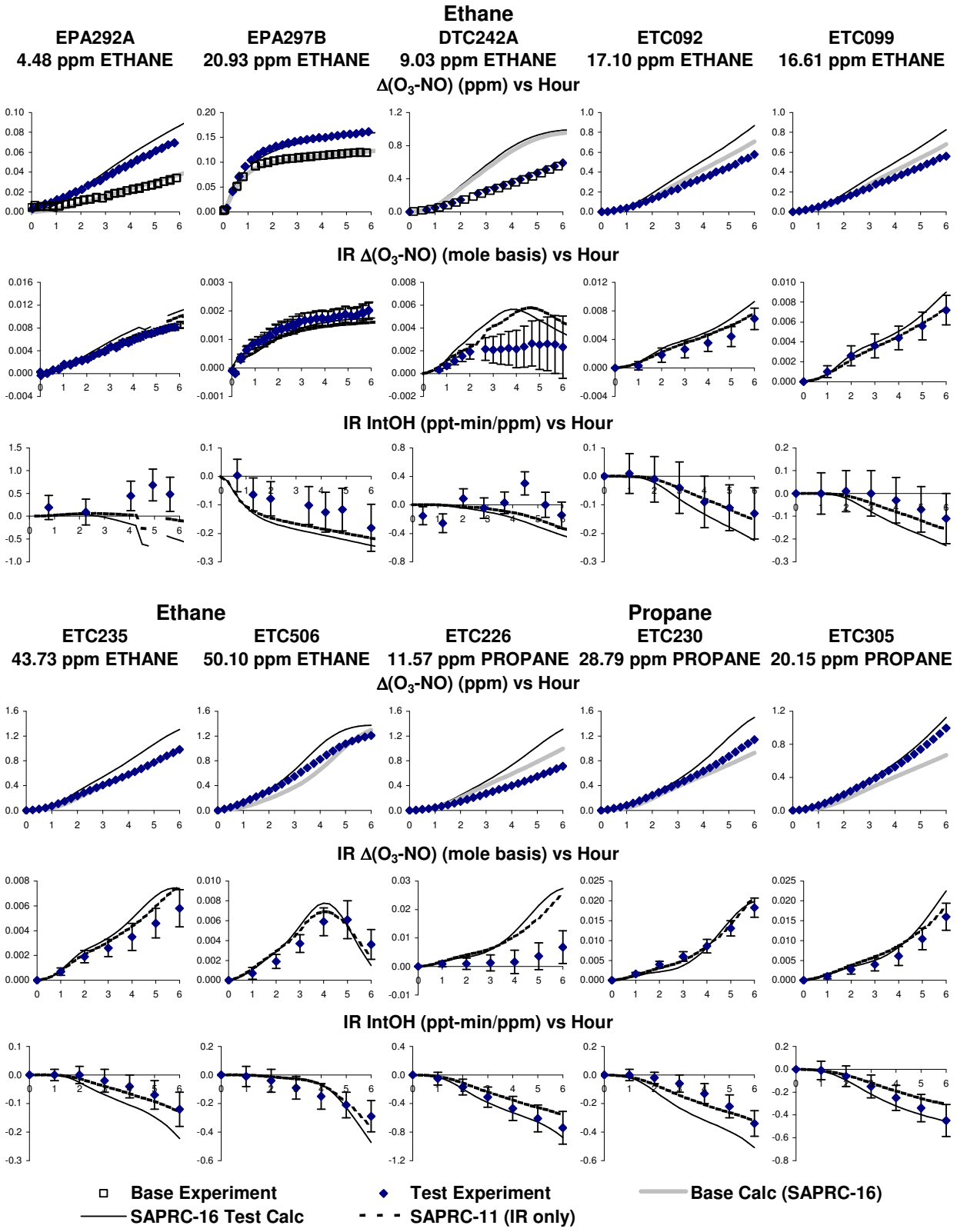
[d] Notes refer to assigned rate constants only. All other rate constants and product yields were derived using the assignments in the mechanism generation system.

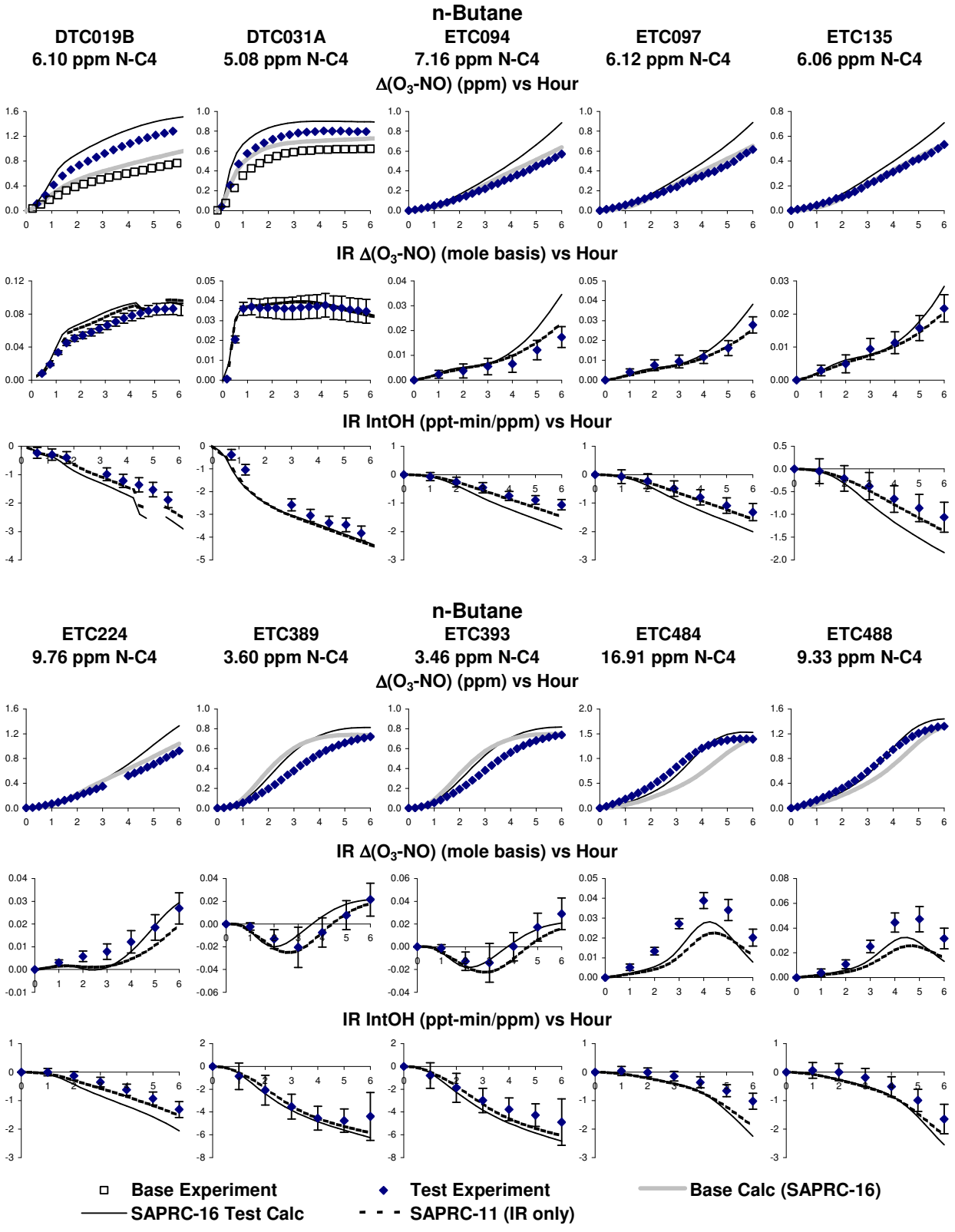
Appendix B. Plots of Results of Incremental Reactivity Experiments

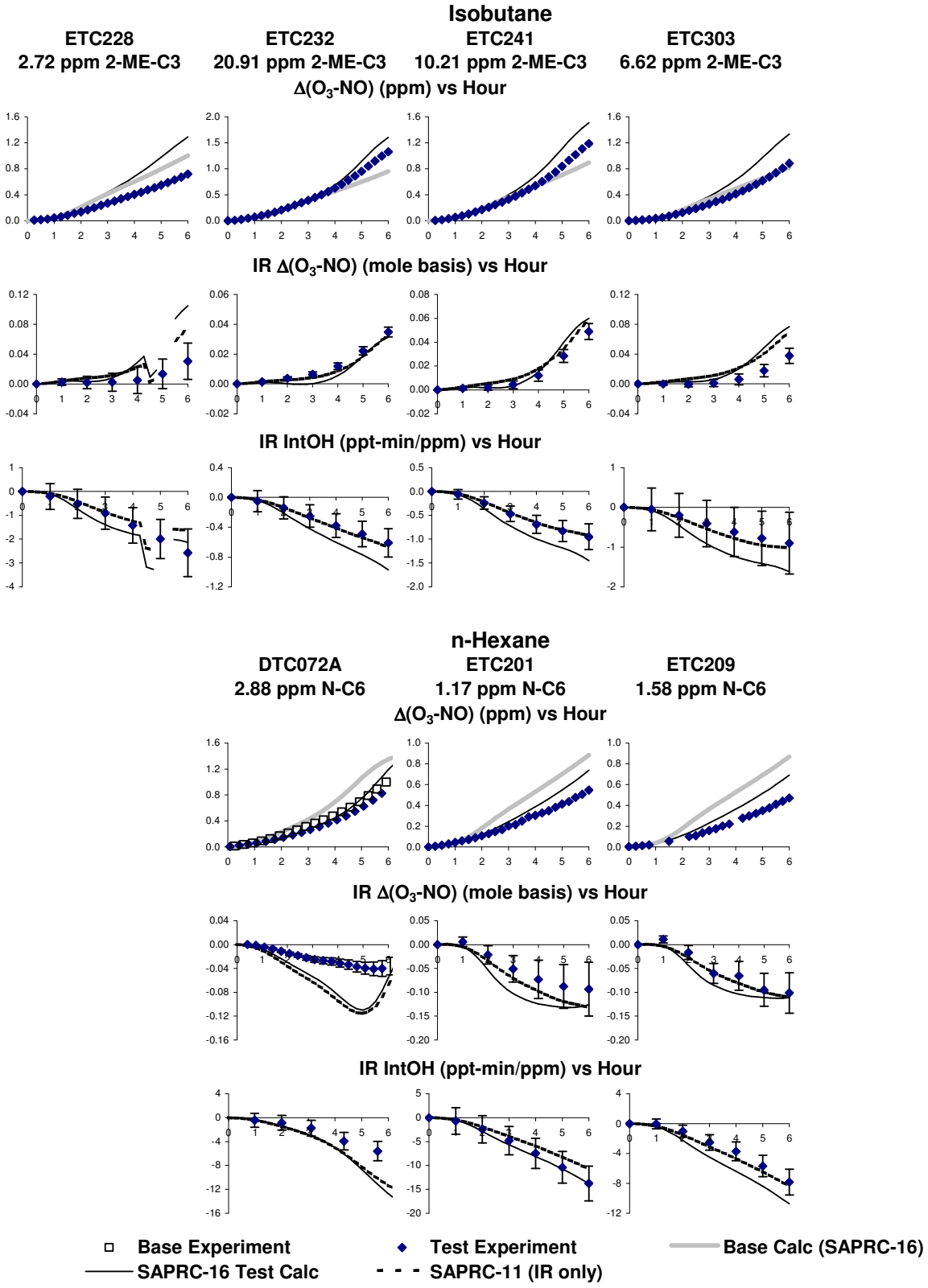
This Appendix contains plots of selected experimental and model calculation data for all of the incremental reactivity experiments used for mechanism evaluation. These experiments are summarized on Table 6 in the main text, with reference to the page number(s) in this Appendix where experiments for a particular compound can be found. Each "figure" in this appendix actually consists of multiple pages showing data for up to 10 experiments, grouped according to the compound studied.

Three plots are shown for each experiment. The top plot shows the experimental and calculated $\Delta([O_3]-[NO])$ data (ozone formed + NO oxidized) data for both the base case experiment and the test experiment where the compound was added, with the run number and amount of compound added indicated above the plots. The points show the experimental data and the lines show the SAPRC-16 model simulations of the base case (thick light lines) and the added VOC (thin darker lines) experiments. The middle plots show the change in $\Delta([O_3]-[NO])$ caused by adding the test compound, divided by the amount of test compound added (incremental reactivity, or IR). The bottom plots show the changes in integrated OH levels (IntOH) caused by adding the test compound, where the integrated OH was derived from the measured rates of consumption of m-xylene or another reactive compound present in the base case experiment. The experimental data are shown as points with error bars indicating approximate uncertainty in the change due to experimental variability. If the addition of the compound causes only a small change in $\Delta([O_3]-[NO])$ or IntOH then the error bars will be relatively large because the effect of the change is small compared to experimental variability, and vise-versa. (Note that the error bars DO NOT reflect systematic uncertainties such as uncertainties in calibrating the compounds or products, difficulties in injecting some compounds into the gas phase, and uncertainties in rate constants used to derive IntOH values.) The solid lines on the middle and bottom plots are the calculation using the SAPRC-16 mechanism, and the dashed lines are the calculations using the SAPRC-11 mechanism, which are shown for comparison. Note that SAPRC-11 calculations are not shown on the top plots (see Table 5 for a summary of differences between the mechanisms in simulating ambient mixture experiments.

Figure B-1. Plots of selected experimental and model calculation results for the incremental reactivity experiments with the alkanes.



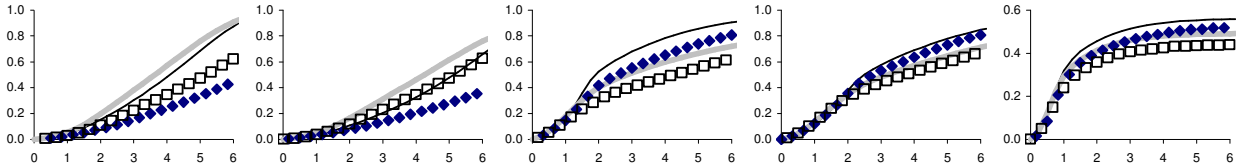

n-Butane
DTC019B
6.10 ppm N-C4
DTC031A
5.08 ppm N-C4
ETC094
7.16 ppm N-C4
ETC097
6.12 ppm N-C4
ETC135
6.06 ppm N-C4
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
n-Butane
ETC224
9.76 ppm N-C4
ETC389
3.60 ppm N-C4
ETC393
3.46 ppm N-C4
ETC484
16.91 ppm N-C4
ETC488
9.33 ppm N-C4
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)


Isobutane
ETC228
2.72 ppm 2-ME-C3
ETC232
20.91 ppm 2-ME-C3
ETC241
10.21 ppm 2-ME-C3
ETC303
6.62 ppm 2-ME-C3
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
n-Hexane
DTC072A
2.88 ppm N-C6
ETC201
1.17 ppm N-C6
ETC209
1.58 ppm N-C6
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

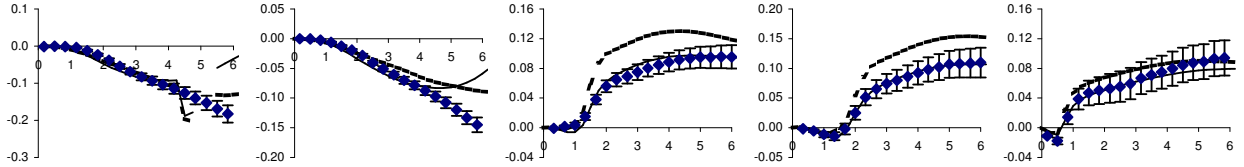
Cyclohexane

DTC541A	DTC551A	DTC543B	DTC552B	DTC544A
0.95 ppm CYCC6	1.71 ppm CYCC6	1.95 ppm CYCC6	1.25 ppm CYCC6	0.86 ppm CYCC6

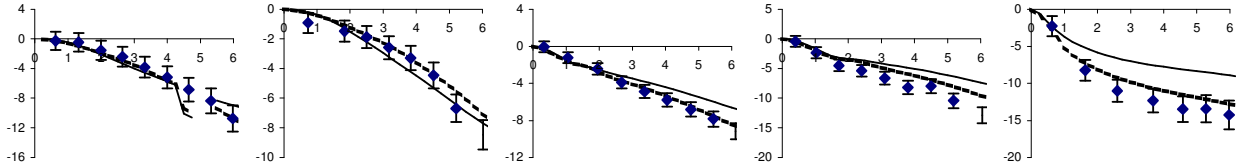
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



IR IntOH (ppt-min/ppm) vs Hour



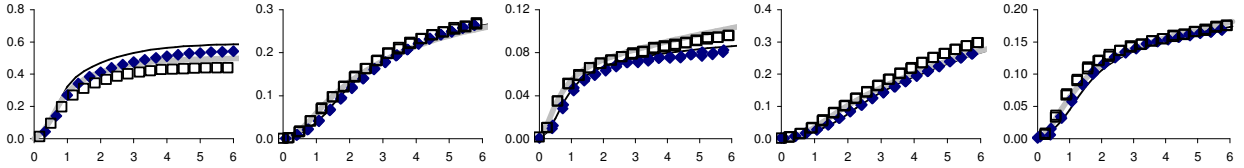
Cyclohexane

DTC553A
1.41 ppm CYCC6

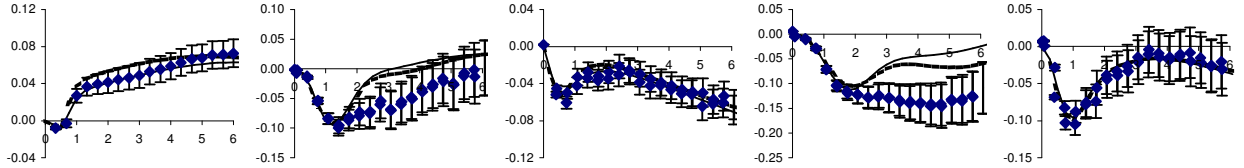
n-Octane (page 1 of 2)

EPA083B	EPA085B	EPA113B	EPA095A
0.25 ppm N-C8	0.24 ppm N-C8	0.23 ppm N-C8	0.20 ppm N-C8

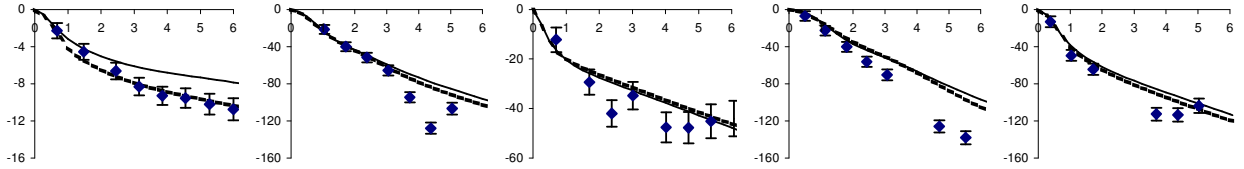
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



IR IntOH (ppt-min/ppm) vs Hour



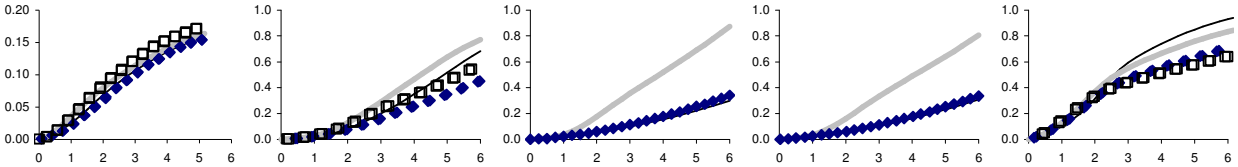
Base Experiment ◆ Test Experiment Base Calc (SAPRC-16)

SAPRC-16 Test Calc - - - SAPRC-11 (IR only)

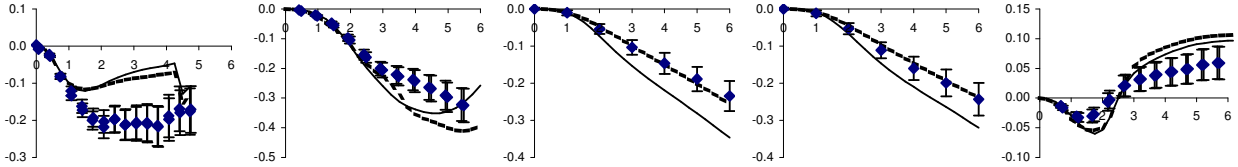
n-Octane (page 2 of 2)

EPA114B	CTC110B	ETC237	ETC239	CTC131A
0.11 ppm N-C8	0.34 ppm N-C8	1.66 ppm N-C8	1.55 ppm N-C8	1.01 ppm N-C8

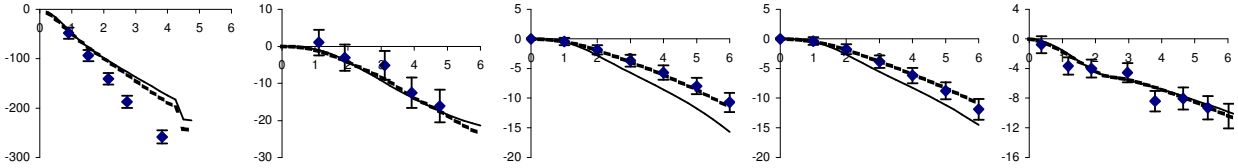
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



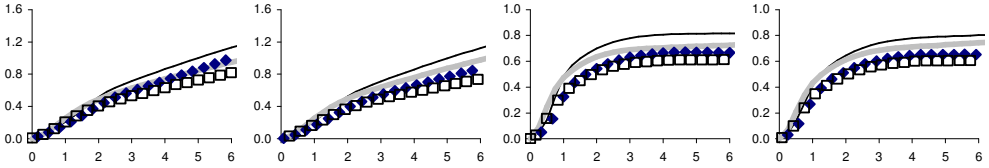
IR IntOH (ppt-min/ppm) vs Hour



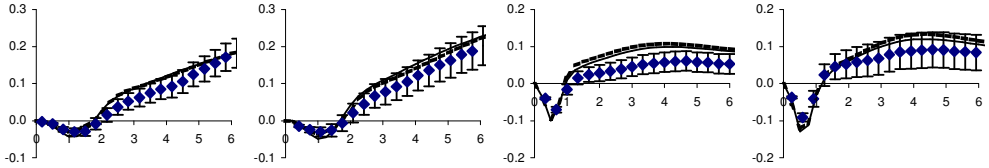
n-Octane

DTC024B	DTC070A	DTC037B	DTC071B
1.01 ppm N-C8	0.65 ppm N-C8	1.03 ppm N-C8	0.56 ppm N-C8

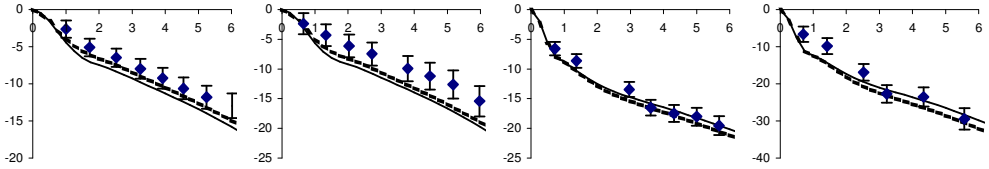
$\Delta(O_3\text{-NO})$ (ppm) vs Hour

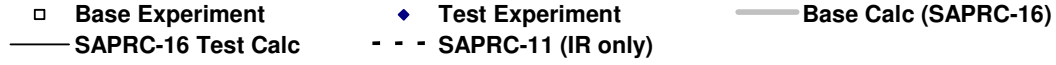


IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



IR IntOH (ppt-min/ppm) vs Hour



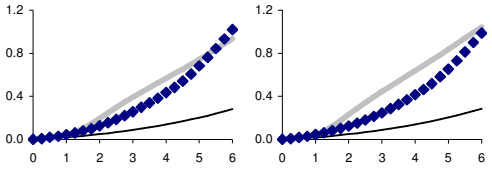


2,2,4-Trimethyl Pentane

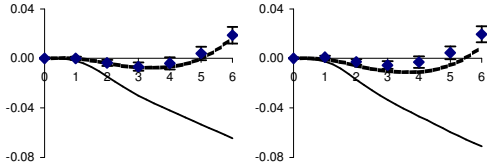
ETC291 — **10.14 ppm 224TM-C5**

ETC293 — **10.64 ppm 224TM-C5**

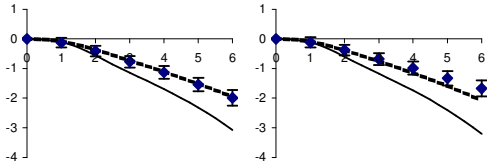
Δ(O_3-NO) (ppm) vs Hour



IR Δ(O_3-NO) (mole basis) vs Hour



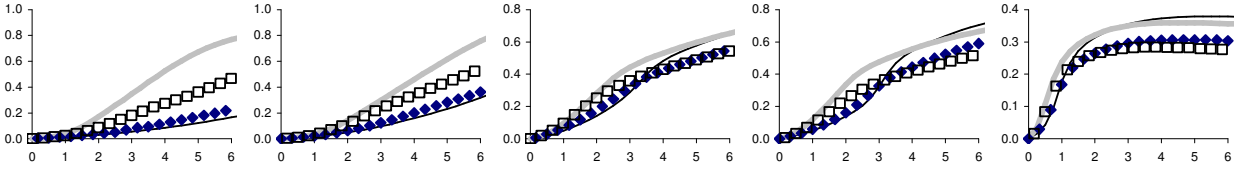
IR IntOH (ppt-min/ppm) vs Hour



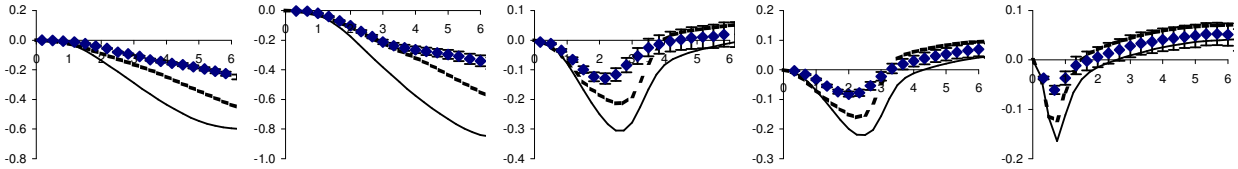
2,6-Dimethyl Octane

DTC733A	DTC749A	DTC738B	DTC747A	DTC739A
1.01 ppm 26DM-C8	0.52 ppm 26DM-C8	0.56 ppm 26DM-C8	0.98 ppm 26DM-C8	0.54 ppm 26DM-C8

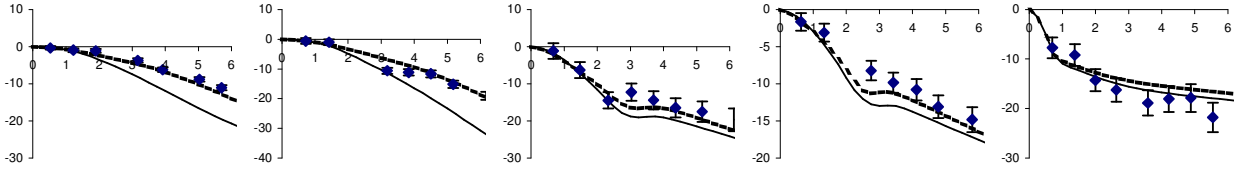
Δ(O_3-NO) (ppm) vs Hour



IR Δ(O_3-NO) (mole basis) vs Hour



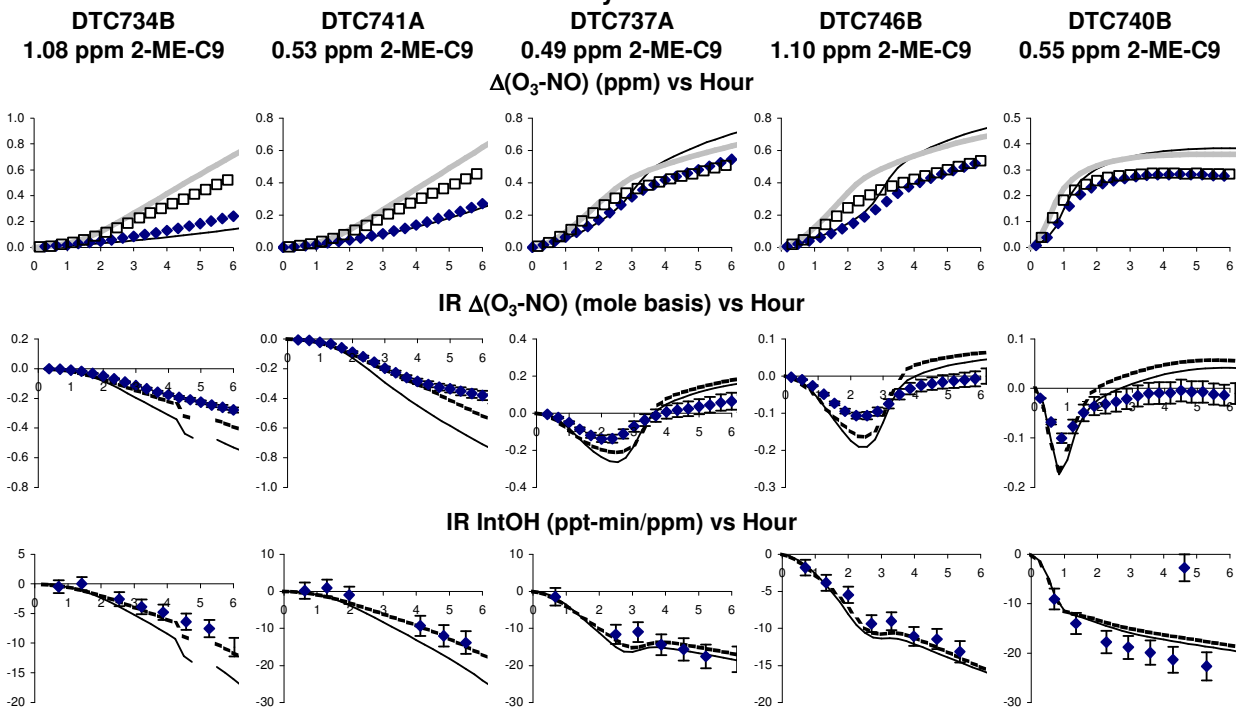
IR IntOH (ppt-min/ppm) vs Hour



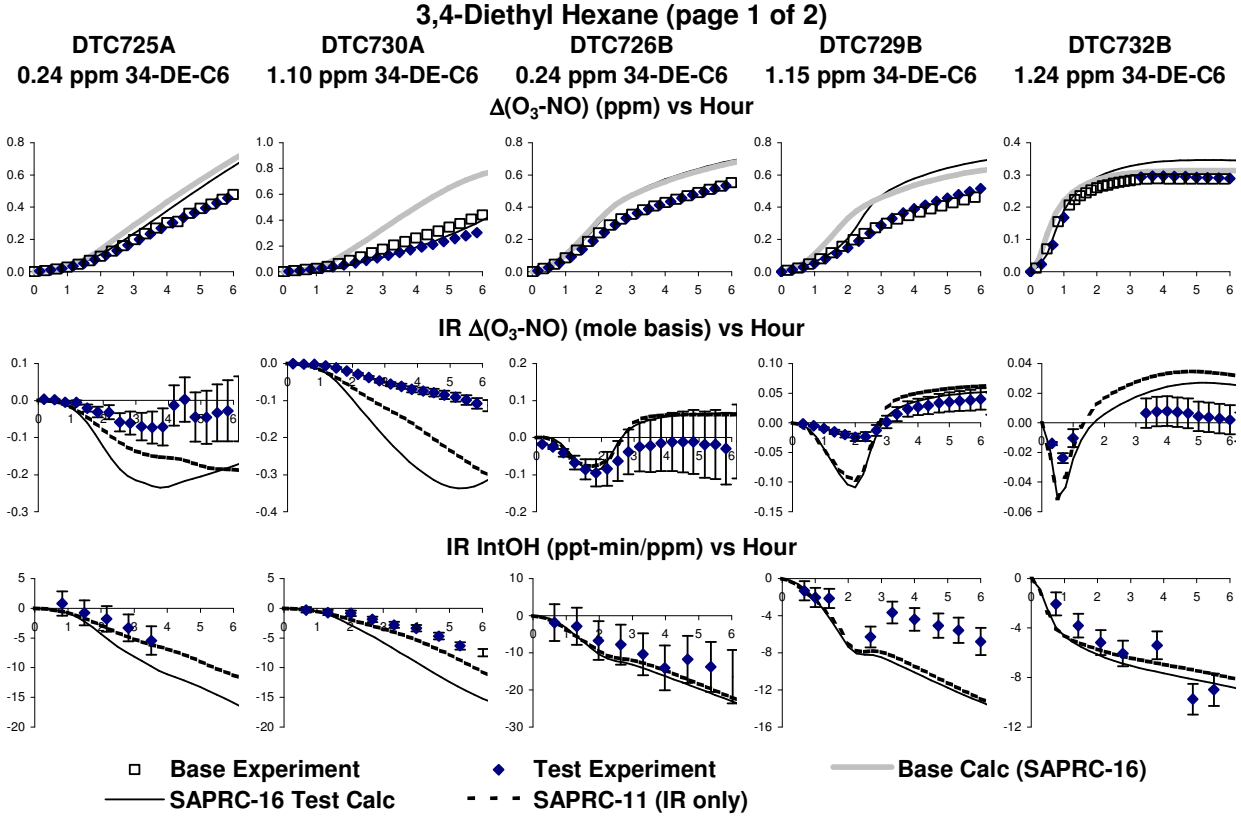
□ **Base Experiment** ◆ **Test Experiment** **Base Calc (SAPRC-16)**

SAPRC-16 Test Calc **SAPRC-11 (IR only)**

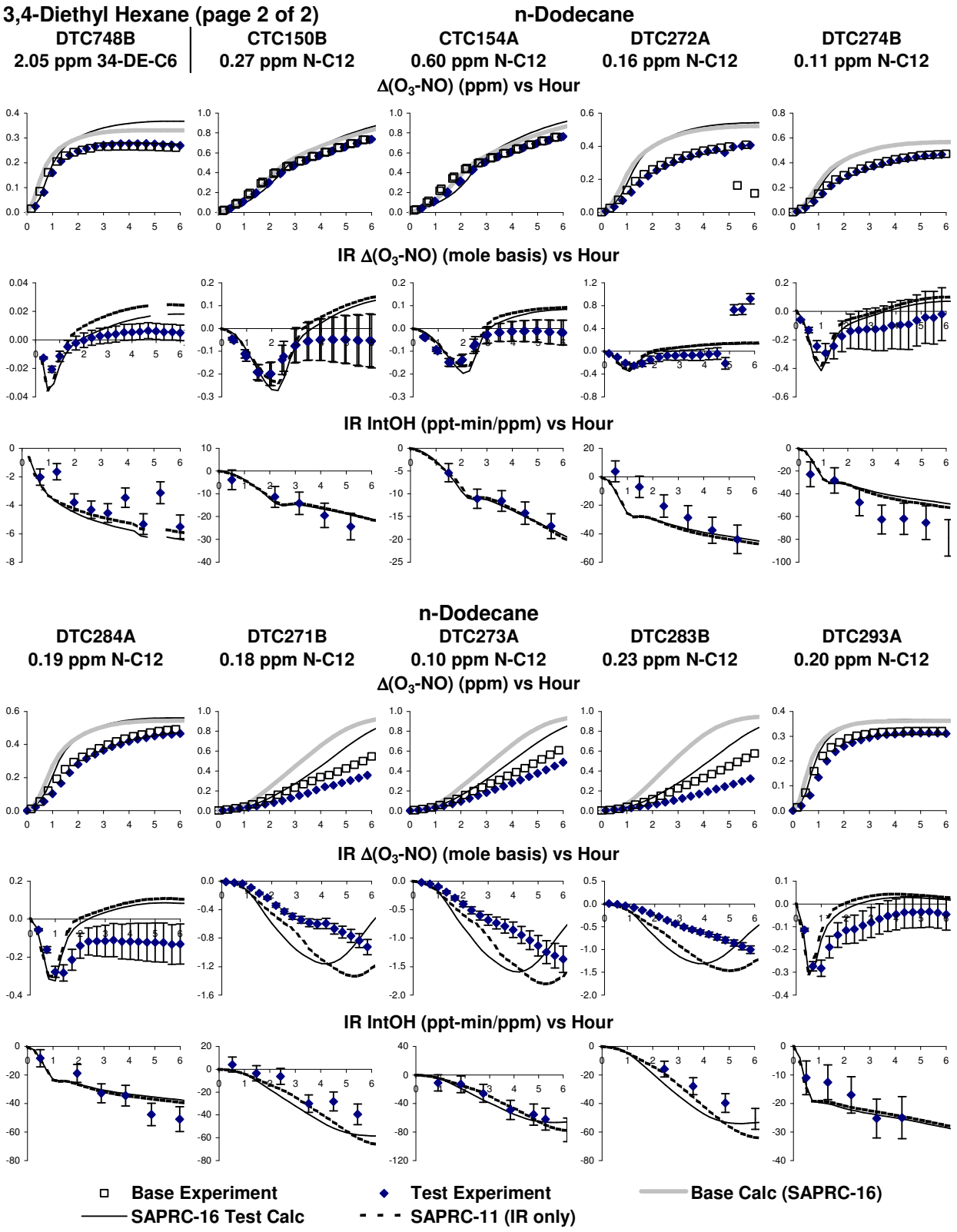
2-Methyl Nonane

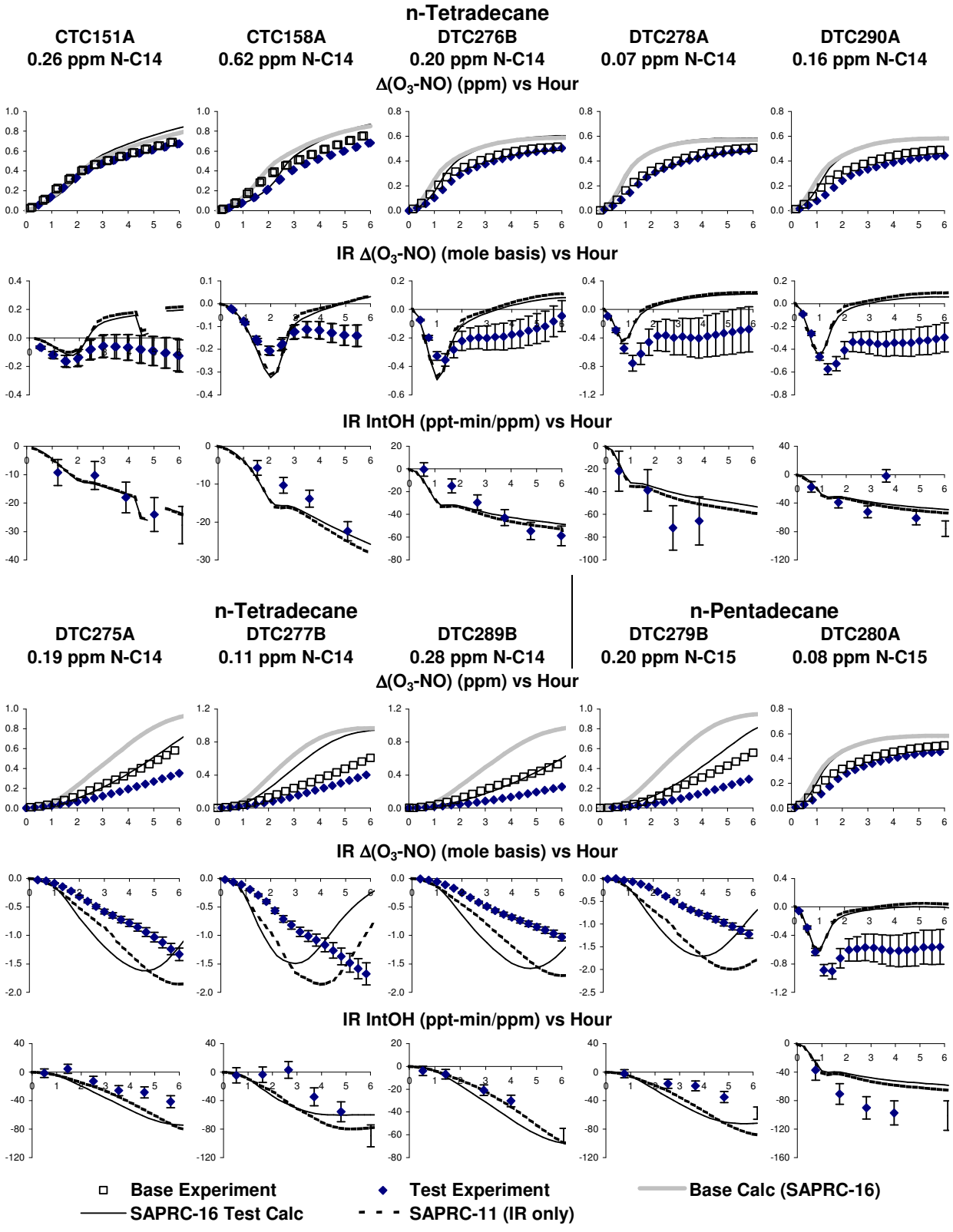


3,4-Diethyl Hexane (page 1 of 2)



Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

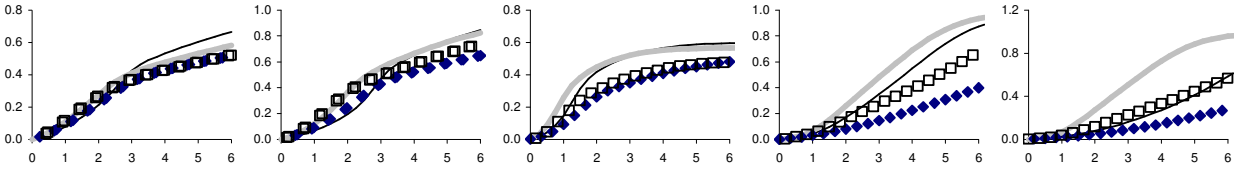

3,4-Diethyl Hexane (page 2 of 2)
n-Dodecane
DTC748B
2.05 ppm 34-DE-C6
CTC150B
0.27 ppm N-C12
CTC154A
0.60 ppm N-C12
DTC272A
0.16 ppm N-C12
DTC274B
0.11 ppm N-C12
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
n-Dodecane
DTC284A
0.19 ppm N-C12
DTC271B
0.18 ppm N-C12
DTC273A
0.10 ppm N-C12
DTC283B
0.23 ppm N-C12
DTC293A
0.20 ppm N-C12
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)


n-Tetradecane
CTC151A
0.26 ppm N-C14
CTC158A
0.62 ppm N-C14
DTC276B
0.20 ppm N-C14
DTC278A
0.07 ppm N-C14
DTC290A
0.16 ppm N-C14
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
n-Tetradecane
DTC275A
0.19 ppm N-C14
DTC277B
0.11 ppm N-C14
DTC289B
0.28 ppm N-C14
n-Pentadecane
DTC279B
0.20 ppm N-C15
DTC280A
0.08 ppm N-C15
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

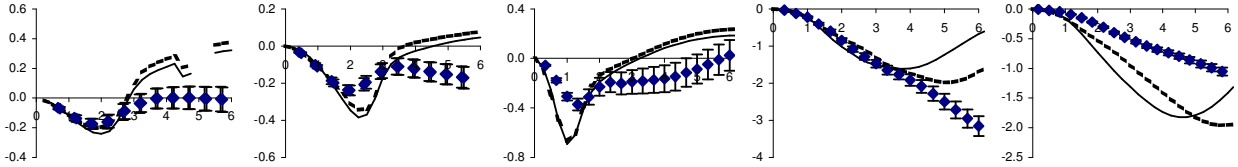
n-Hexadecane

CTC152B 0.26 ppm N-C16 | CTC156B 0.48 ppm N-C16 | DTC281B 0.16 ppm N-C16 | DTC282A 0.09 ppm N-C16 | DTC291B 0.26 ppm N-C16

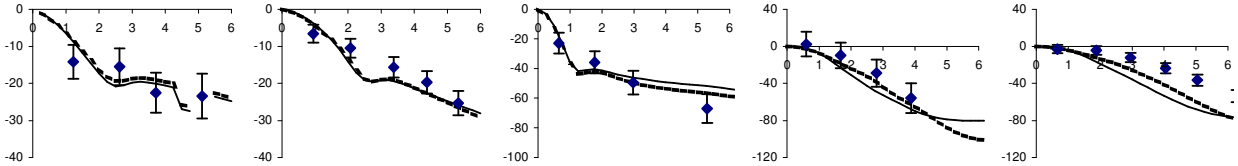
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



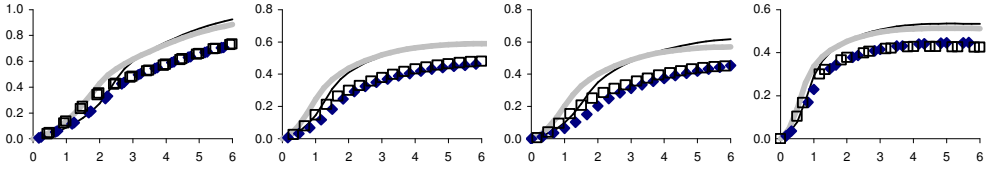
IR IntOH (ppt-min/ppm) vs Hour



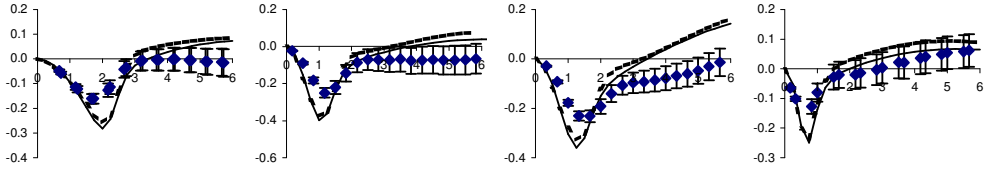
Hexyl Cyclohexane (page 1 of 2)

CTC167A 0.55 ppm C6-CYCC6 | DTC317A 0.25 ppm C6-CYCC6 | DTC319B 0.34 ppm C6-CYCC6 | CTC233A 0.33 ppm C6-CYCC6

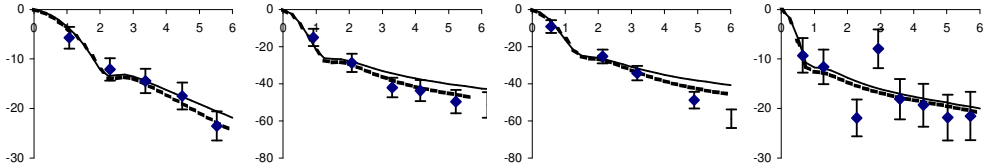
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



IR IntOH (ppt-min/ppm) vs Hour



Base Experiment | Test Experiment | Base Calc (SAPRC-16)

SAPRC-16 Test Calc | SAPRC-11 (IR only)

Hexyl Cyclohexane (page 2 of 2)

DTC315B
0.22 ppm C6-CYCC6

DTC318B
0.13 ppm C6-CYCC6

Octyl Cyclohexane

CTC168B
0.47 ppm C8-CYCC6

CTC232B
0.31 ppm C8-CYCC6

Δ(O_3-NO) (ppm) vs Hour

IR Δ(O_3-NO) (mole basis) vs Hour

IR IntOH (ppt-min/ppm) vs Hour

Octyl Cyclohexane

CTC239B
0.49 ppm C8-CYCC6

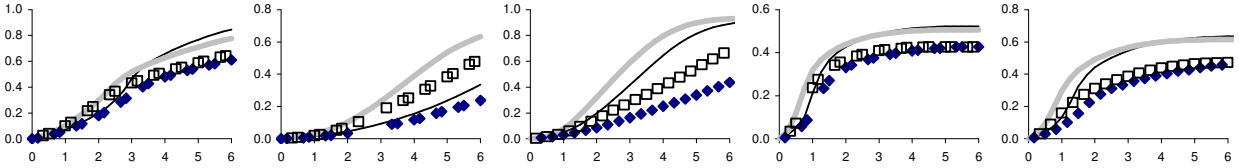
CTC231A
0.25 ppm C8-CYCC6

DTC324A
0.12 ppm C8-CYCC6

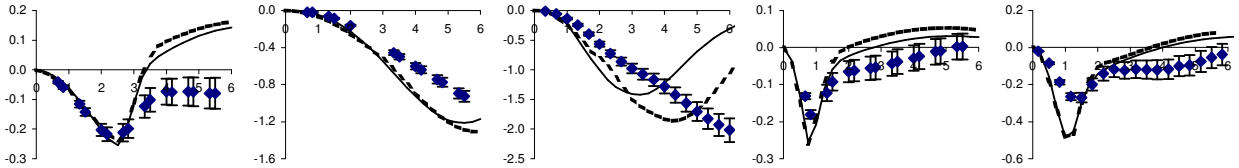
CTC240A
0.52 ppm C8-CYCC6

DTC325B
0.34 ppm C8-CYCC6

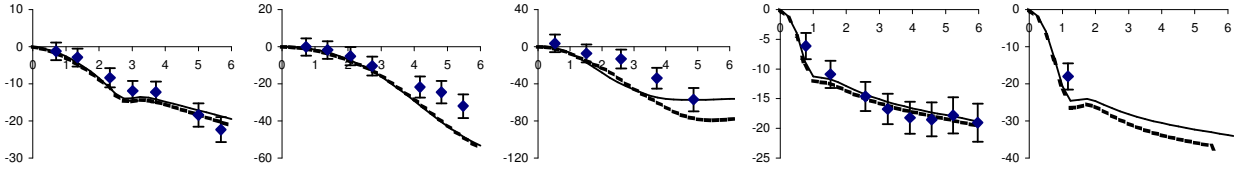
Δ(O_3-NO) (ppm) vs Hour



IR Δ(O_3-NO) (mole basis) vs Hour



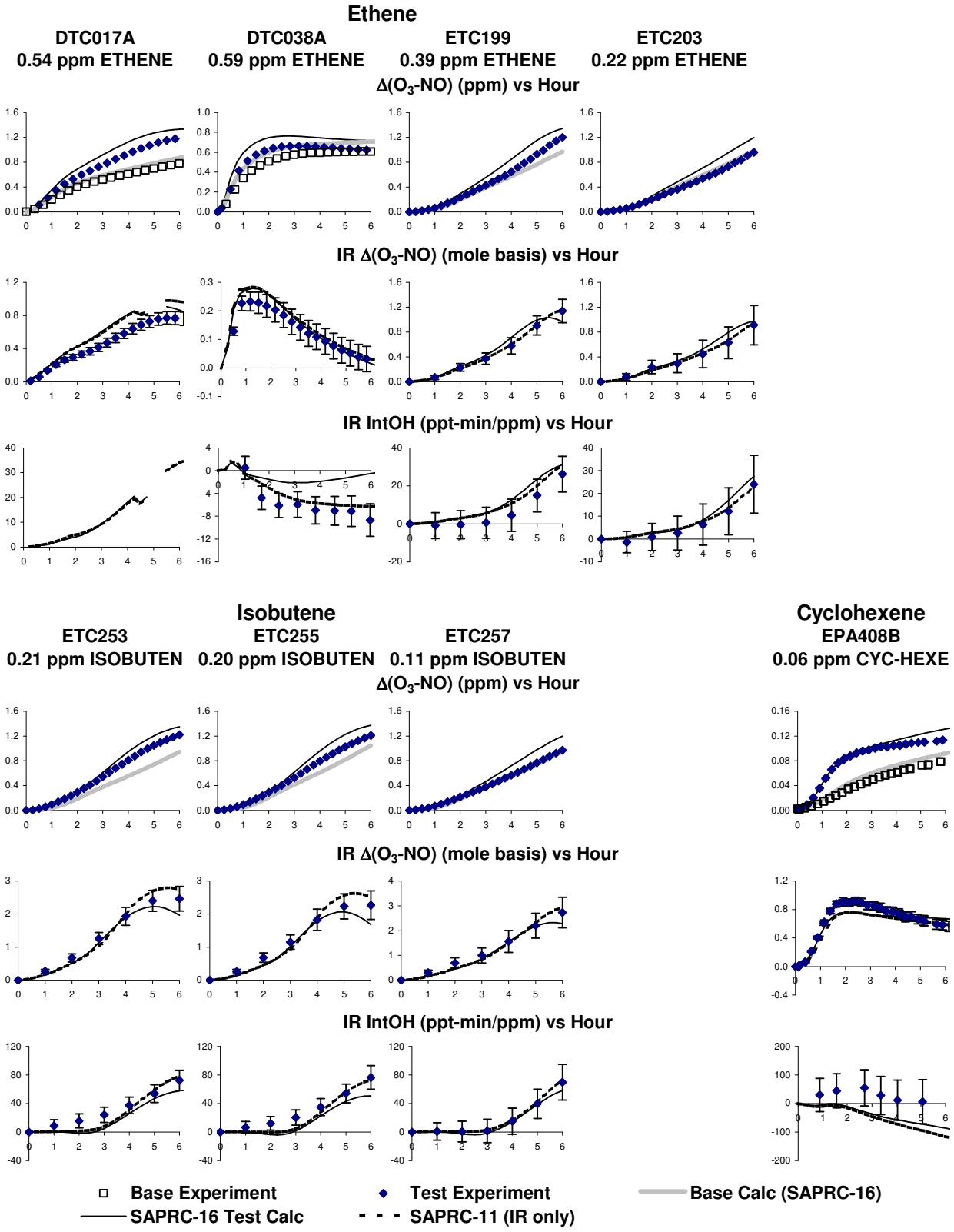
IR IntOH (ppt-min/ppm) vs Hour

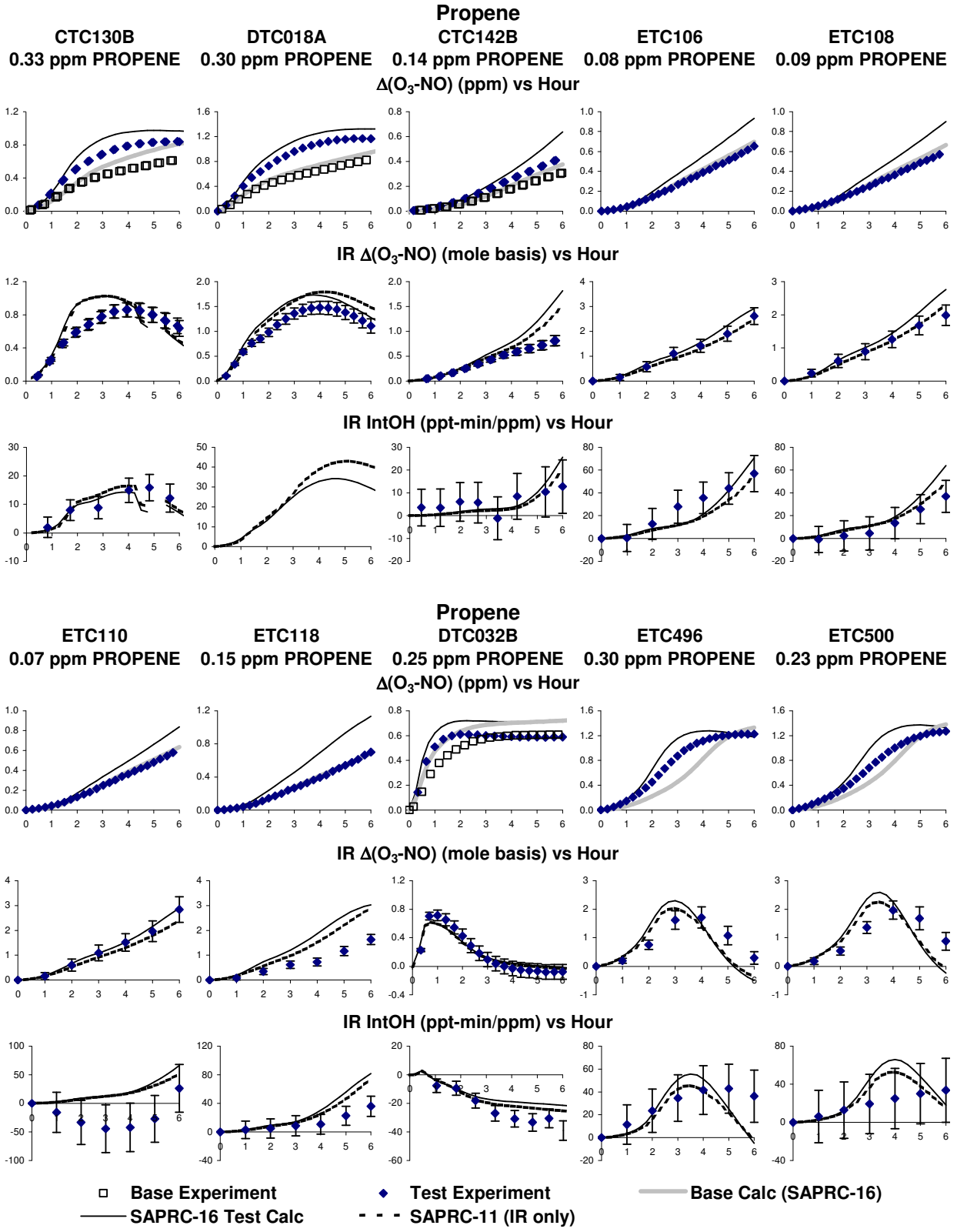


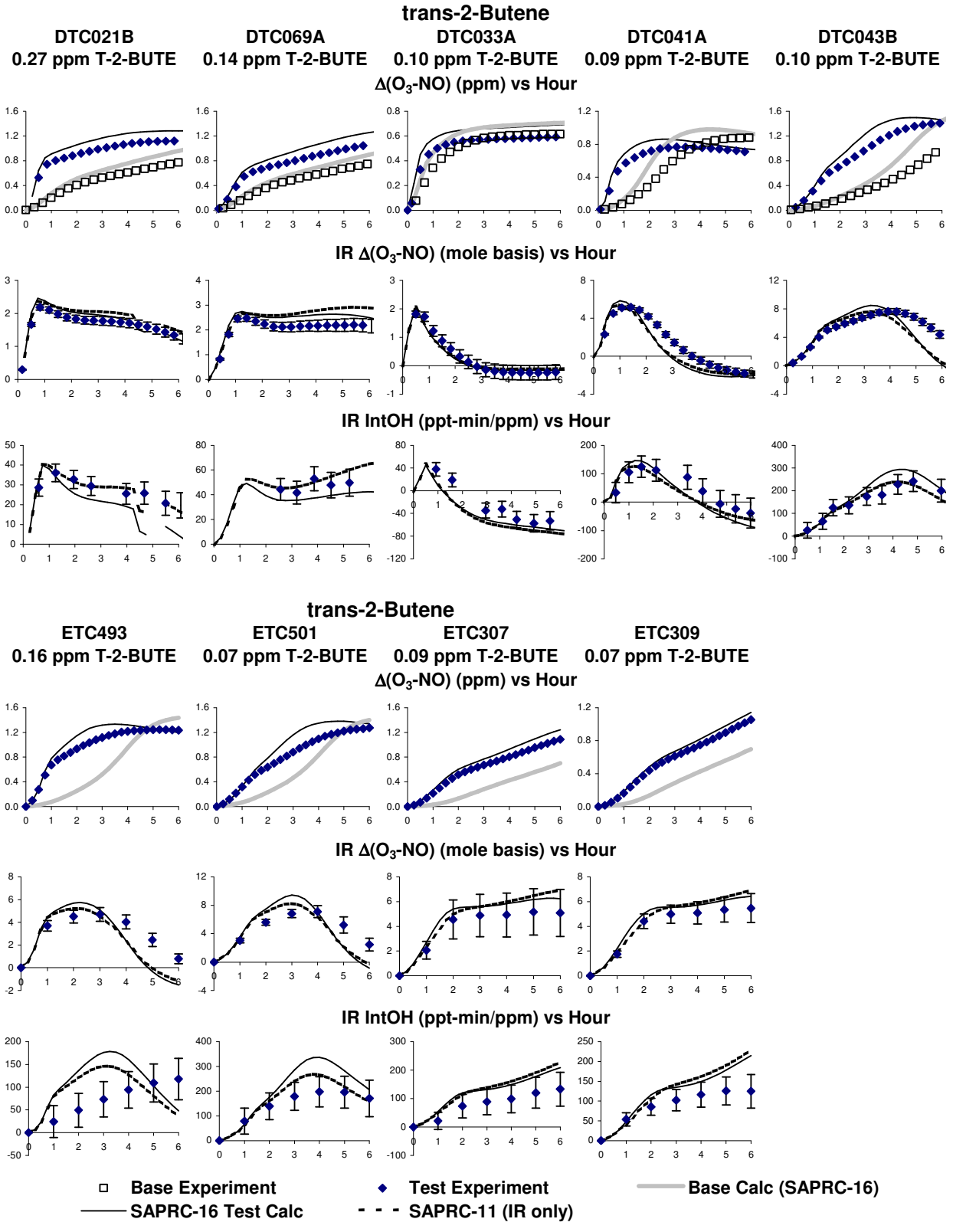
□ **Base Experiment** ◆ **Test Experiment** **Base Calc (SAPRC-16)**

SAPRC-16 Test Calc **SAPRC-11 (IR only)**

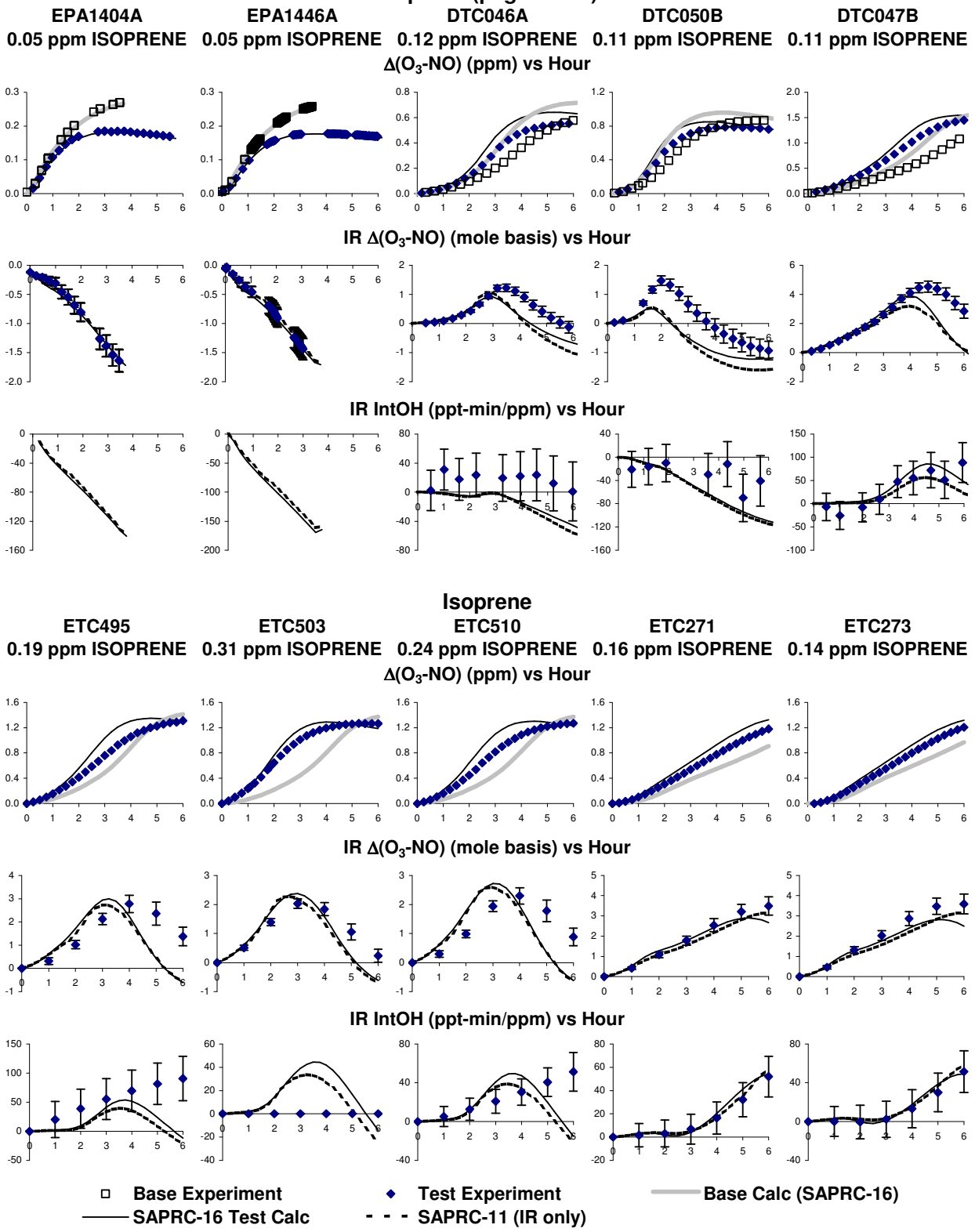
Figure B-2. Plots of selected experimental and model calculation results for the incremental reactivity experiments with the alkenes and acetylene.




Propene
CTC130B
0.33 ppm PROPENE
DTC018A
0.30 ppm PROPENE
CTC142B
0.14 ppm PROPENE
ETC106
0.08 ppm PROPENE
ETC108
0.09 ppm PROPENE
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Propene
ETC110
0.07 ppm PROPENE
ETC118
0.15 ppm PROPENE
DTC032B
0.25 ppm PROPENE
ETC496
0.30 ppm PROPENE
ETC500
0.23 ppm PROPENE
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)


trans-2-Butene
DTC021B
0.27 ppm T-2-BUTE
DTC069A
0.14 ppm T-2-BUTE
DTC033A
0.10 ppm T-2-BUTE
DTC041A
0.09 ppm T-2-BUTE
DTC043B
0.10 ppm T-2-BUTE
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
trans-2-Butene
ETC493
0.16 ppm T-2-BUTE
ETC501
0.07 ppm T-2-BUTE
ETC307
0.09 ppm T-2-BUTE
ETC309
0.07 ppm T-2-BUTE
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

Isoprene (page 1 of 2)



Isoprene

Isoprene (page 2 of 2)

b-Pinene

ETC275 — 0.11 ppm ISOPRENE

ETC277 — 0.08 ppm ISOPRENE

DTC048A — 0.10 ppm B-PINENE

DTC051B — 0.11 ppm B-PINENE

$\Delta(O_3\text{-NO})$ (ppm) vs Hour

IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour

IR IntOH (ppt-min/ppm) vs Hour

a-Pinene

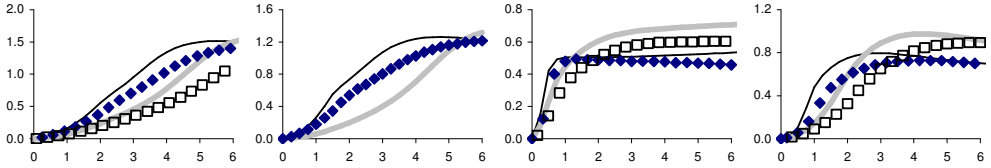
DTC045B — 0.11 ppm A-PINENE

ETC508 — 0.15 ppm A-PINENE

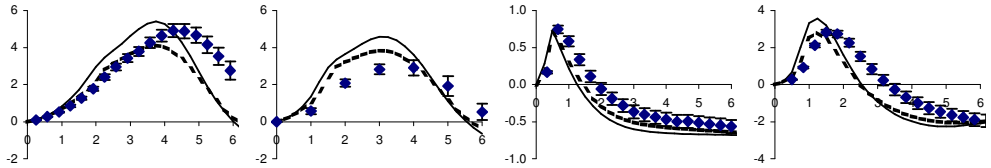
DTC034B — 0.26 ppm A-PINENE

DTC044A — 0.10 ppm A-PINENE

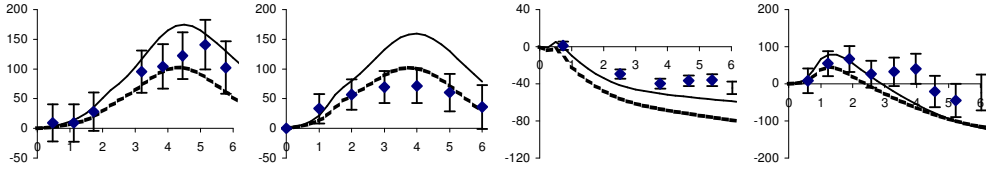
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



IR IntOH (ppt-min/ppm) vs Hour



□ Base Experiment ◆ Test Experiment ——— Base Calc (SAPRC-16)

——— SAPRC-16 Test Calc - - - SAPRC-11 (IR only)

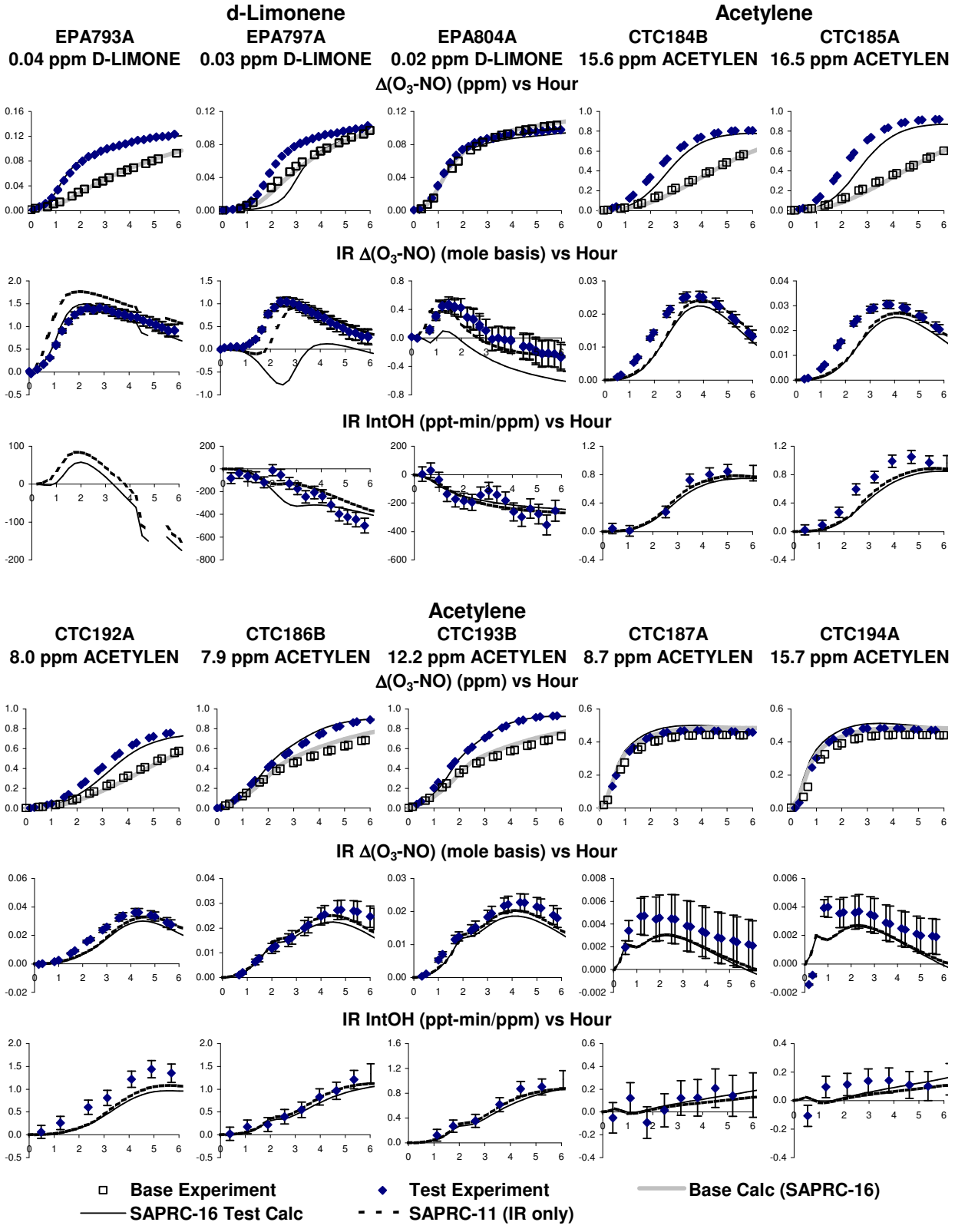
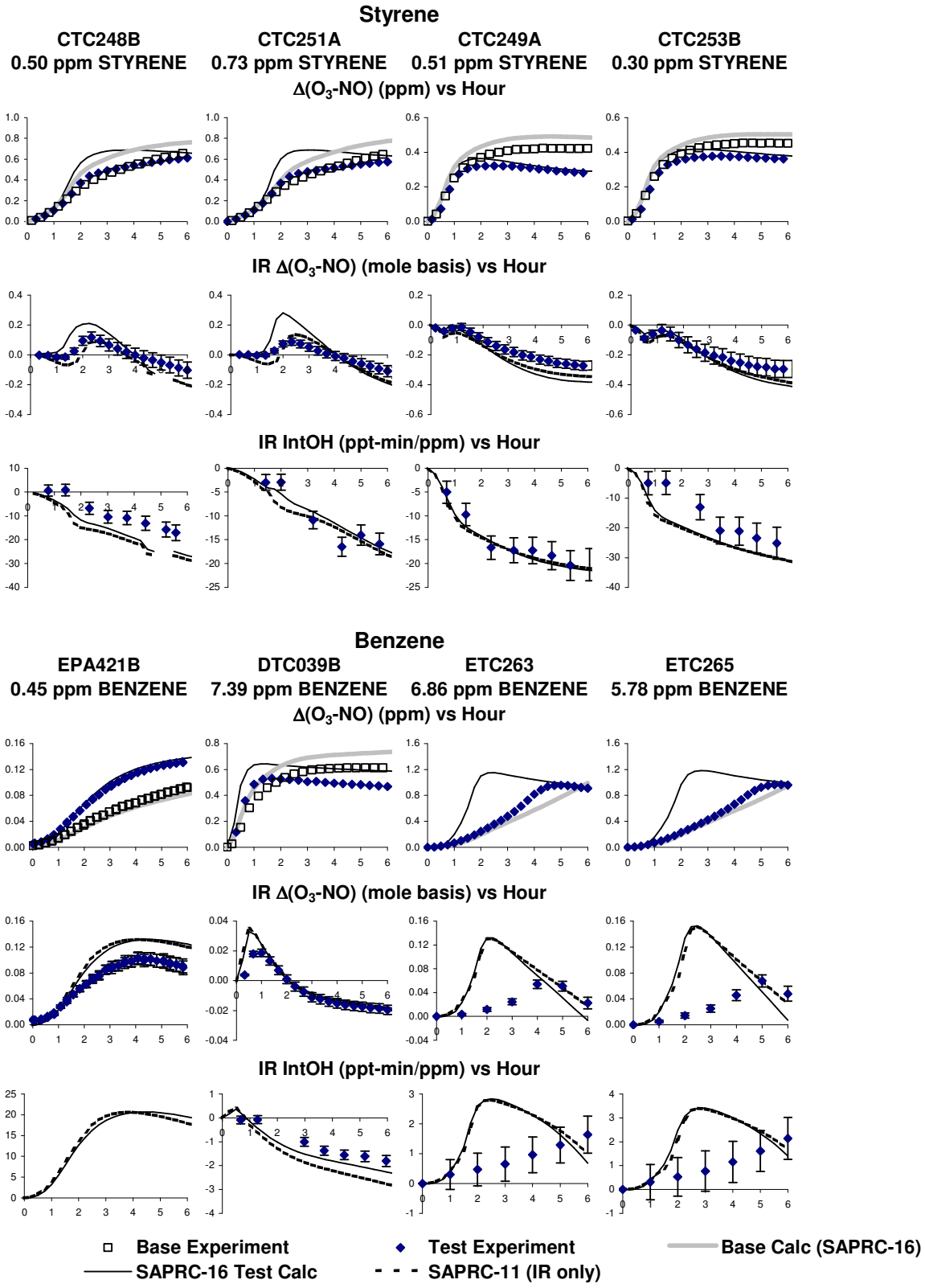
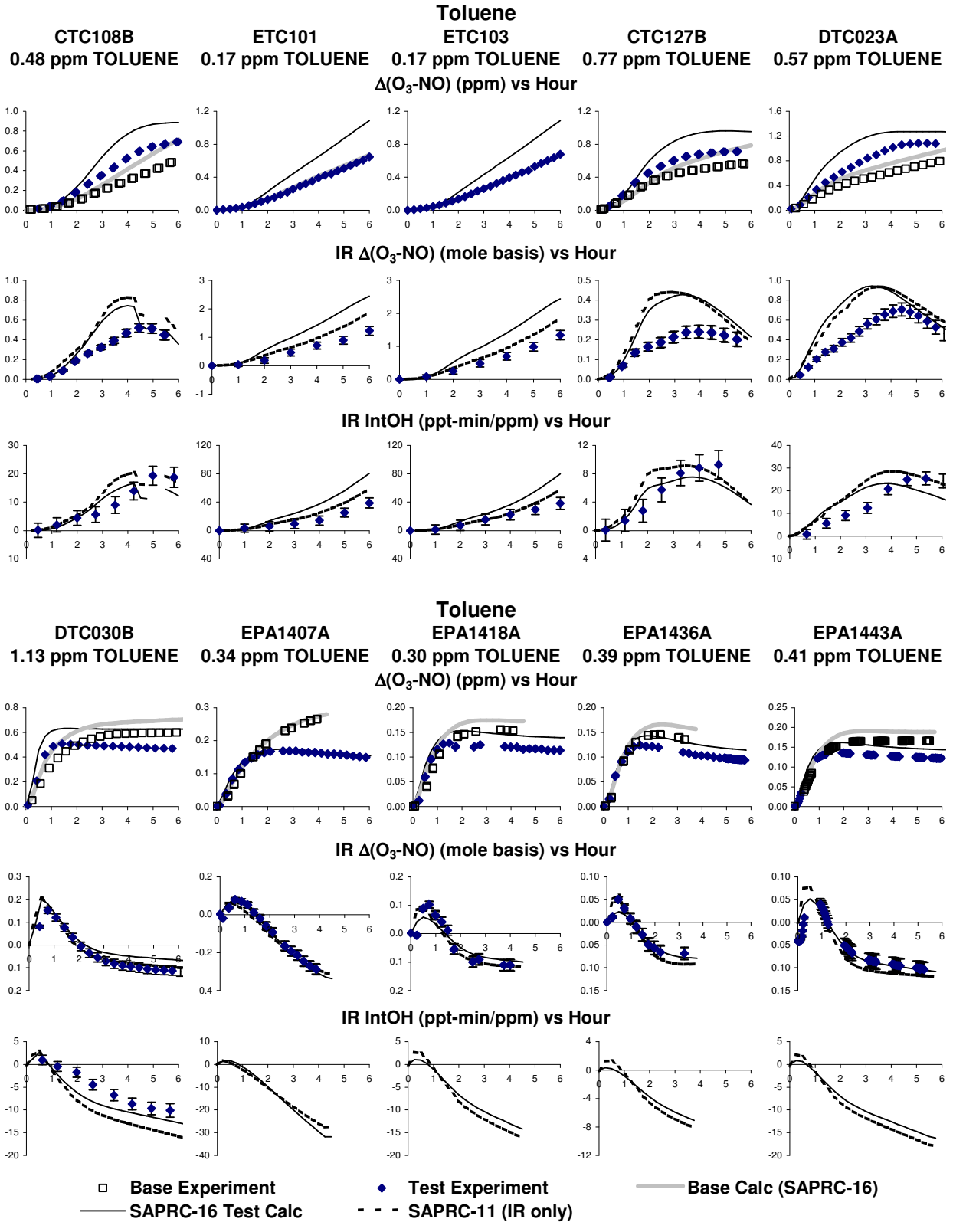

d-Limonene
Acetylene
EPA793A
0.04 ppm D-LIMONE
EPA797A
0.03 ppm D-LIMONE
EPA804A
0.02 ppm D-LIMONE
CTC184B
15.6 ppm ACETYLEN
CTC185A
16.5 ppm ACETYLEN
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Acetylene
CTC192A
8.0 ppm ACETYLEN
CTC186B
7.9 ppm ACETYLEN
CTC193B
12.2 ppm ACETYLEN
CTC187A
8.7 ppm ACETYLEN
CTC194A
15.7 ppm ACETYLEN
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

Figure B-3. Plots of selected experimental and model calculation results for the incremental reactivity experiments with styrene and the aromatics.

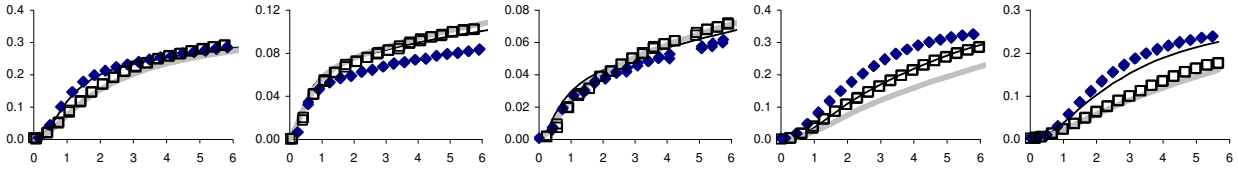



Toluene
CTC108B
0.48 ppm TOLUENE
ETC101
0.17 ppm TOLUENE
ETC103
0.17 ppm TOLUENE
CTC127B
0.77 ppm TOLUENE
DTC023A
0.57 ppm TOLUENE
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Toluene
DTC030B
1.13 ppm TOLUENE
EPA1407A
0.34 ppm TOLUENE
EPA1418A
0.30 ppm TOLUENE
EPA1436A
0.39 ppm TOLUENE
EPA1443A
0.41 ppm TOLUENE
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

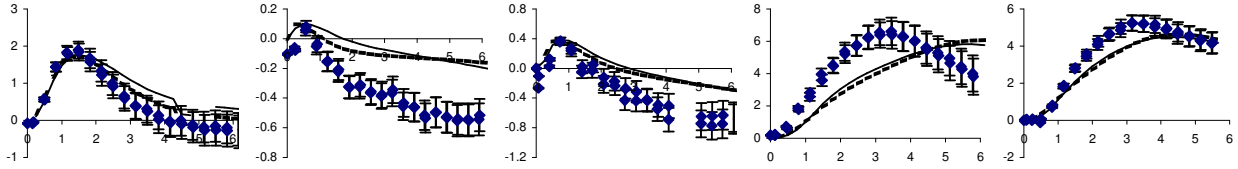
m-Xylene (page 1 of 2)

EPA084A	EPA086B	EPA100B	EPA108A	EPA128B
0.03 ppm M-XYLENE	0.04 ppm M-XYLENE	0.01 ppm M-XYLENE	0.01 ppm M-XYLENE	0.02 ppm M-XYLENE

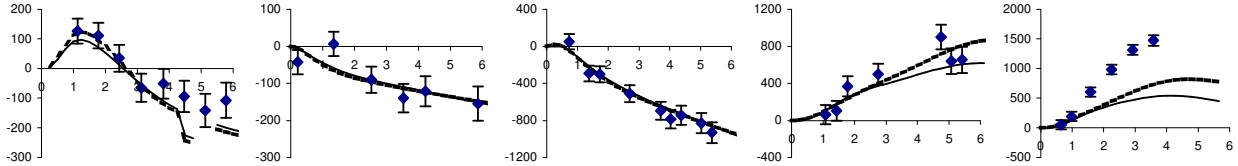
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



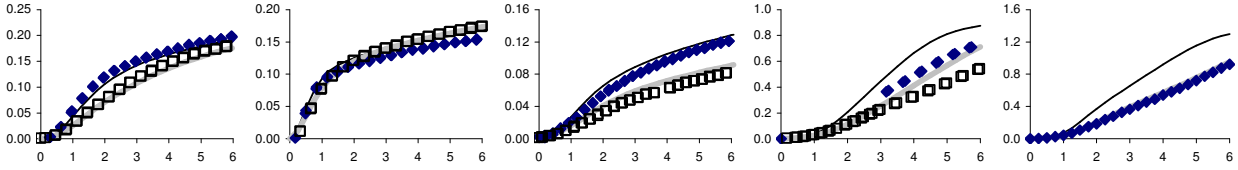
IR IntOH (ppt-min/ppm) vs Hour



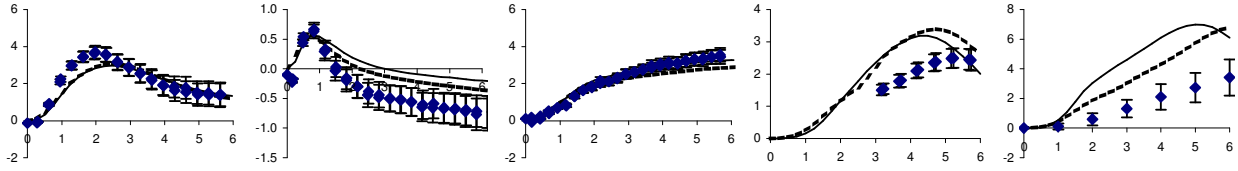
m-Xylene

EPA110A	EPA123B	EPA406B	CTC109A	ETC196
0.01 ppm M-XYLENE	0.03 ppm M-XYLENE	0.01 ppm M-XYLENE	0.08 ppm M-XYLENE	0.06 ppm M-XYLENE

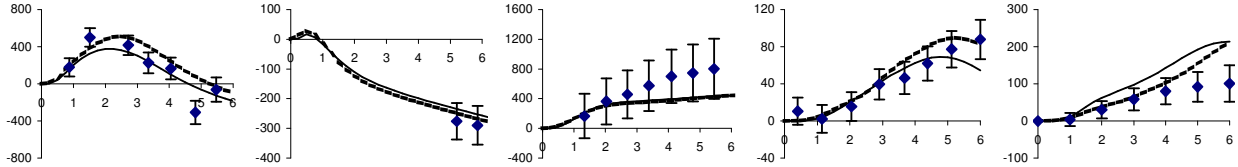
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



IR IntOH (ppt-min/ppm) vs Hour



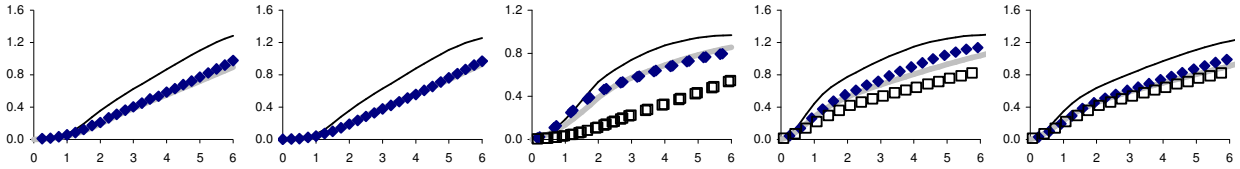
Base Experiment ◆ Test Experiment Base Calc (SAPRC-16)

SAPRC-16 Test Calc - - - SAPRC-11 (IR only)

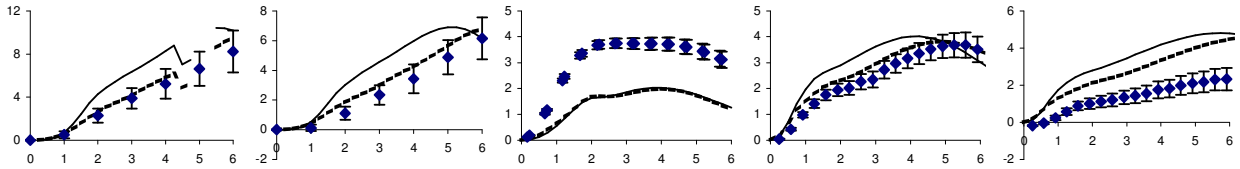
m-Xylene (page 2 of 2)

ETC207	ETC301	CTC128A	DTC025A	DTC068B
0.04 ppm M-XYLENE	0.05 ppm M-XYLENE	0.09 ppm M-XYLENE	0.08 ppm M-XYLENE	0.06 ppm M-XYLENE

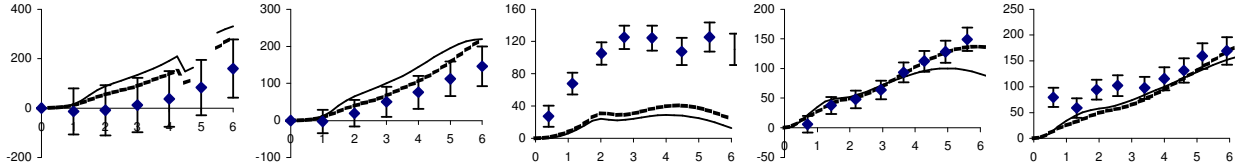
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour

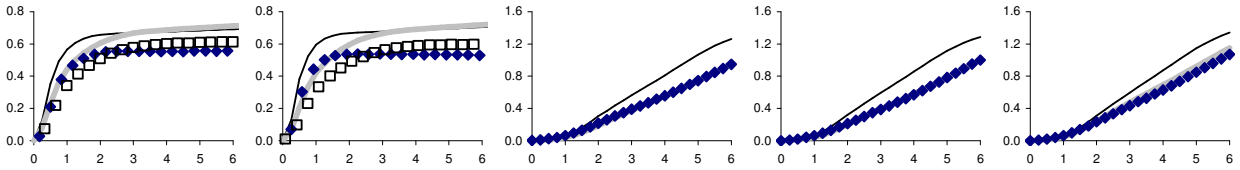


IR IntOH (ppt-min/ppm) vs Hour

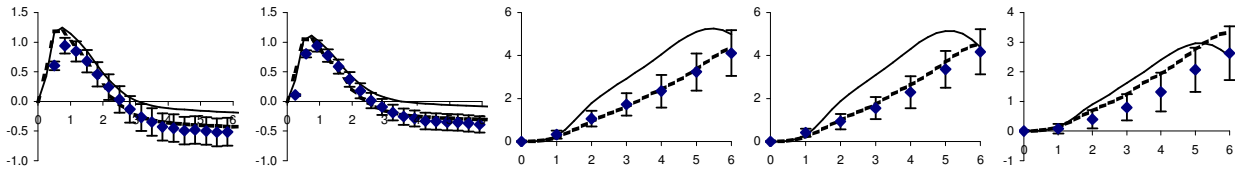


m-Xylene		o-Xylene		p-Xylene
DTC035A	DTC067B	ETC259	ETC261	ETC348
0.11 ppm M-XYLENE	0.17 ppm M-XYLENE	0.06 ppm O-XYLENE	0.06 ppm O-XYLENE	0.08 ppm P-XYLENE

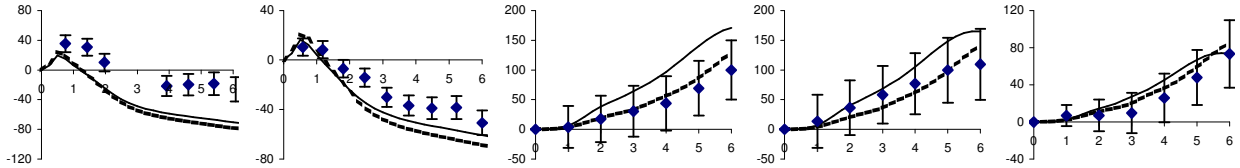
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour

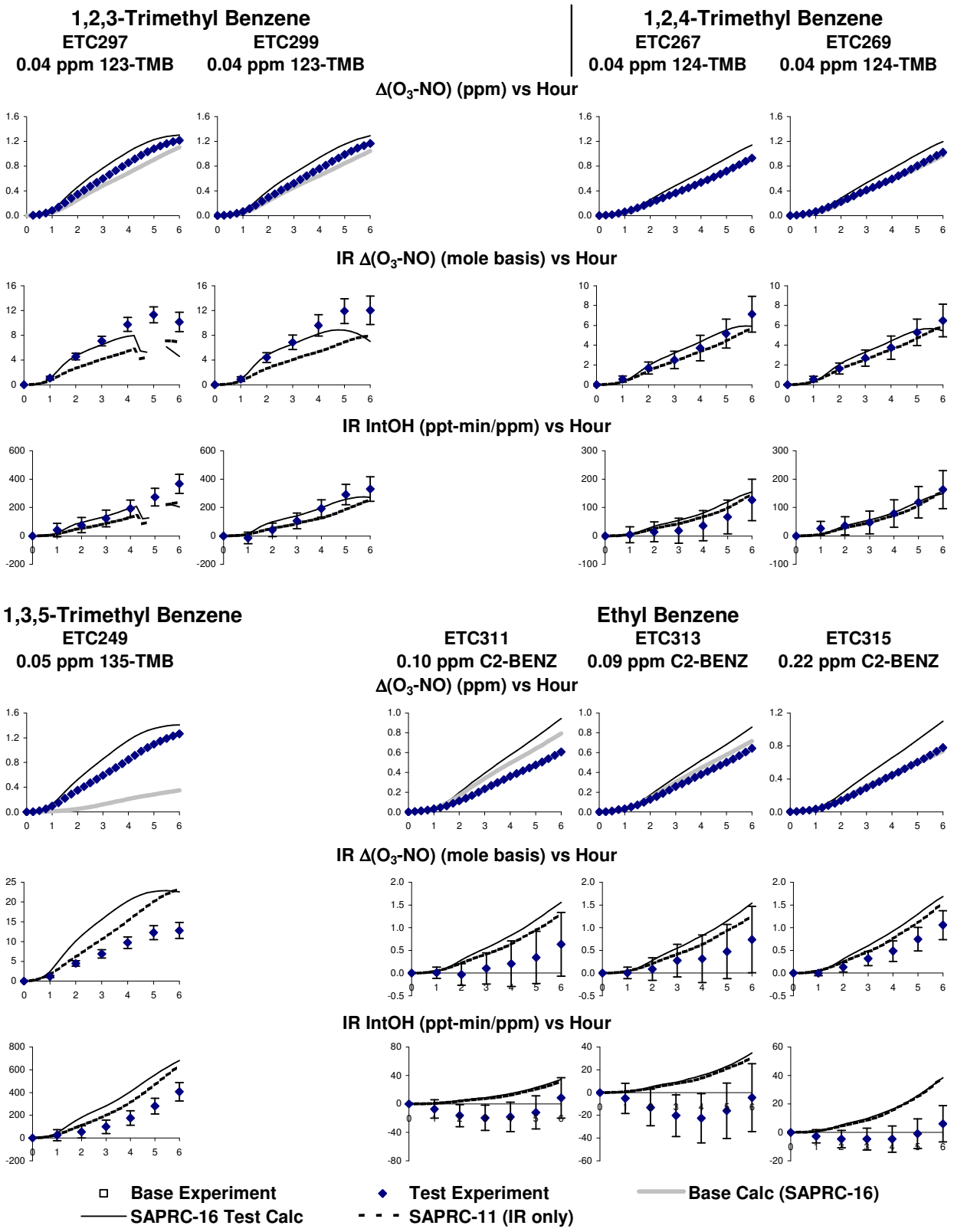


IR IntOH (ppt-min/ppm) vs Hour



Base Experiment Test Experiment Base Calc (SAPRC-16)

SAPRC-16 Test Calc SAPRC-11 (IR only)


1,2,3-Trimethyl Benzene
ETC297
0.04 ppm 123-TMB
ETC299
0.04 ppm 123-TMB
1,2,4-Trimethyl Benzene
ETC267
0.04 ppm 124-TMB
ETC269
0.04 ppm 124-TMB
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
1,3,5-Trimethyl Benzene
ETC249
0.05 ppm 135-TMB
Ethyl Benzene
ETC311
0.10 ppm C2-BENZ
ETC313
0.09 ppm C2-BENZ
ETC315
0.22 ppm C2-BENZ
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

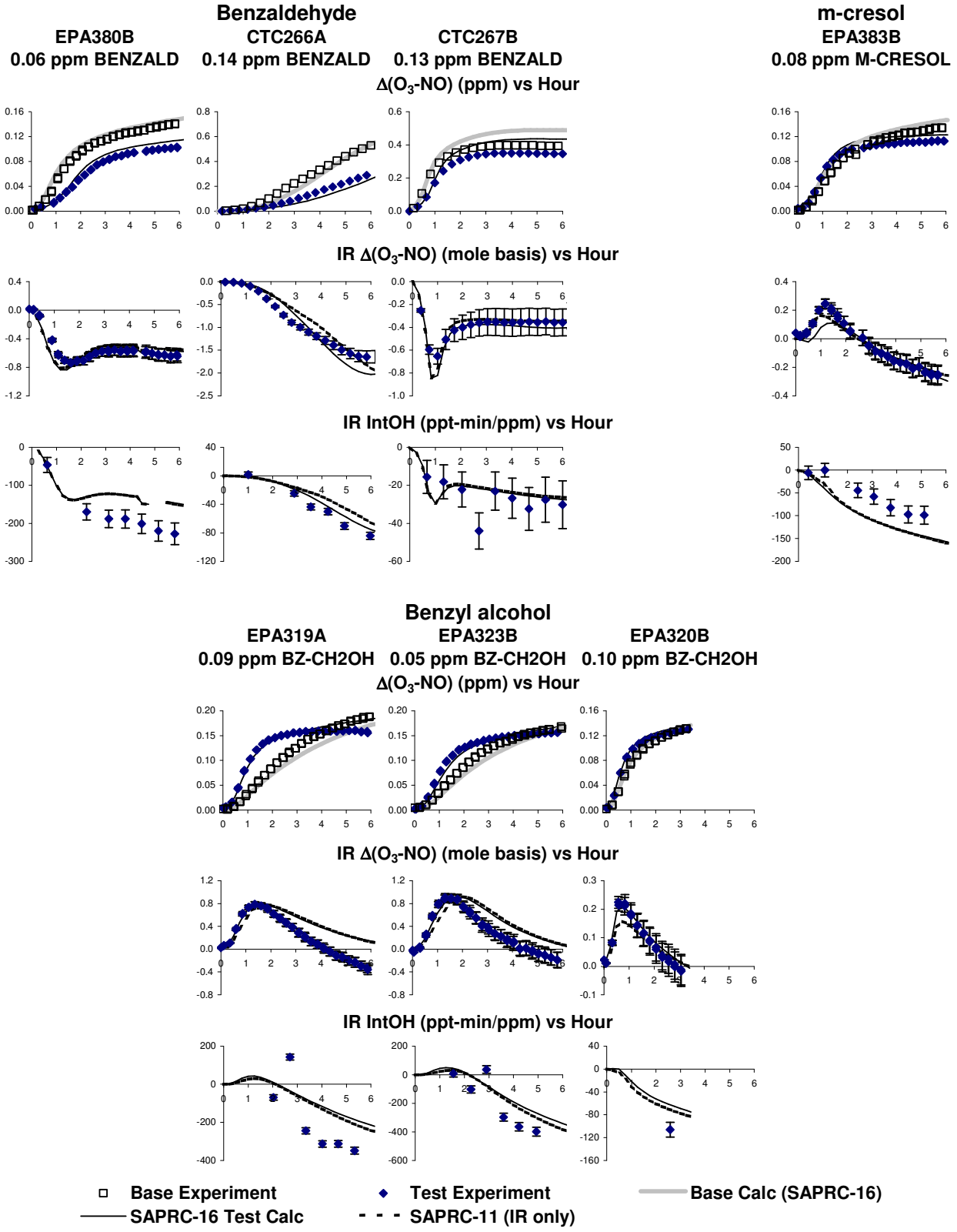
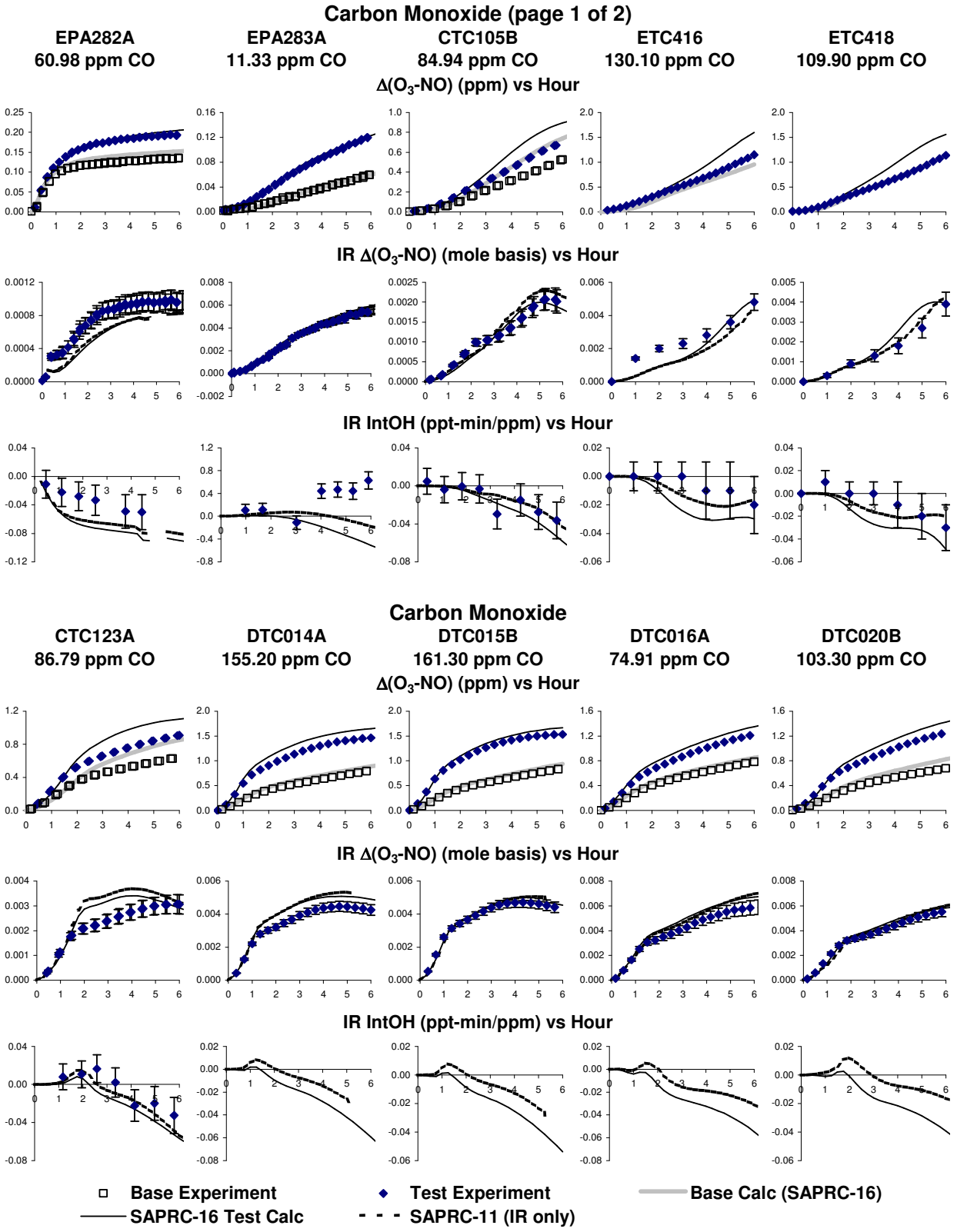
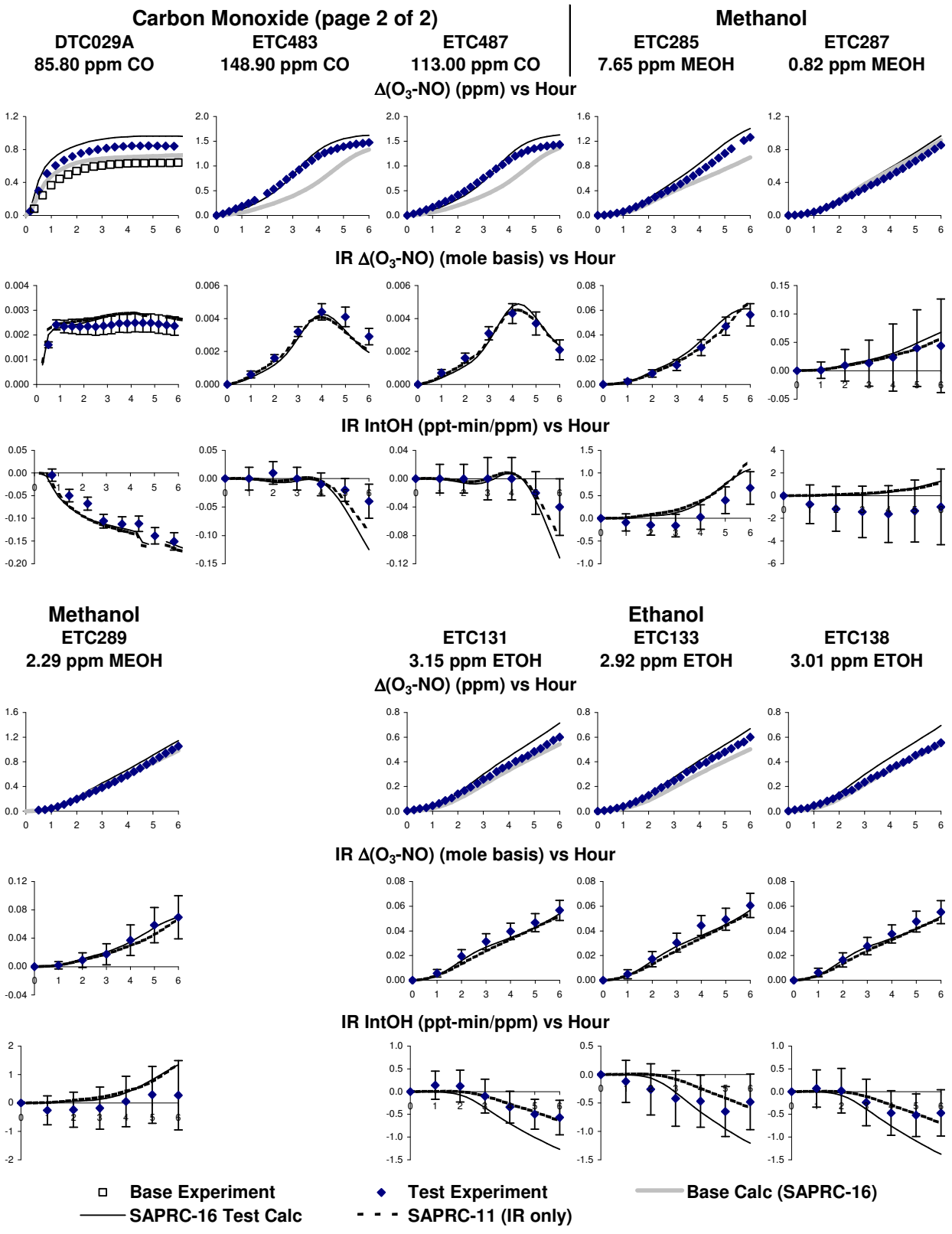
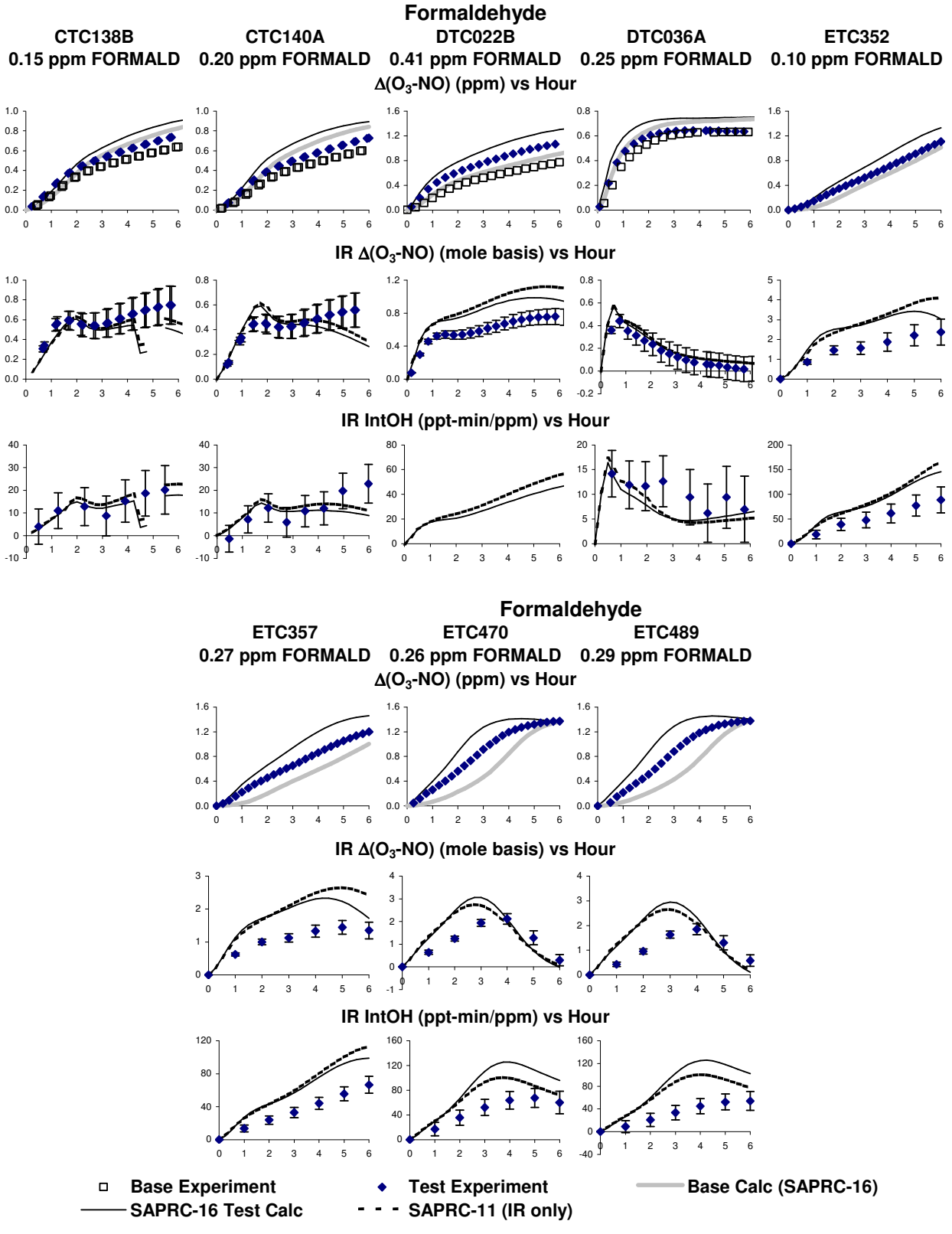

Benzaldehyde
m-cresol
EPA380B
0.06 ppm BENZALD
CTC266A
0.14 ppm BENZALD
CTC267B
0.13 ppm BENZALD
EPA383B
0.08 ppm M-CRESOL
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Benzyl alcohol
EPA319A
0.09 ppm BZ-CH2OH
EPA323B
0.05 ppm BZ-CH2OH
EPA320B
0.10 ppm BZ-CH2OH
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

Figure B-4. Plots of selected experimental and model calculation results for the incremental reactivity experiments with CO and representative oxidation products.



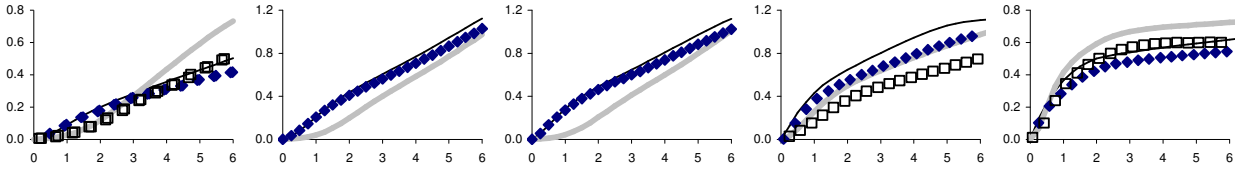

Carbon Monoxide (page 2 of 2)
Methanol
DTC029A
85.80 ppm CO
ETC483
148.90 ppm CO
ETC487
113.00 ppm CO
ETC285
7.65 ppm MEOH
ETC287
0.82 ppm MEOH
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Methanol
ETC289
2.29 ppm MEOH
Ethanol
ETC131
3.15 ppm ETOH
ETC133
2.92 ppm ETOH
ETC138
3.01 ppm ETOH
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)


Formaldehyde
CTC138B
0.15 ppm FORMALD
CTC140A
0.20 ppm FORMALD
DTC022B
0.41 ppm FORMALD
DTC036A
0.25 ppm FORMALD
ETC352
0.10 ppm FORMALD
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Formaldehyde
ETC357
0.27 ppm FORMALD
ETC470
0.26 ppm FORMALD
ETC489
0.29 ppm FORMALD
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

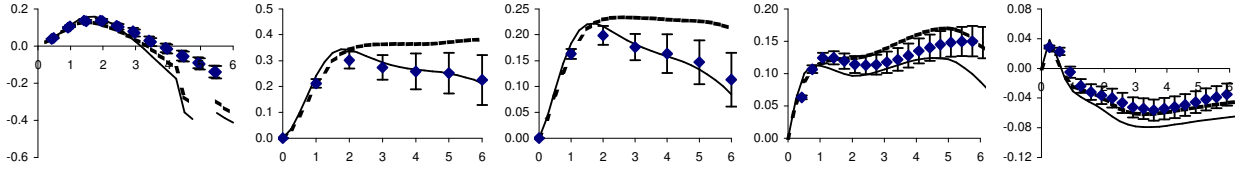
Acetaldehyde

CTC107A	ETC335	ETC338	DTC065A	DTC066B
0.56 ppm ACETALD	0.70 ppm ACETALD	1.31 ppm ACETALD	1.54 ppm ACETALD	1.62 ppm ACETALD

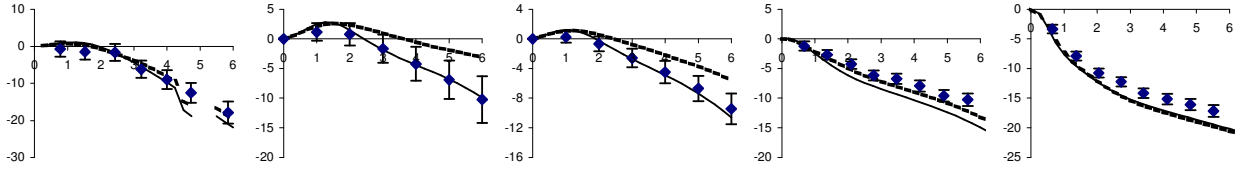
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



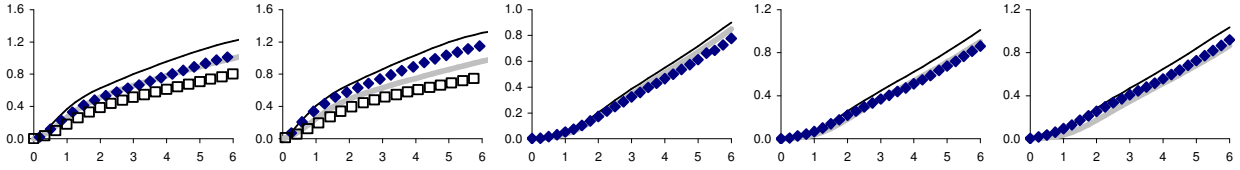
IR IntOH (ppt-min/ppm) vs Hour



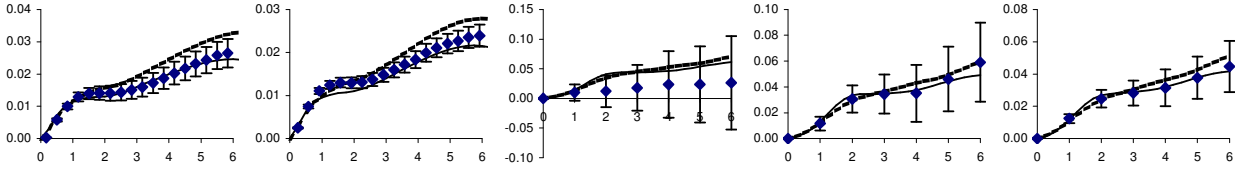
Acetone (page 1 of 2)

DTC028A	DTC064B	ETC243	ETC245	ETC247
8.72 ppm ACETONE	16.27 ppm ACETONE	0.85 ppm ACETONE	2.19 ppm ACETONE	4.15 ppm ACETONE

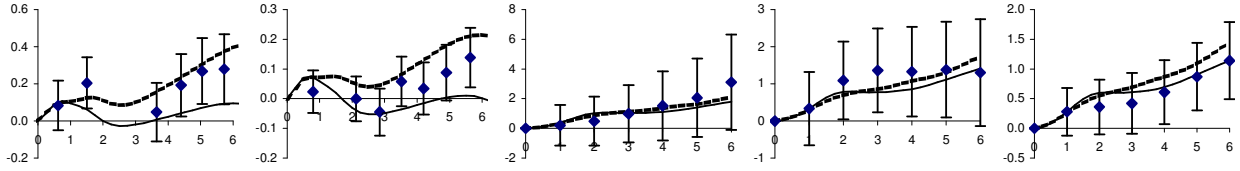
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour

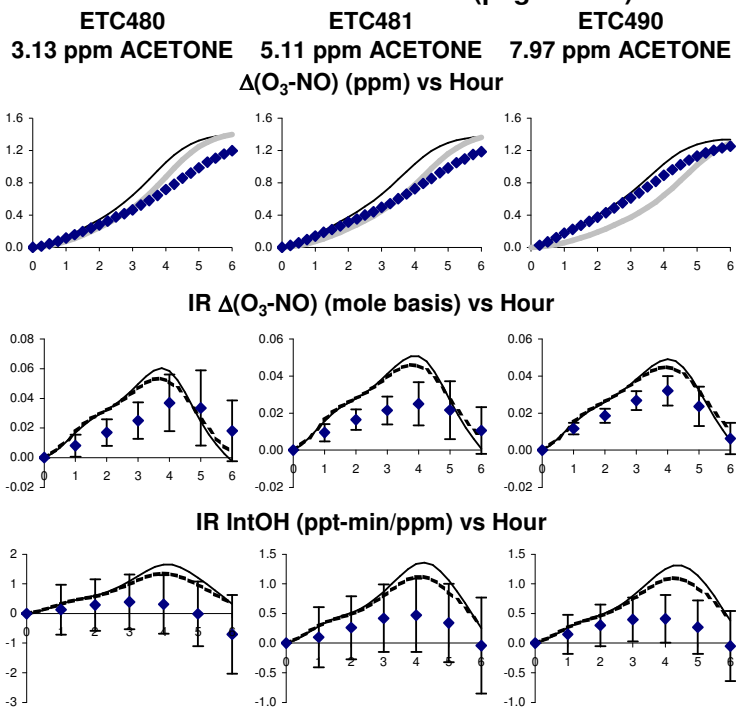


IR IntOH (ppt-min/ppm) vs Hour

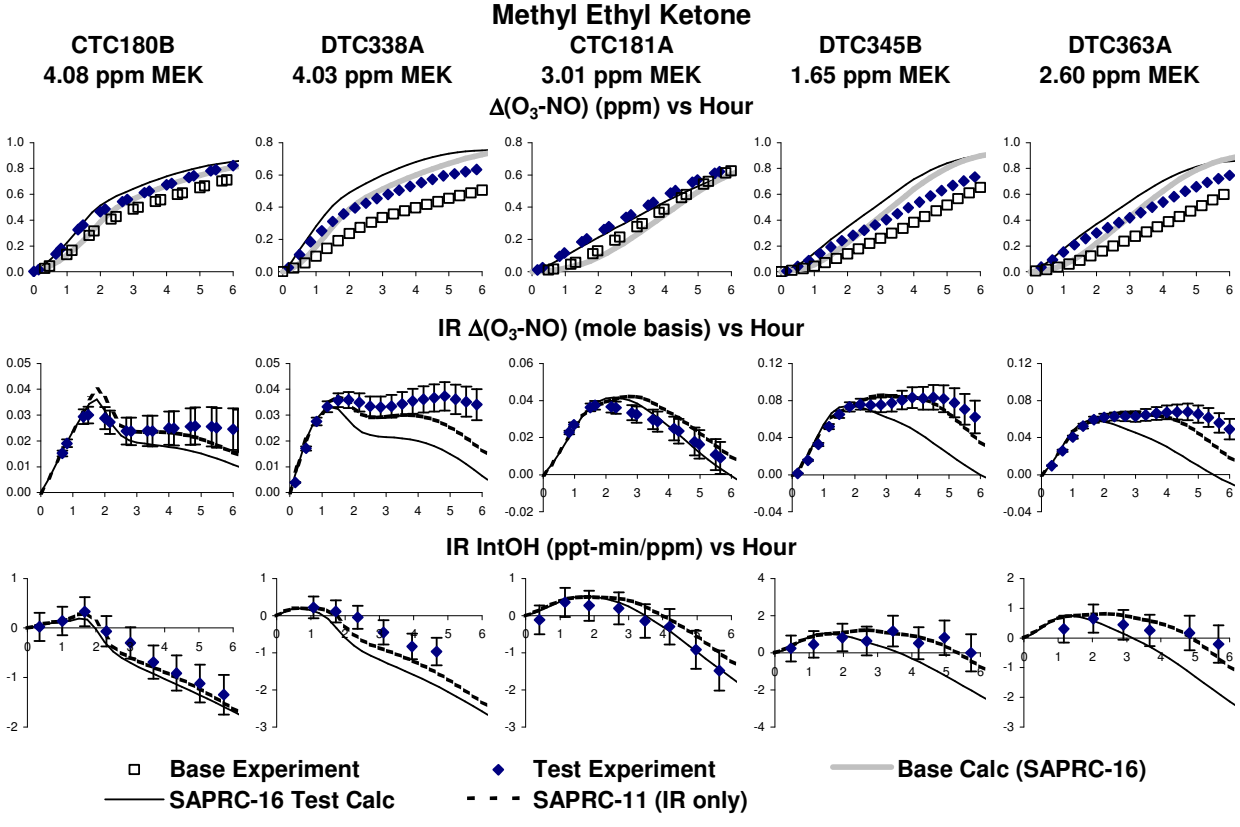


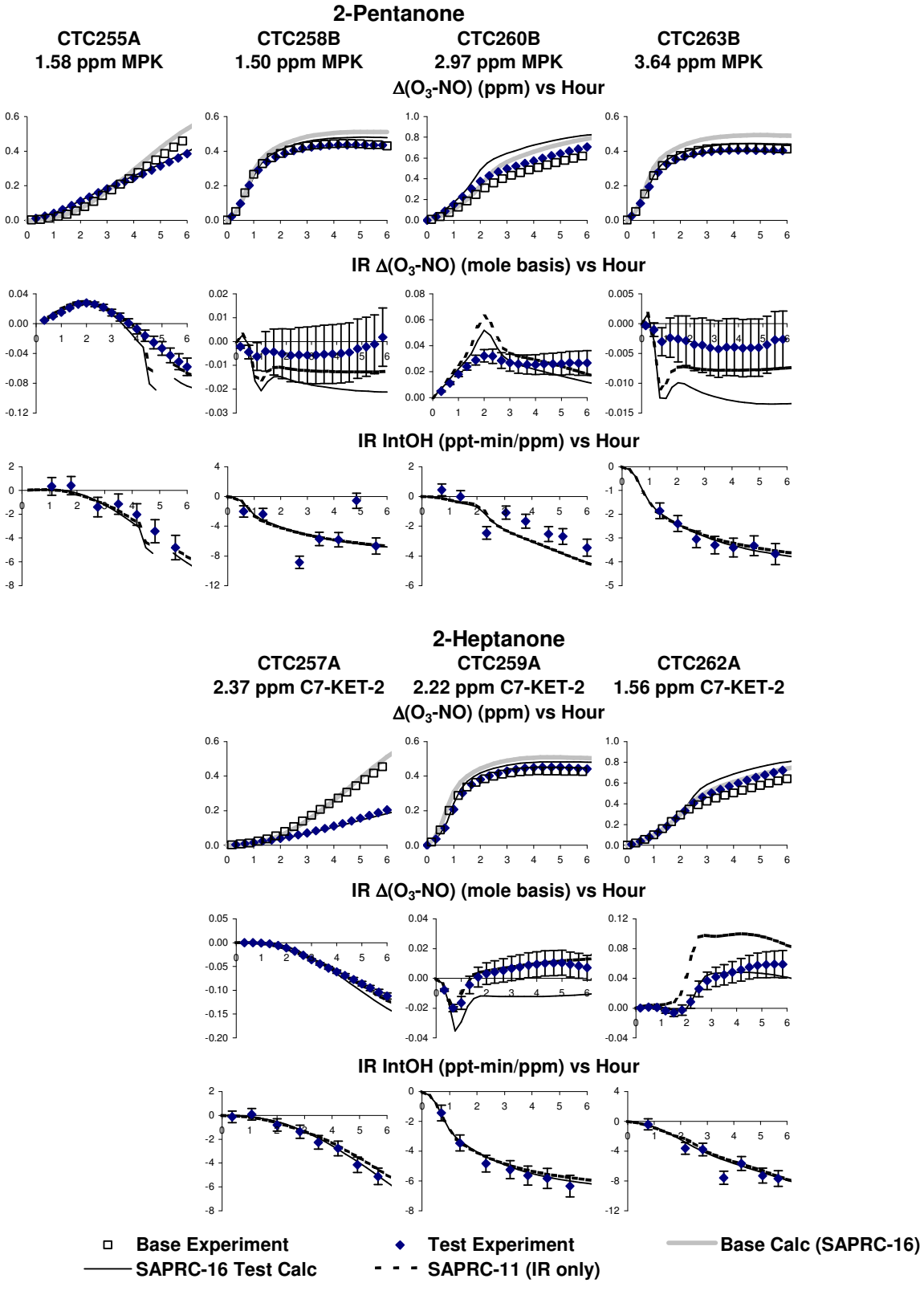
Base Experiment Test Experiment Base Calc (SAPRC-16)
SAPRC-16 Test Calc SAPRC-11 (IR only)

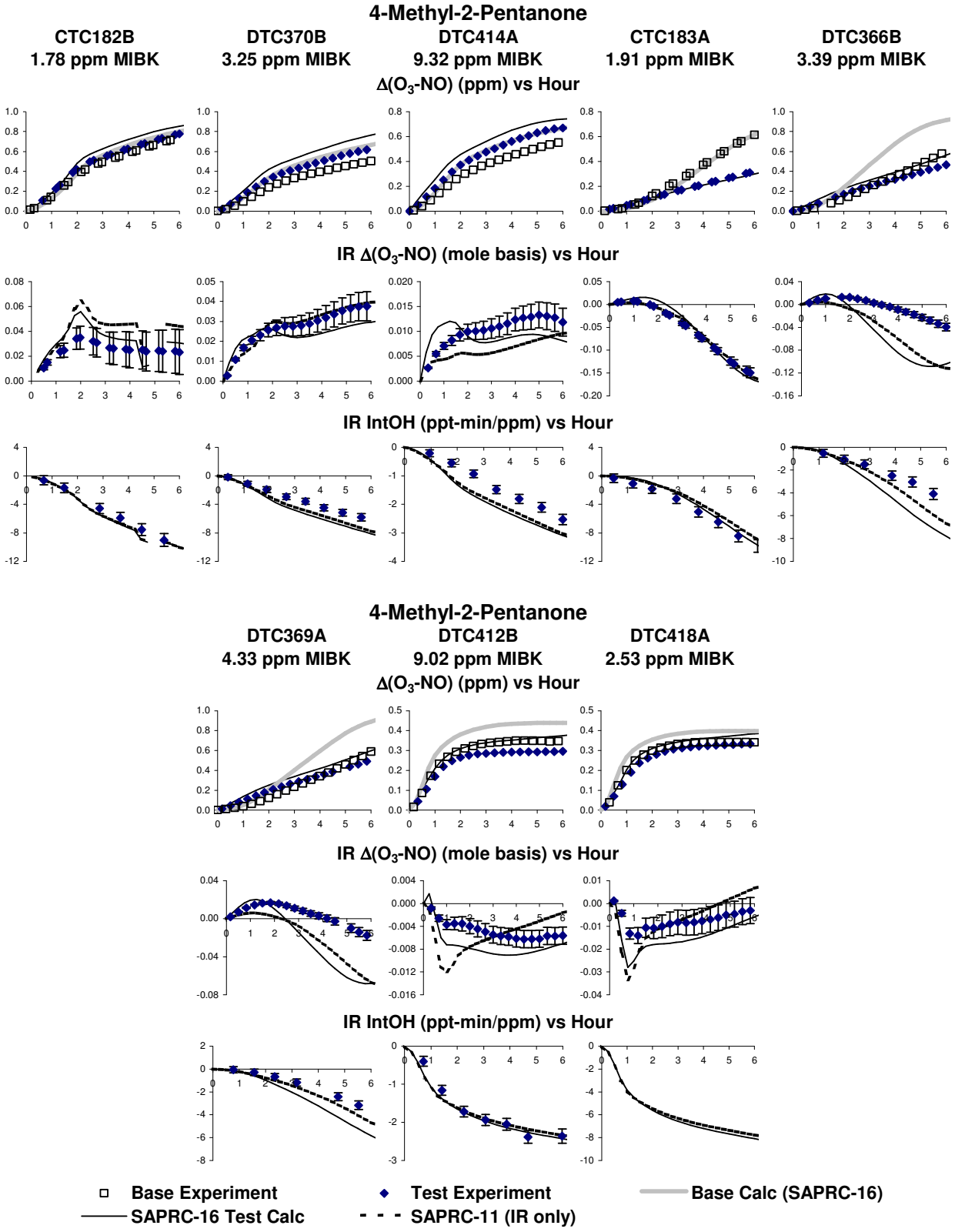
Acetone (page 2 of 2)



Methyl Ethyl Ketone




2-Pentanone
CTC255A
1.58 ppm MPK
CTC258B
1.50 ppm MPK
CTC260B
2.97 ppm MPK
CTC263B
3.64 ppm MPK
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
2-Heptanone
CTC257A
2.37 ppm C7-KET-2
CTC259A
2.22 ppm C7-KET-2
CTC262A
1.56 ppm C7-KET-2
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)


4-Methyl-2-Pentanone
CTC182B
1.78 ppm MIBK
DTC370B
3.25 ppm MIBK
DTC414A
9.32 ppm MIBK
CTC183A
1.91 ppm MIBK
DTC366B
3.39 ppm MIBK
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
4-Methyl-2-Pentanone
DTC369A
4.33 ppm MIBK
DTC412B
9.02 ppm MIBK
DTC418A
2.53 ppm MIBK
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

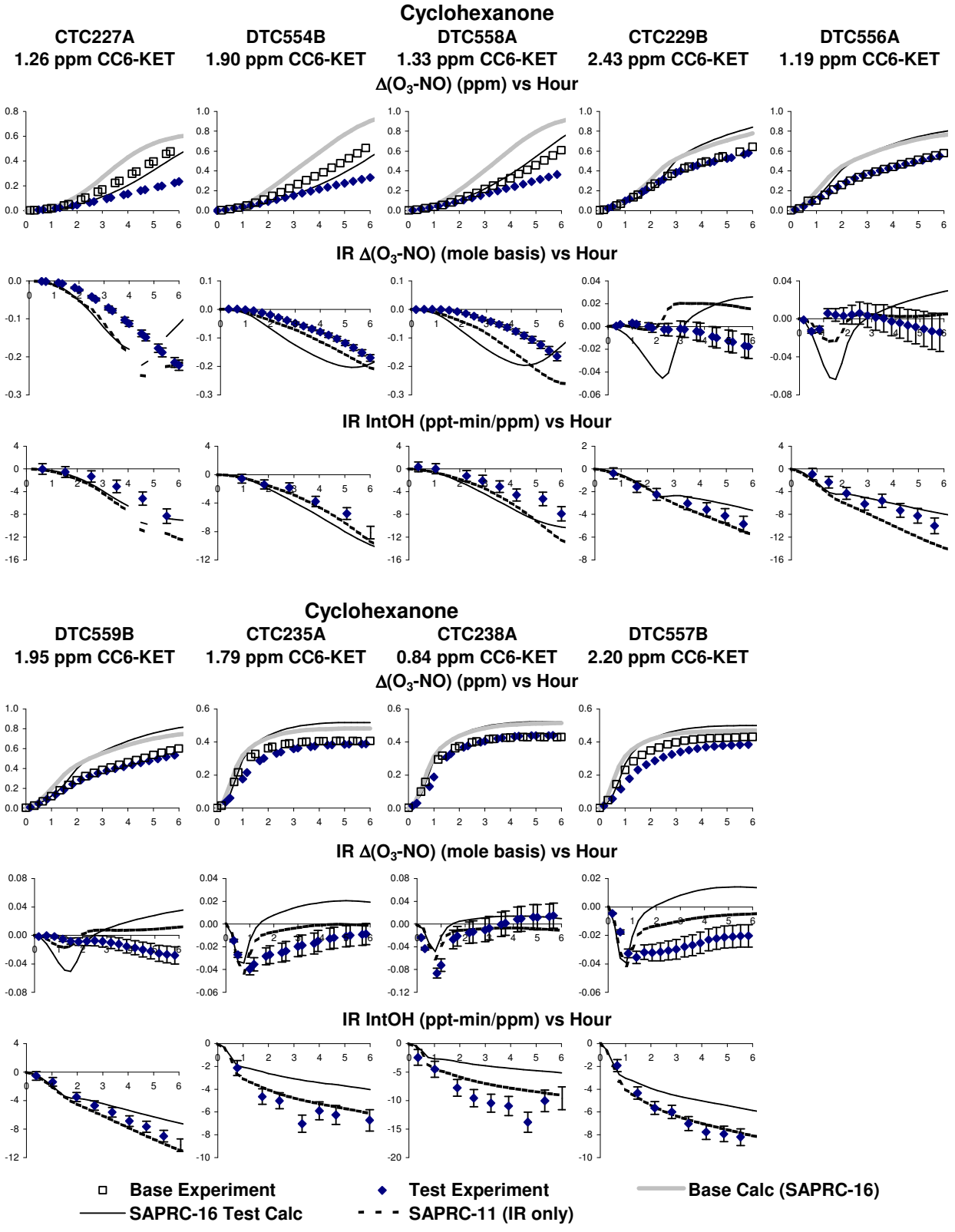
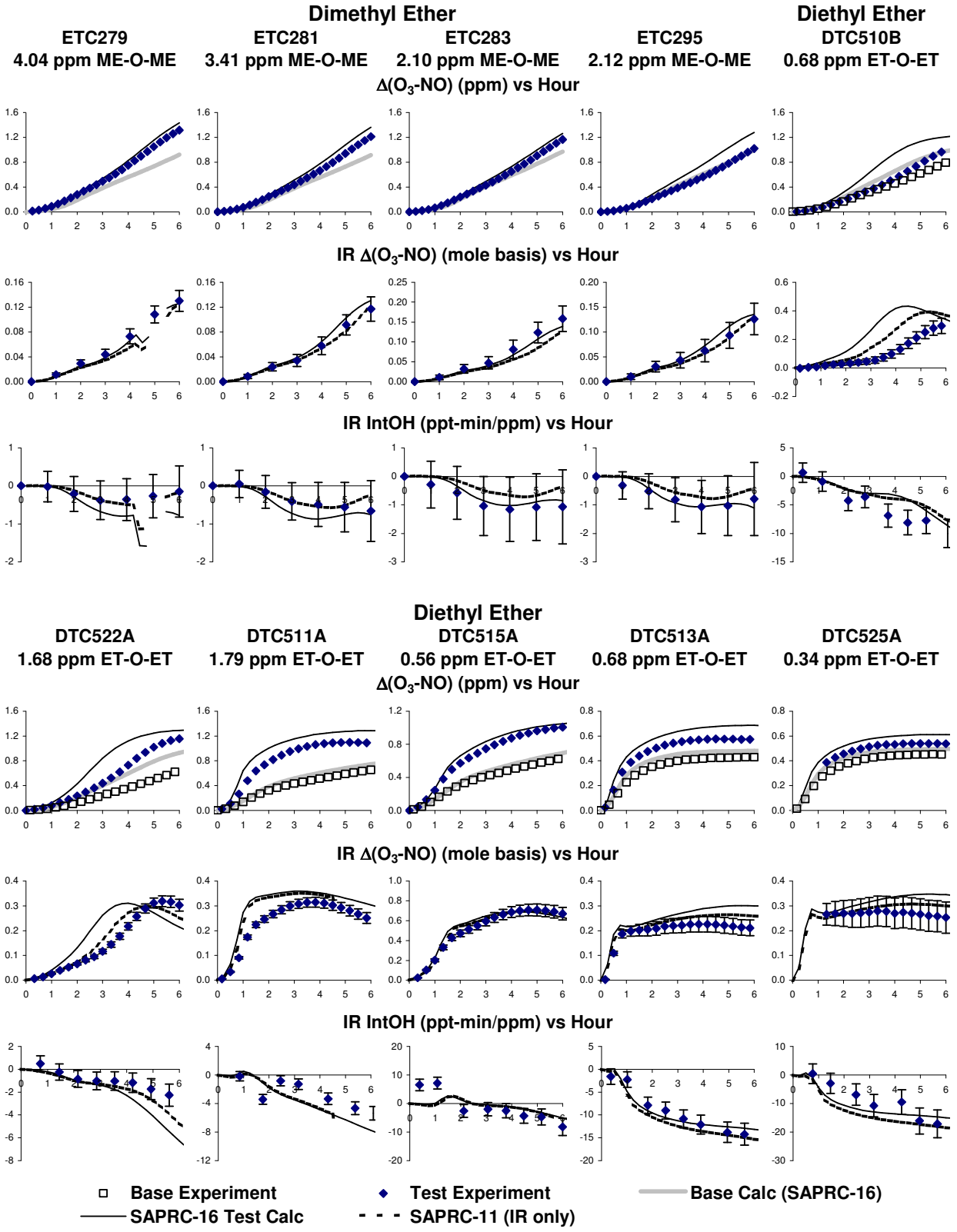
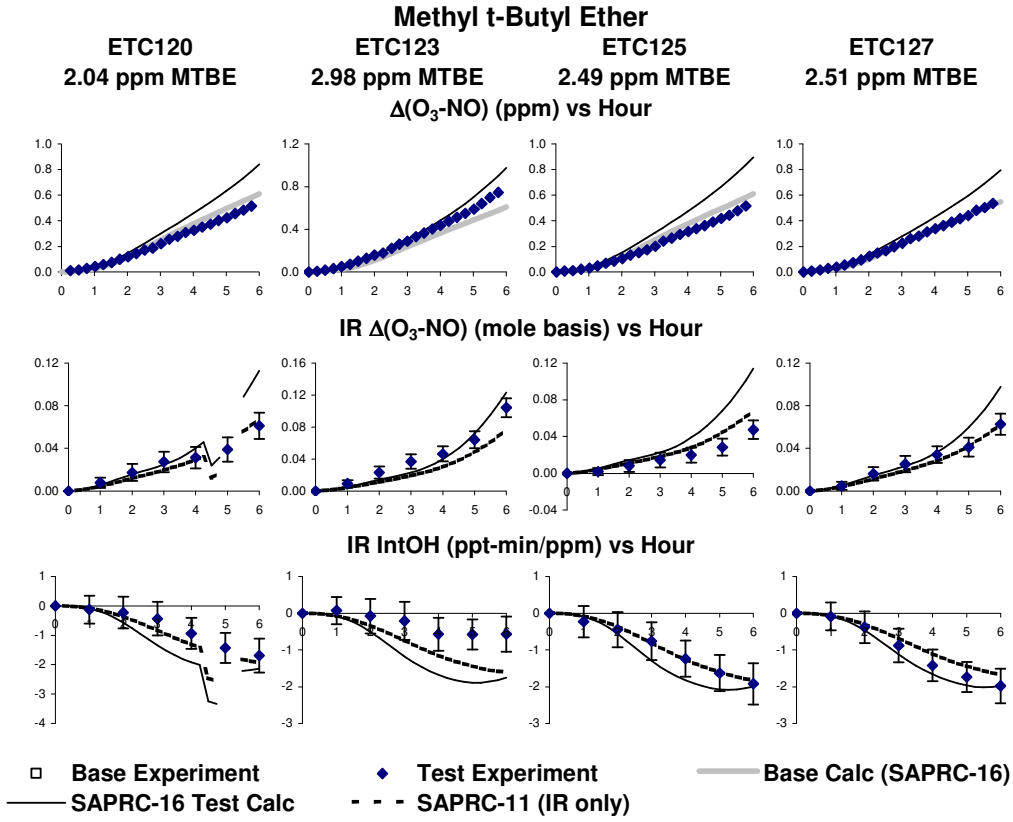
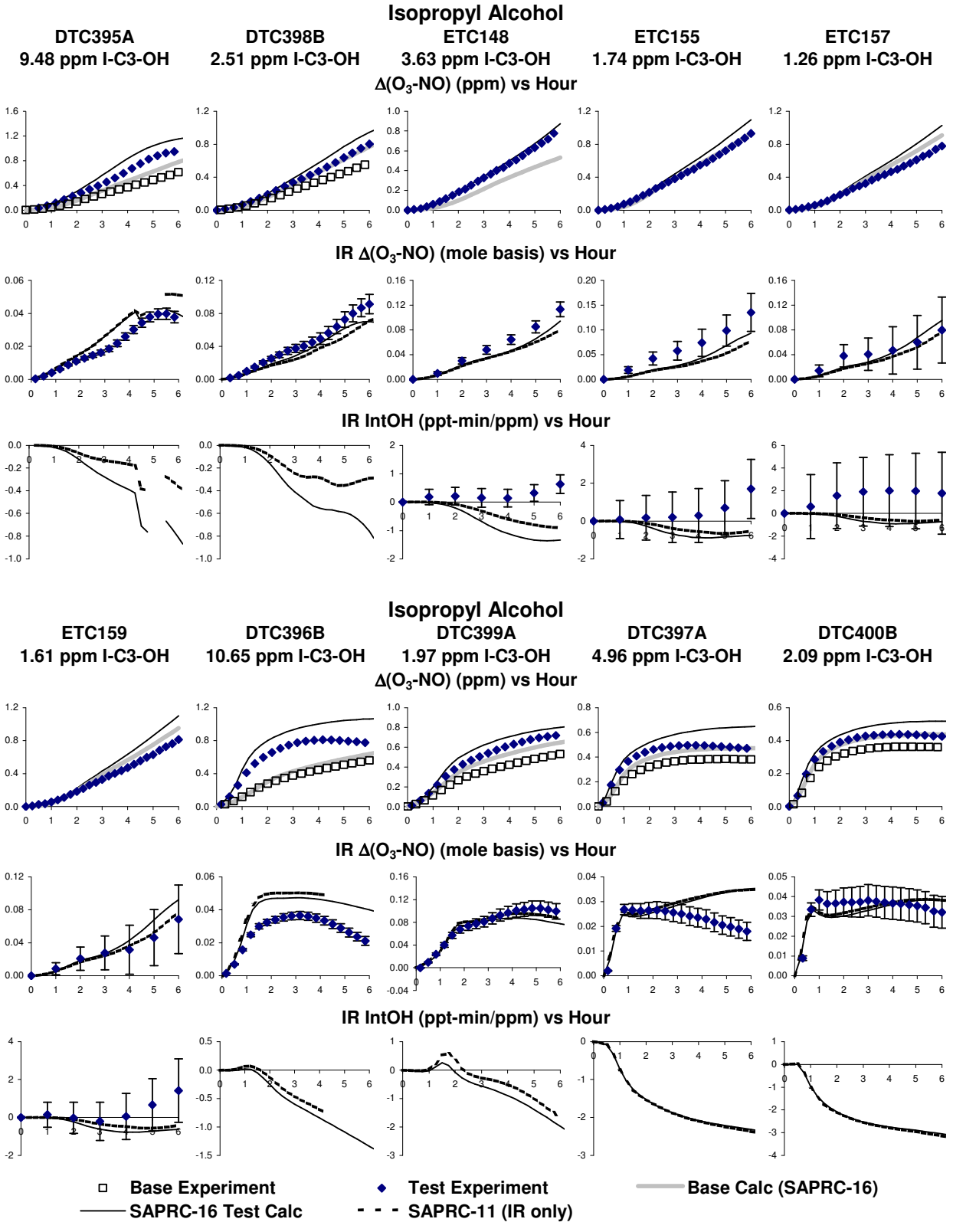
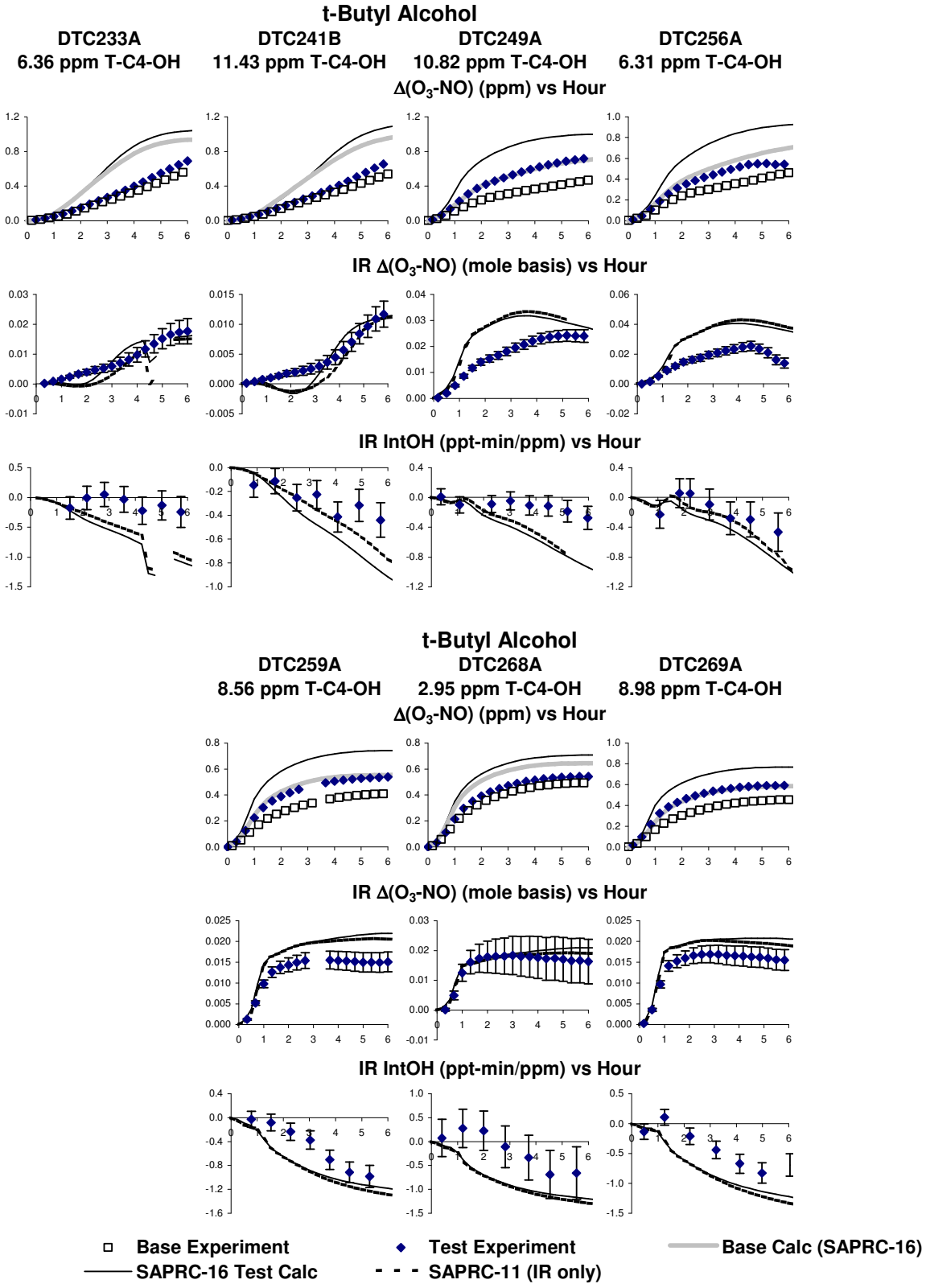

Cyclohexanone
CTC227A
1.26 ppm CC6-KET
DTC554B
1.90 ppm CC6-KET
DTC558A
1.33 ppm CC6-KET
CTC229B
2.43 ppm CC6-KET
DTC556A
1.19 ppm CC6-KET
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Cyclohexanone
DTC559B
1.95 ppm CC6-KET
CTC235A
1.79 ppm CC6-KET
CTC238A
0.84 ppm CC6-KET
DTC557B
2.20 ppm CC6-KET
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

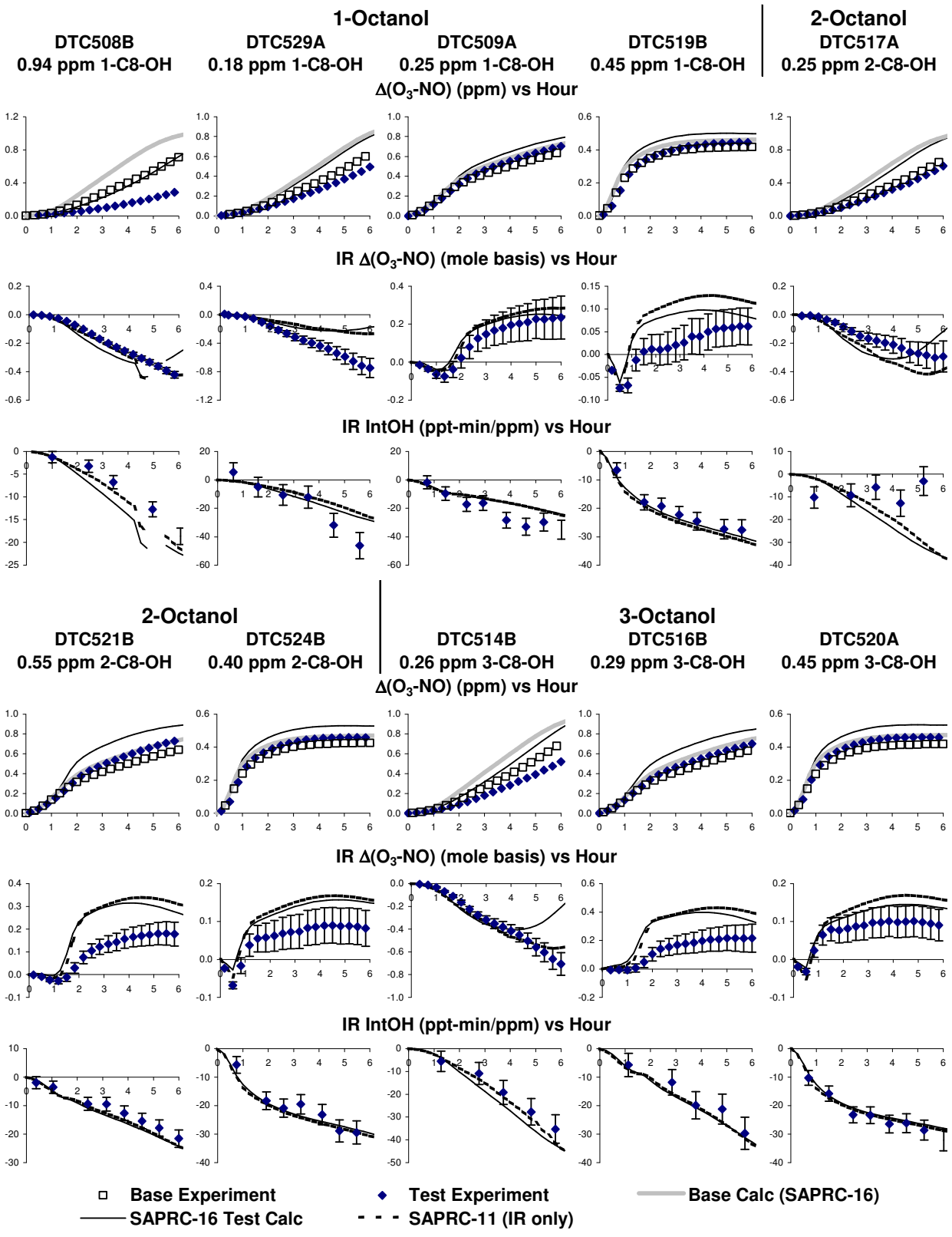
Figure B-5. Plots of selected experimental and model calculation results for the incremental reactivity experiments with various types of emitted oxygenated compounds.



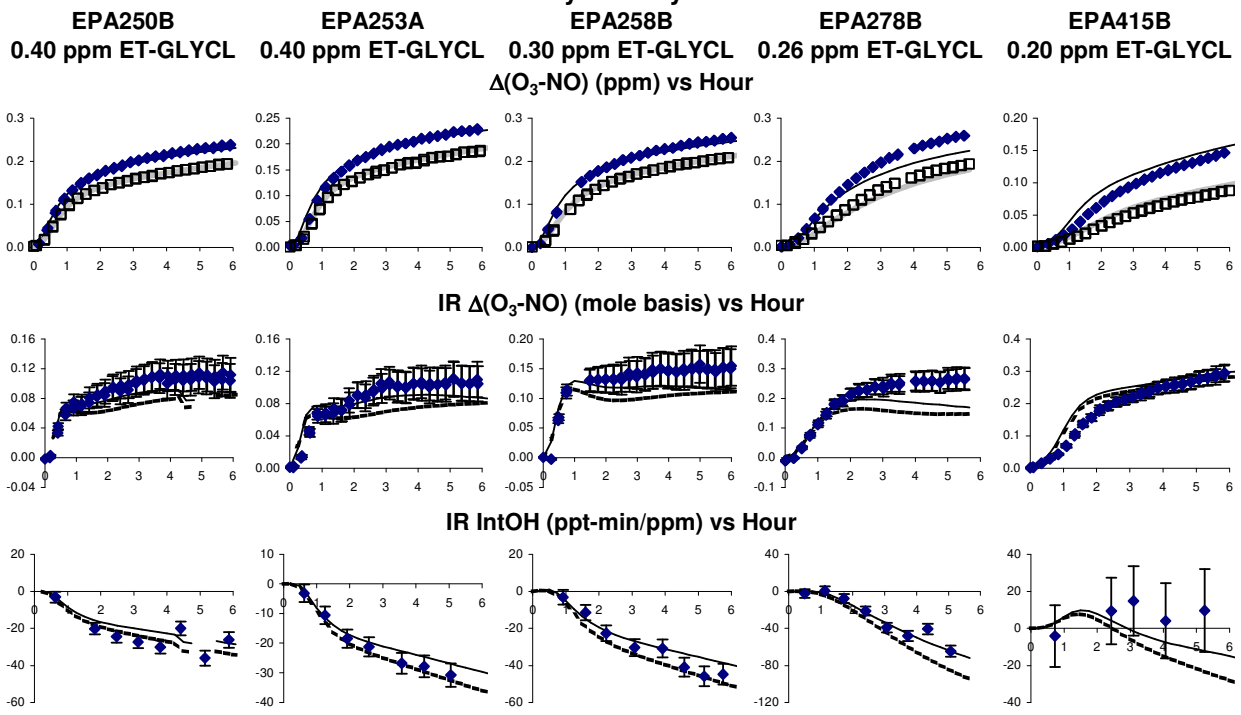

Methyl t-Butyl Ether
ETC120
2.04 ppm MTBE
ETC123
2.98 ppm MTBE
ETC125
2.49 ppm MTBE
ETC127
2.51 ppm MTBE
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)


Isopropyl Alcohol
DTC395A
9.48 ppm I-C3-OH
DTC398B
2.51 ppm I-C3-OH
ETC148
3.63 ppm I-C3-OH
ETC155
1.74 ppm I-C3-OH
ETC157
1.26 ppm I-C3-OH
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Isopropyl Alcohol
ETC159
1.61 ppm I-C3-OH
DTC396B
10.65 ppm I-C3-OH
DTC399A
1.97 ppm I-C3-OH
DTC397A
4.96 ppm I-C3-OH
DTC400B
2.09 ppm I-C3-OH
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

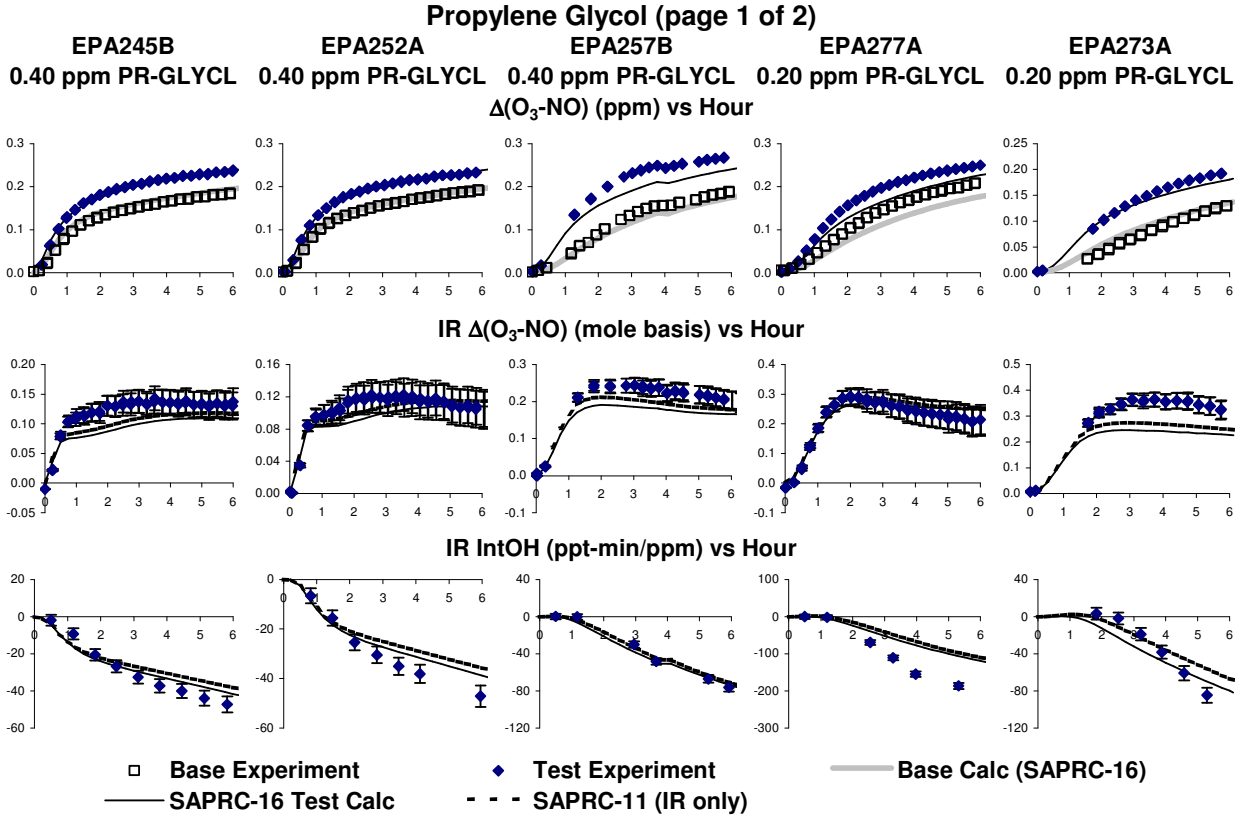

t-Butyl Alcohol
DTC233A
6.36 ppm T-C4-OH
DTC241B
11.43 ppm T-C4-OH
DTC249A
10.82 ppm T-C4-OH
DTC256A
6.31 ppm T-C4-OH
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
t-Butyl Alcohol
DTC259A
8.56 ppm T-C4-OH
DTC268A
2.95 ppm T-C4-OH
DTC269A
8.98 ppm T-C4-OH
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)


1-Octanol
2-Octanol
DTC508B
0.94 ppm 1-C8-OH
DTC529A
0.18 ppm 1-C8-OH
DTC509A
0.25 ppm 1-C8-OH
DTC519B
0.45 ppm 1-C8-OH
DTC517A
0.25 ppm 2-C8-OH
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
2-Octanol
3-Octanol
DTC521B
0.55 ppm 2-C8-OH
DTC524B
0.40 ppm 2-C8-OH
DTC514B
0.26 ppm 3-C8-OH
DTC516B
0.29 ppm 3-C8-OH
DTC520A
0.45 ppm 3-C8-OH
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

Ethylene Glycol



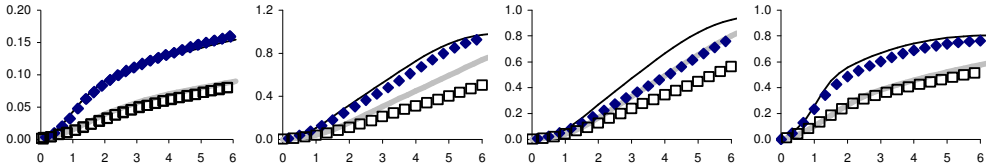
Propylene Glycol (page 1 of 2)



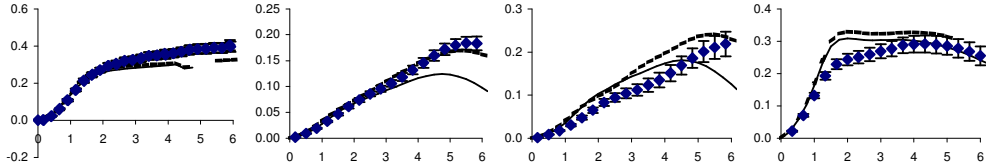
Propylene Glycol (page 2 of 2)

EPA404B	DTC385A	DTC389B	DTC386B
0.20 ppm PR-GLYCL	2.40 ppm PR-GLYCL	0.99 ppm PR-GLYCL	0.94 ppm PR-GLYCL

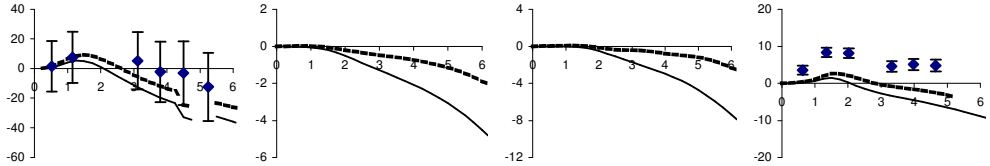
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



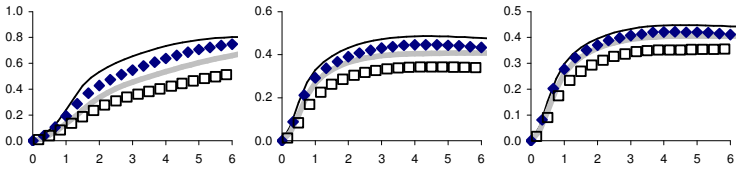
IR IntOH (ppt-min/ppm) vs Hour



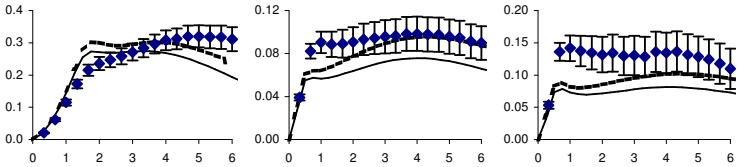
Propylene Glycol

DTC390A	DTC388A	DTC391B
0.74 ppm PR-GLYCL	1.06 ppm PR-GLYCL	0.52 ppm PR-GLYCL

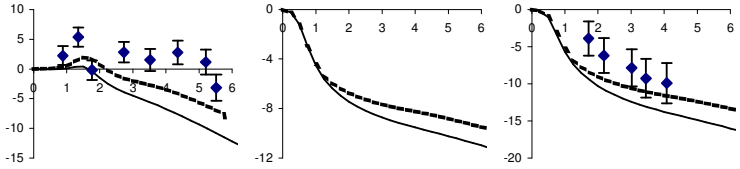
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour

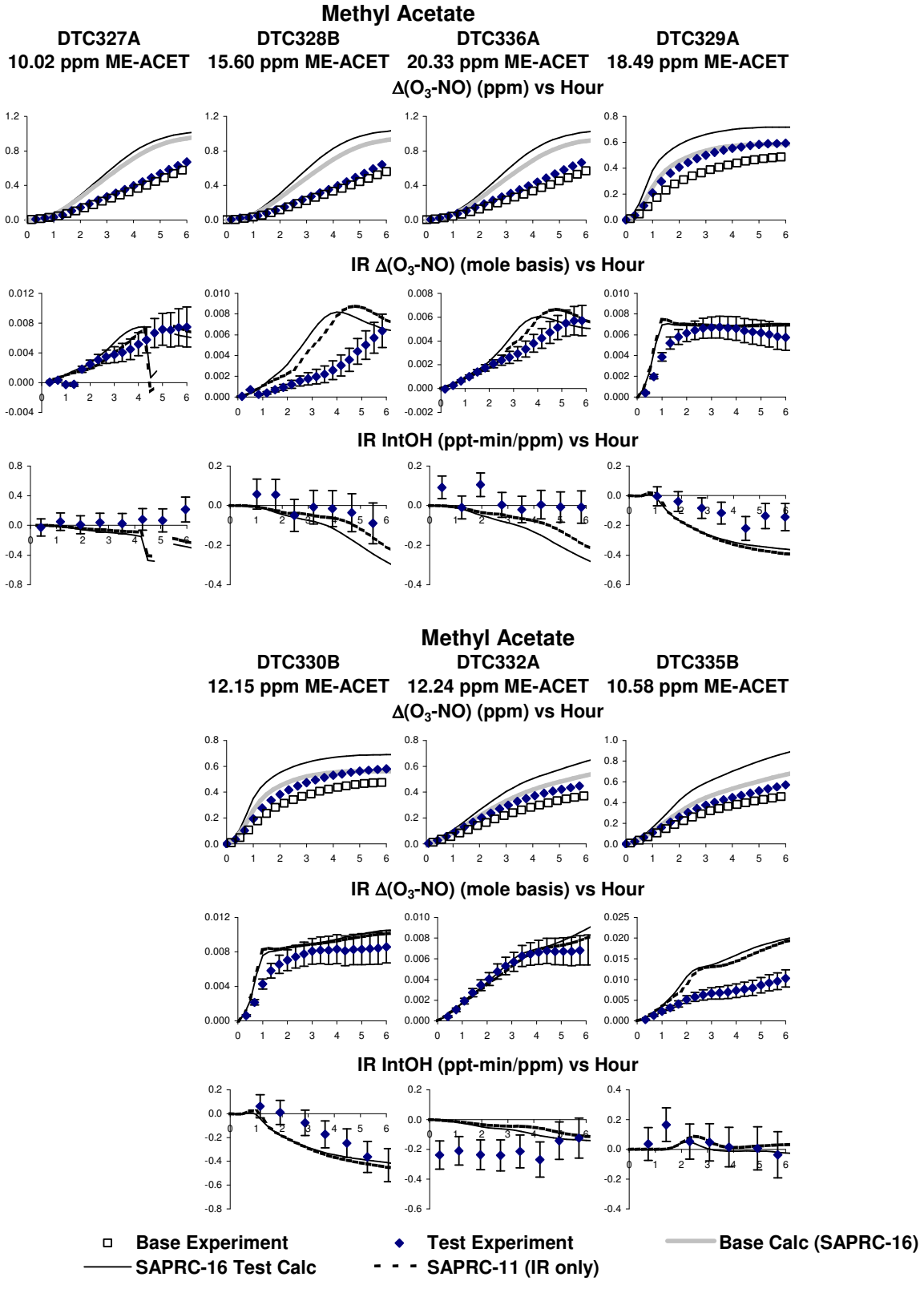


IR IntOH (ppt-min/ppm) vs Hour



□ Base Experiment ◆ Test Experiment ——— Base Calc (SAPRC-16)

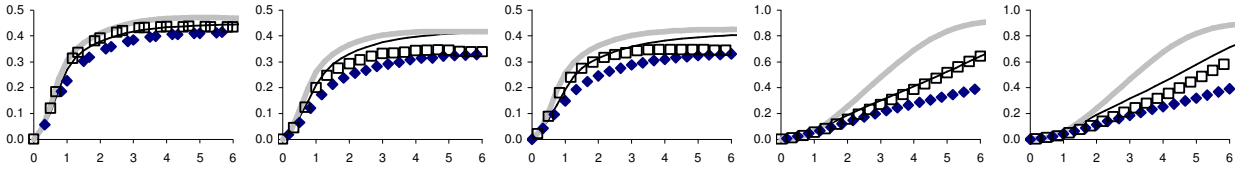
——— SAPRC-16 Test Calc - - - SAPRC-11 (IR only)


Methyl Acetate
DTC327A
10.02 ppm ME-ACET
DTC328B
15.60 ppm ME-ACET
DTC336A
20.33 ppm ME-ACET
DTC329A
18.49 ppm ME-ACET
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Methyl Acetate
DTC330B
12.15 ppm ME-ACET
DTC332A
12.24 ppm ME-ACET
DTC335B
10.58 ppm ME-ACET
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

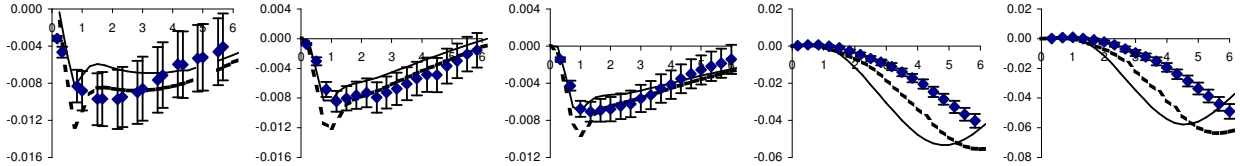
Ethyl Acetate

CTC195B 4.99 ppm ET-ACET | **DTC394A** 6.06 ppm ET-ACET | **DTC409A** 9.03 ppm ET-ACET | **DTC358A** 5.88 ppm ET-ACET | **DTC362B** 4.29 ppm ET-ACET

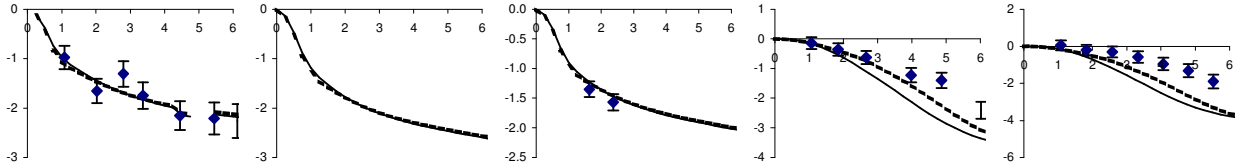
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



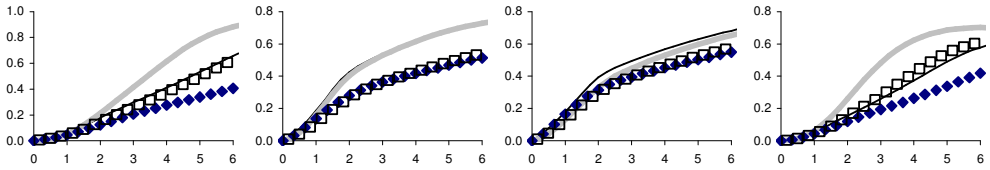
IR IntOH (ppt-min/ppm) vs Hour



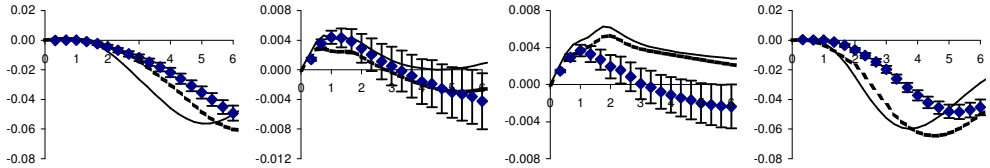
Ethyl Acetate

DTC364B 4.48 ppm ET-ACET | **DTC359B** 5.91 ppm ET-ACET | **DTC408B** 10.12 ppm ET-ACET | **DTC415B** 4.24 ppm ET-ACET

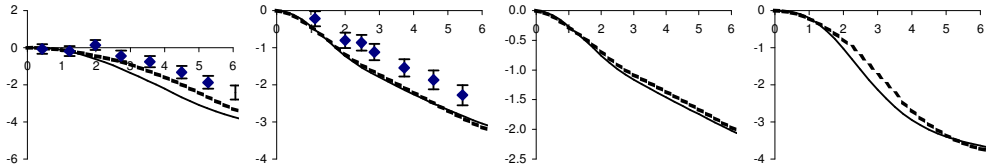
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour

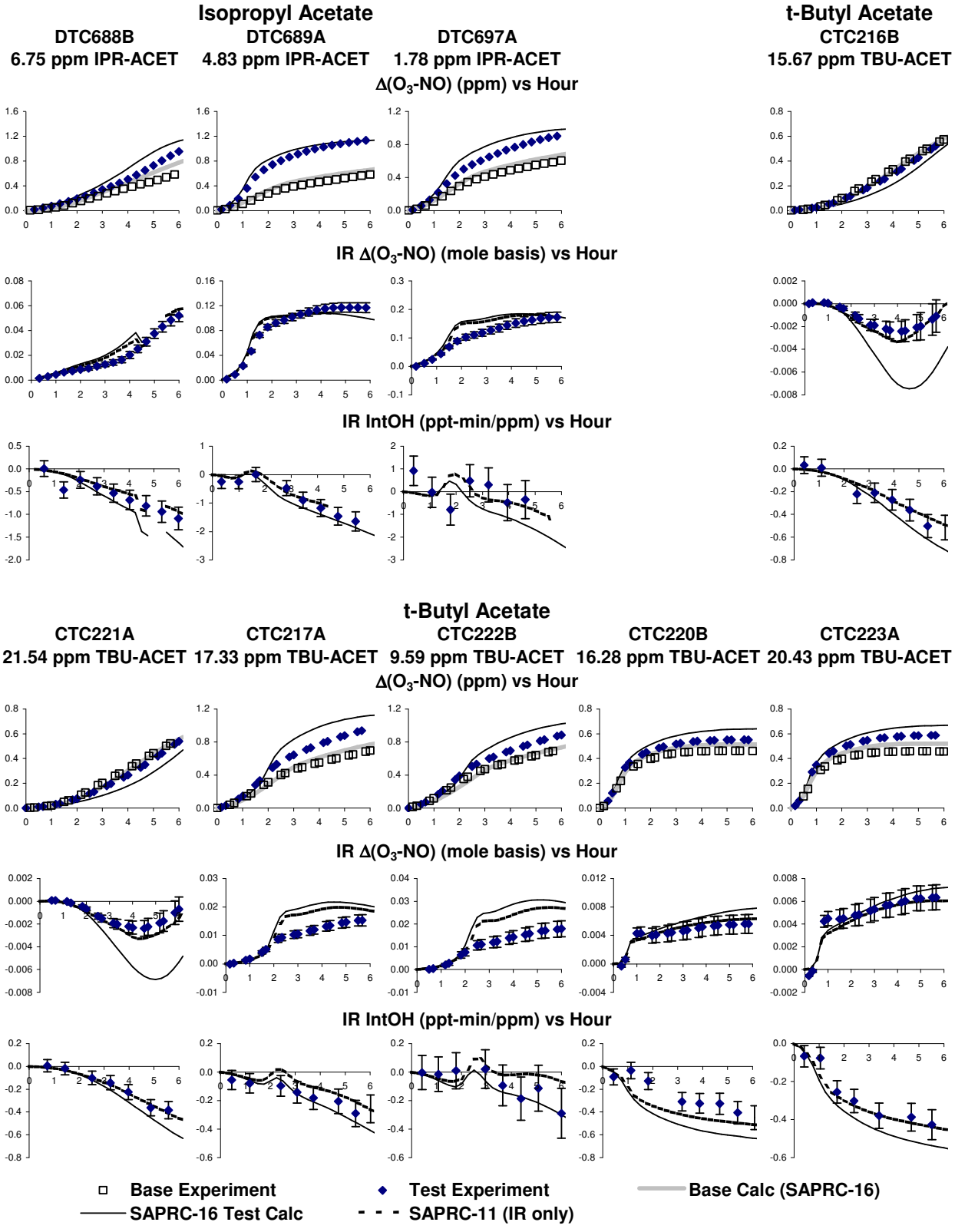


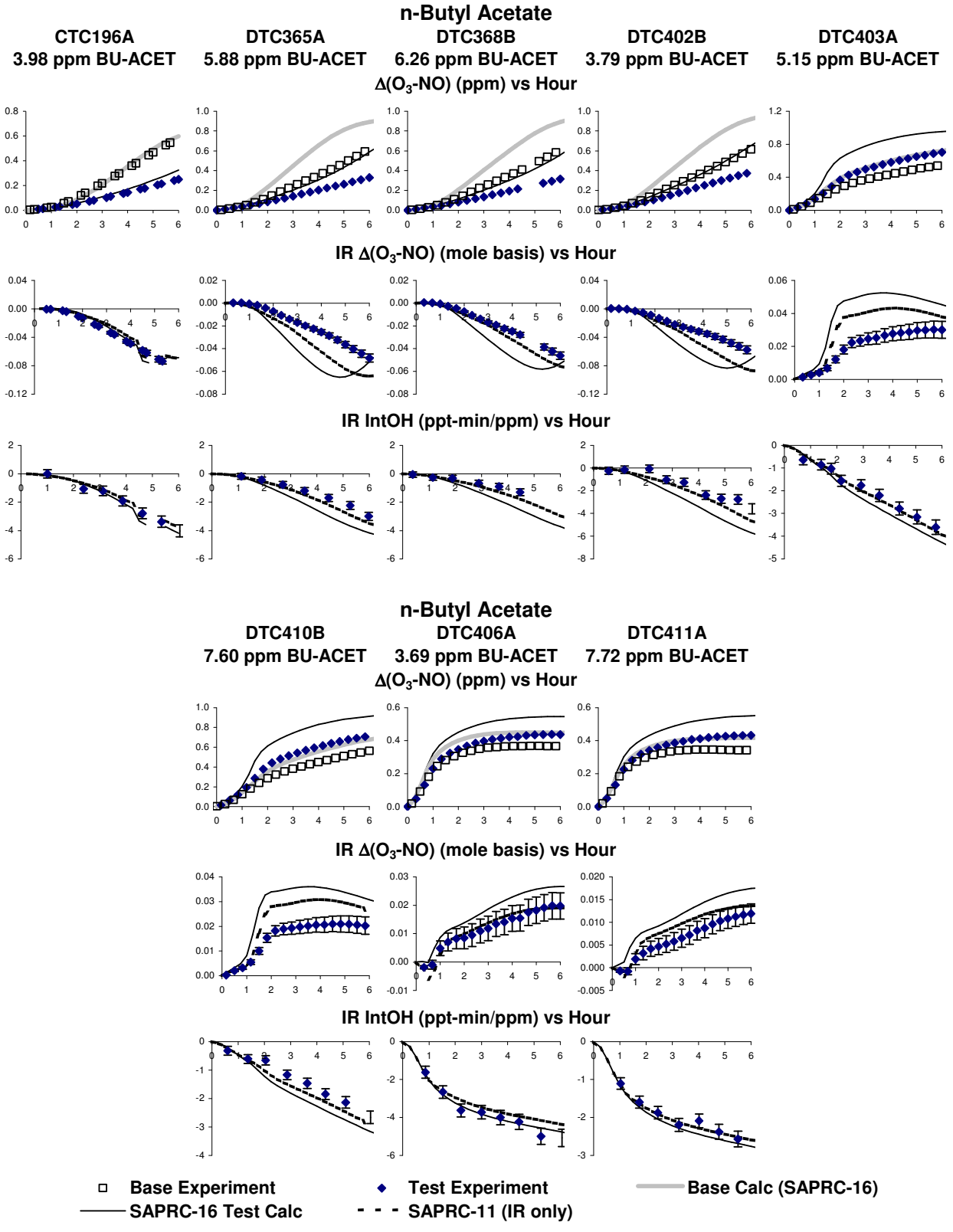
IR IntOH (ppt-min/ppm) vs Hour

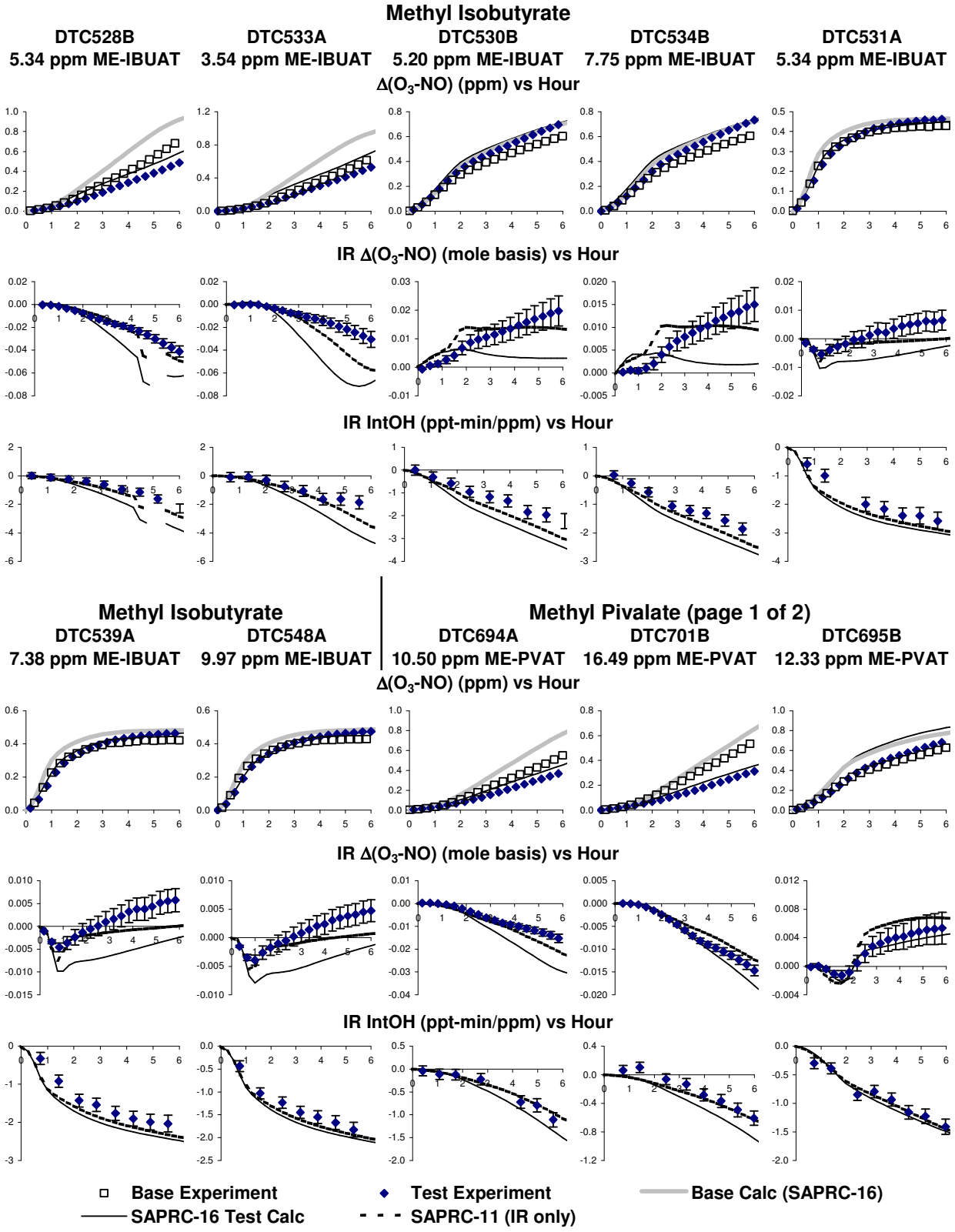


□ Base Experiment ◆ Test Experiment Base Calc (SAPRC-16)

SAPRC-16 Test Calc - - - SAPRC-11 (IR only)


Isopropyl Acetate
t-Butyl Acetate
DTC688B
6.75 ppm IPR-ACET
DTC689A
4.83 ppm IPR-ACET
DTC697A
1.78 ppm IPR-ACET
CTC216B
15.67 ppm TBU-ACET
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
t-Butyl Acetate
CTC221A
21.54 ppm TBU-ACET
CTC217A
17.33 ppm TBU-ACET
CTC222B
9.59 ppm TBU-ACET
CTC220B
16.28 ppm TBU-ACET
CTC223A
20.43 ppm TBU-ACET
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)


n-Butyl Acetate
CTC196A
3.98 ppm BU-ACET
DTC365A
5.88 ppm BU-ACET
DTC368B
6.26 ppm BU-ACET
DTC402B
3.79 ppm BU-ACET
DTC403A
5.15 ppm BU-ACET
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
n-Butyl Acetate
DTC410B
7.60 ppm BU-ACET
DTC406A
3.69 ppm BU-ACET
DTC411A
7.72 ppm BU-ACET
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)


Methyl Isobutyrate
DTC528B
5.34 ppm ME-IBUAT
DTC533A
3.54 ppm ME-IBUAT
DTC530B
5.20 ppm ME-IBUAT
DTC534B
7.75 ppm ME-IBUAT
DTC531A
5.34 ppm ME-IBUAT
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Methyl Isobutyrate
DTC539A
7.38 ppm ME-IBUAT
DTC548A
9.97 ppm ME-IBUAT
Methyl Pivalate (page 1 of 2)
DTC694A
10.50 ppm ME-PVAT
DTC701B
16.49 ppm ME-PVAT
DTC695B
12.33 ppm ME-PVAT
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

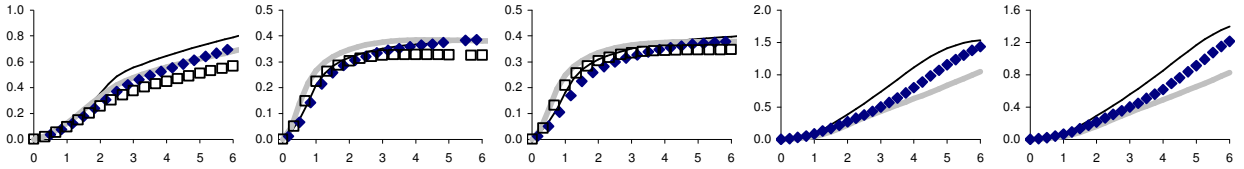
Methyl Pivalate (page 2 of 2)

DTC702A	DTC700A	DTC707B
20.41 ppm ME-PVAT	19.04 ppm ME-PVAT	29.19 ppm ME-PVAT

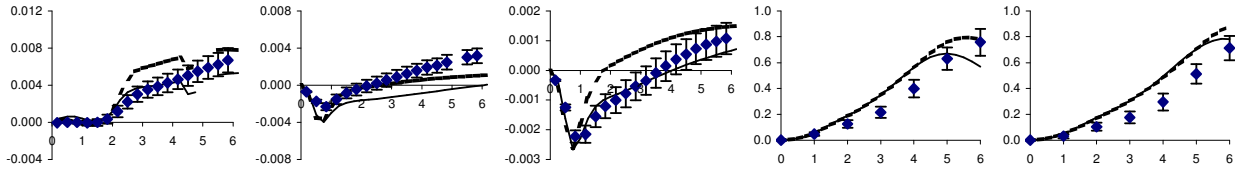
2-Ethoxyethanol

ETC163	ETC171
0.86 ppm ETO-ETOH	0.73 ppm ETO-ETOH

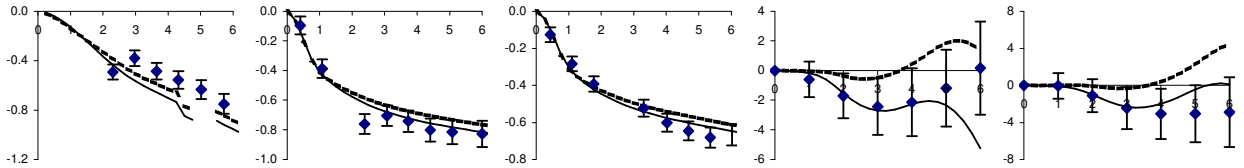
Δ(O_3-NO) (ppm) vs Hour



IR Δ(O_3-NO) (mole basis) vs Hour



IR IntOH (ppt-min/ppm) vs Hour



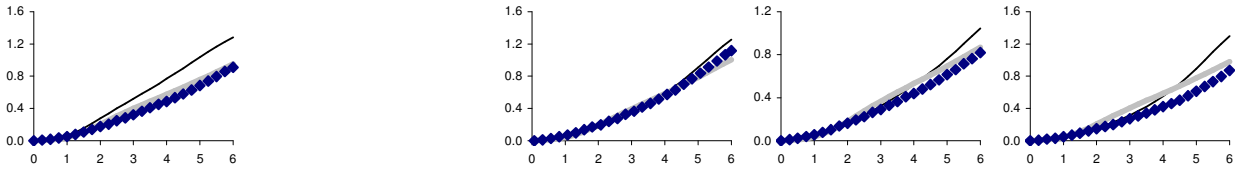
2-Ethoxyethanol

ETC175
0.40 ppm ETO-ETOH

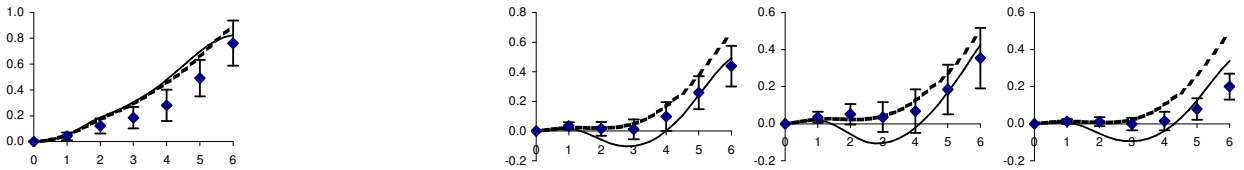
2-(2-Ethoxyethoxy) Ethanol

ETC166	ETC169	ETC173
0.50 ppm DGEE	0.41 ppm DGEE	0.95 ppm DGEE

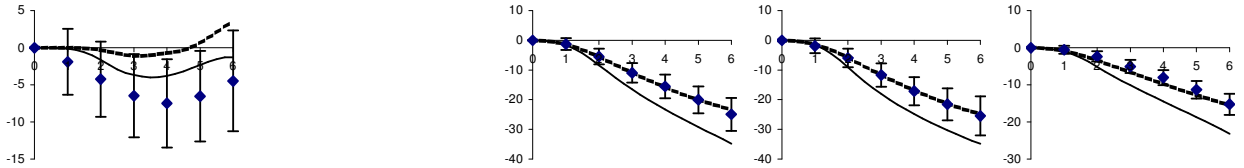
Δ(O_3-NO) (ppm) vs Hour



IR Δ(O_3-NO) (mole basis) vs Hour



IR IntOH (ppt-min/ppm) vs Hour



□ Base Experiment ◆ Test Experiment ——— Base Calc (SAPRC-16)

——— SAPRC-16 Test Calc - - - SAPRC-11 (IR only)

1-Methoxy-2-Propanol

DTC489A
1.97 ppm MEOC3OH

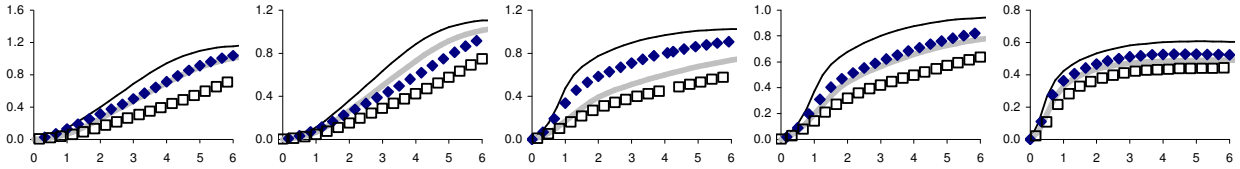
DTC495A
1.05 ppm MEOC3OH

DTC492A
1.29 ppm MEOC3OH

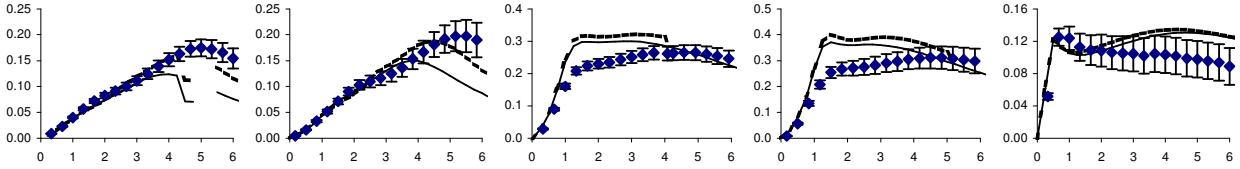
DTC500A
0.65 ppm MEOC3OH

DTC496B
0.91 ppm MEOC3OH

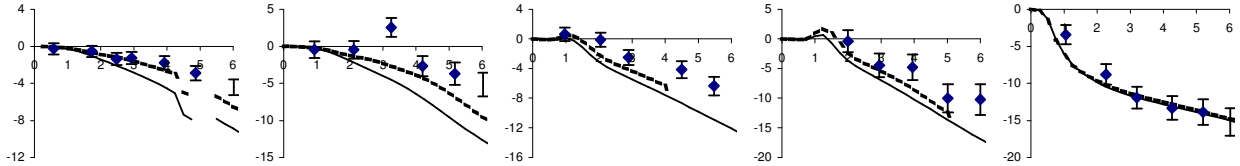
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



IR IntOH (ppt-min/ppm) vs Hour



1-Methoxy-2-Propanol

DTC501B
0.57 ppm MEOC3OH

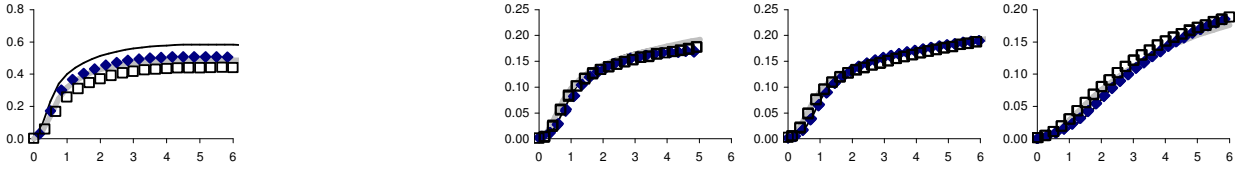
2-(2-Butoxyethoxy)-Ethanol

EPA335A
0.05 ppm DGBE

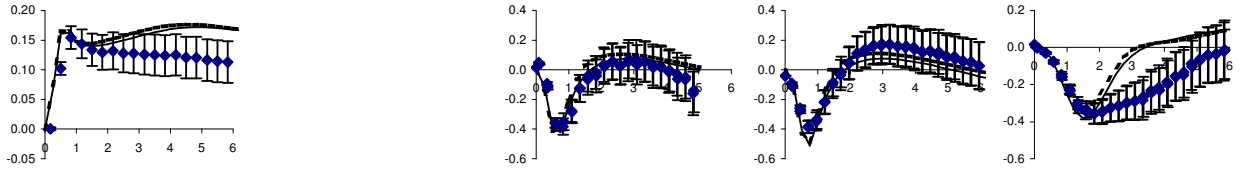
EPA353B
0.05 ppm DGBE

EPA352B
0.05 ppm DGBE

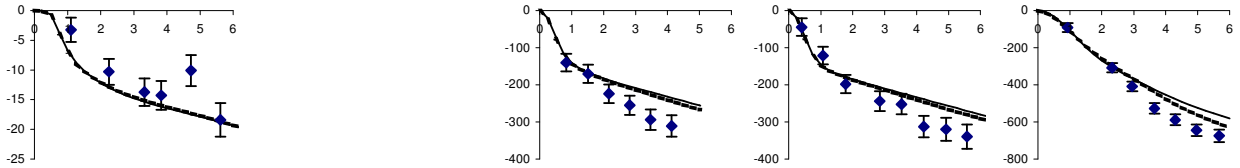
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



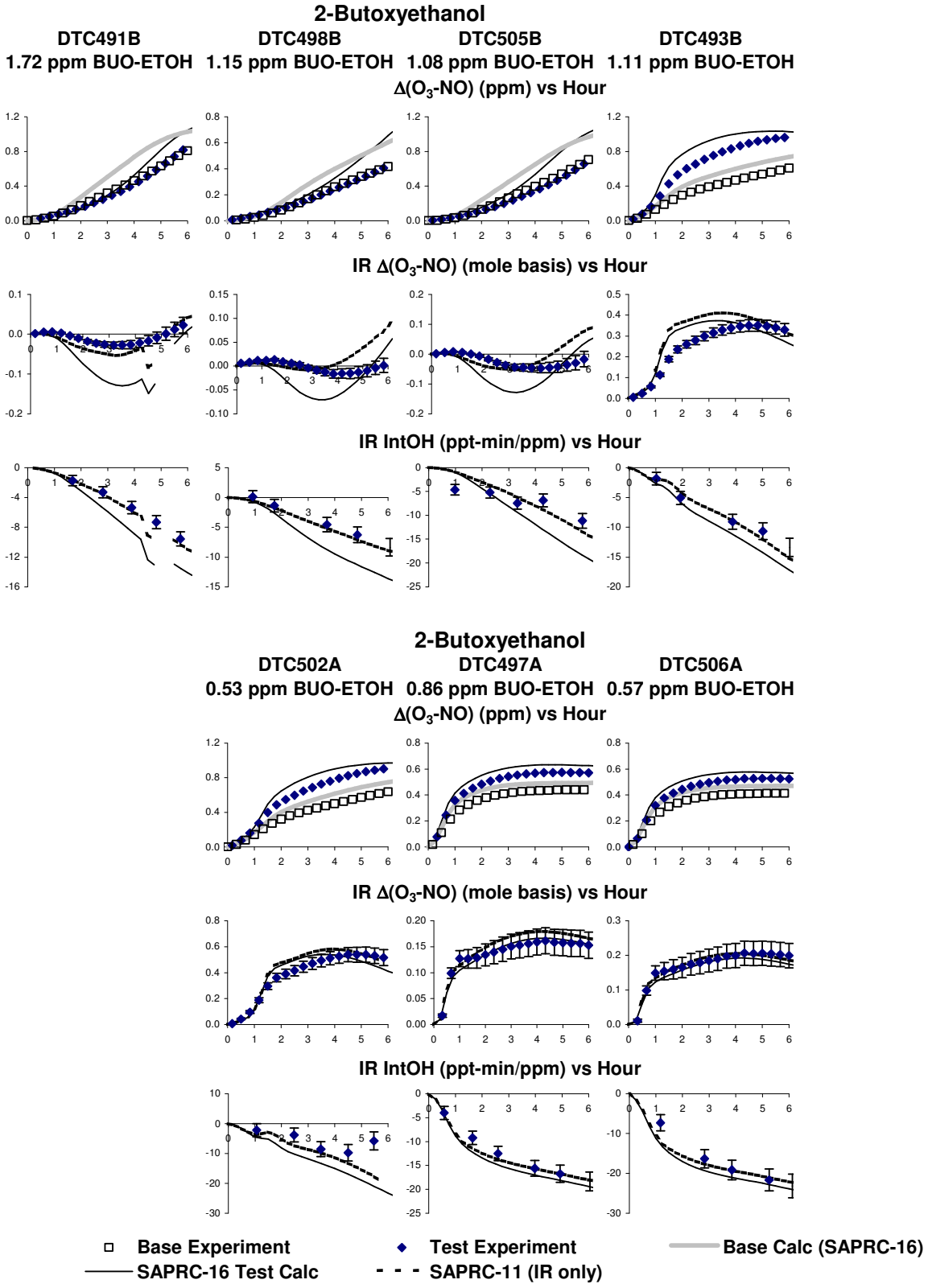
IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



IR IntOH (ppt-min/ppm) vs Hour



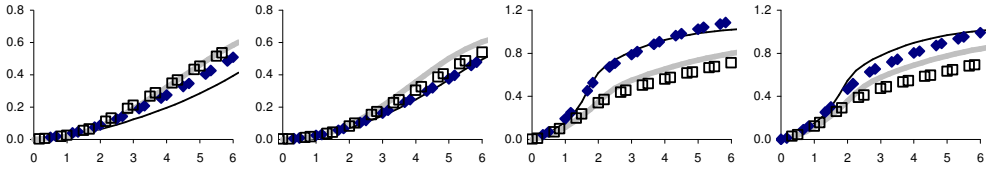
Base Experiment Test Experiment Base Calc (SAPRC-16)
SAPRC-16 Test Calc SAPRC-11 (IR only)


2-Butoxyethanol
DTC491B
1.72 ppm BUO-ETOH
DTC498B
1.15 ppm BUO-ETOH
DTC505B
1.08 ppm BUO-ETOH
DTC493B
1.11 ppm BUO-ETOH
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
2-Butoxyethanol
DTC502A
0.53 ppm BUO-ETOH
DTC497A
0.86 ppm BUO-ETOH
DTC506A
0.57 ppm BUO-ETOH
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

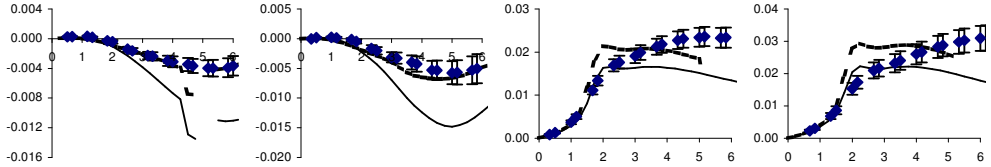
Dimethyl Succinate

CTC197B 17.26 ppm DBE-4 | **CTC211B** 8.73 ppm DBE-4 | **CTC198A** 16.49 ppm DBE-4 | **CTC208A** 9.36 ppm DBE-4

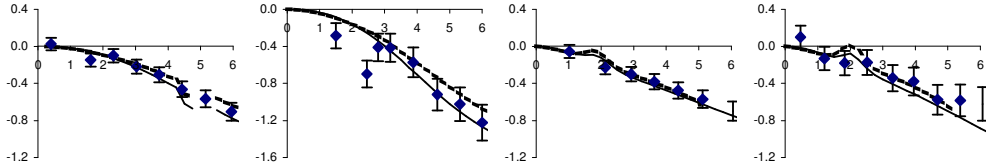
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



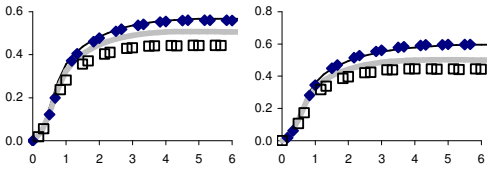
IR IntOH (ppt-min/ppm) vs Hour



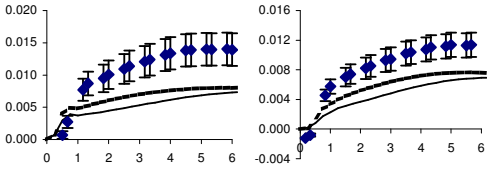
Dimethyl Succinate

CTC199B 8.48 ppm DBE-4 | **CTC210A** 13.58 ppm DBE-4

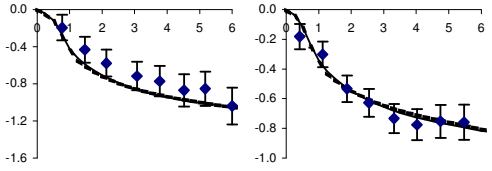
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour

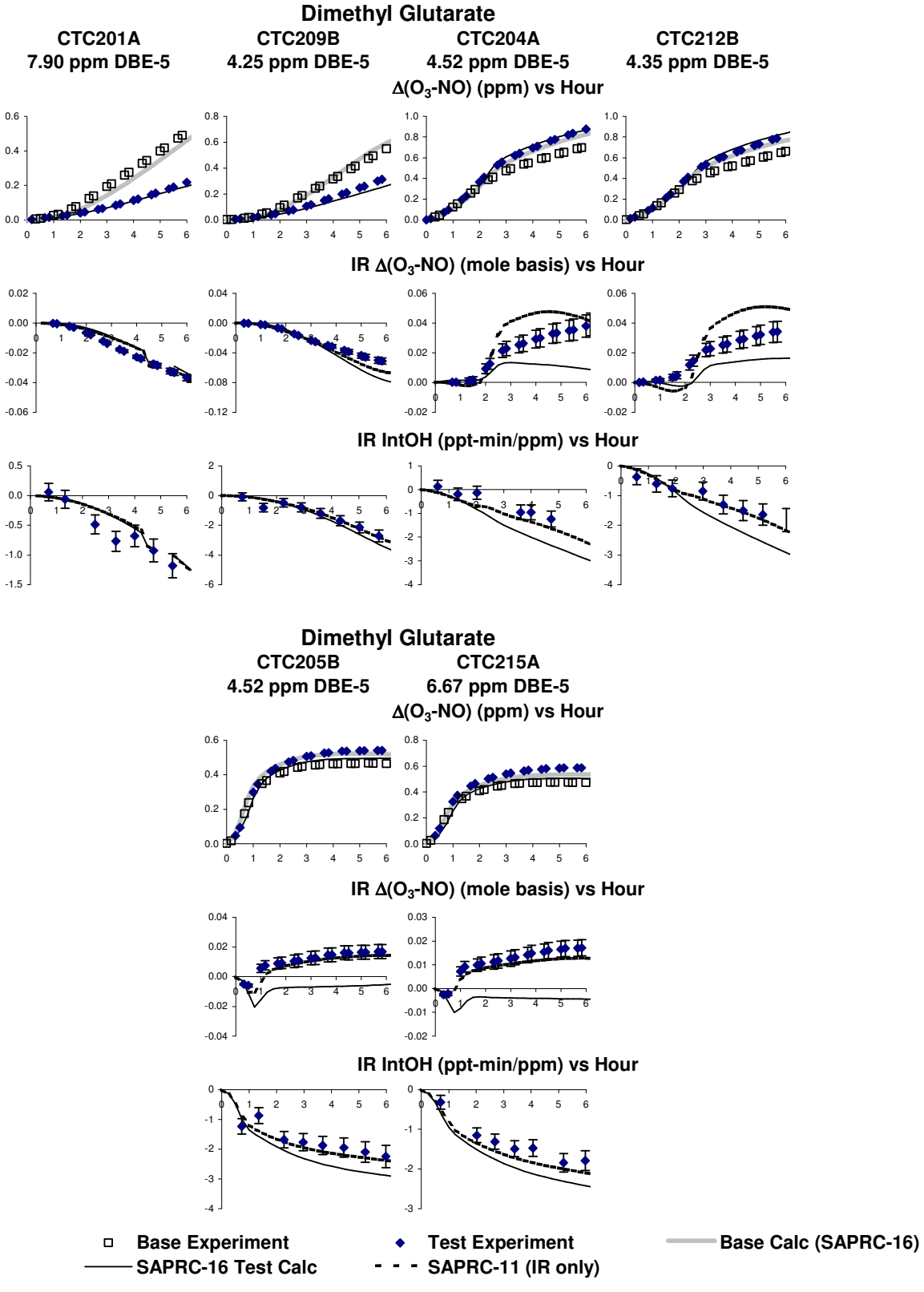


IR IntOH (ppt-min/ppm) vs Hour

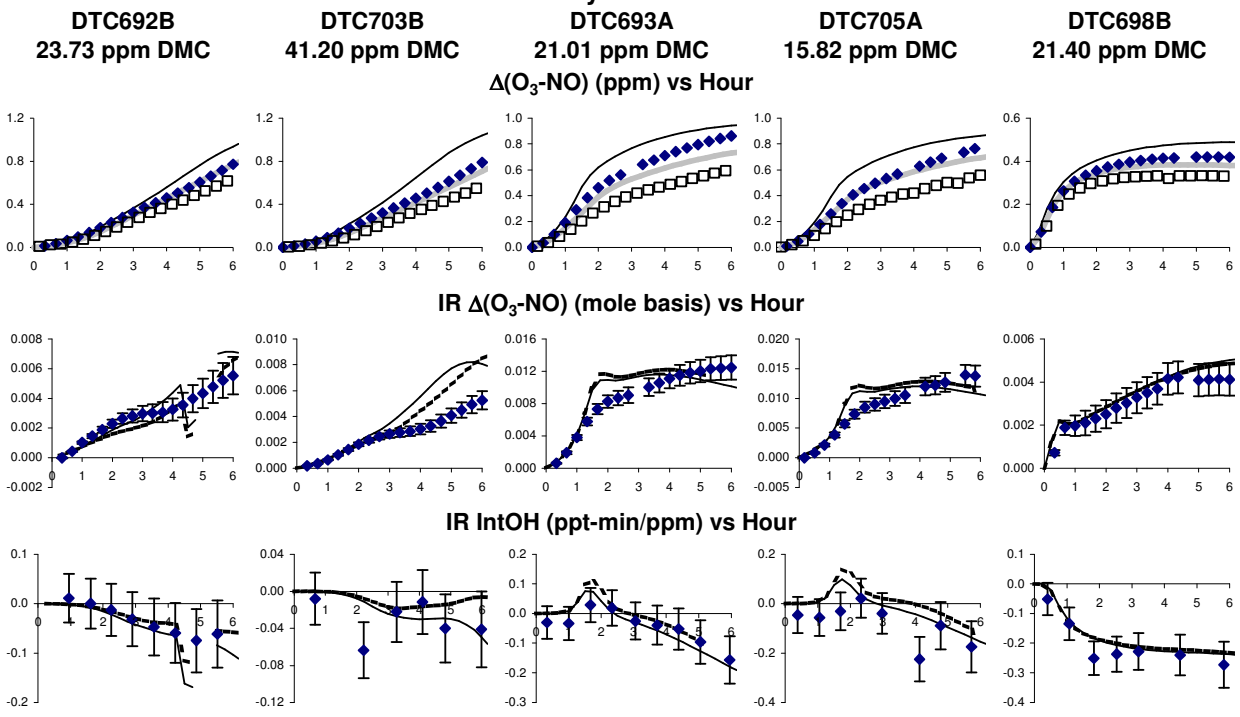


Base Experiment | Test Experiment | Base Calc (SAPRC-16)

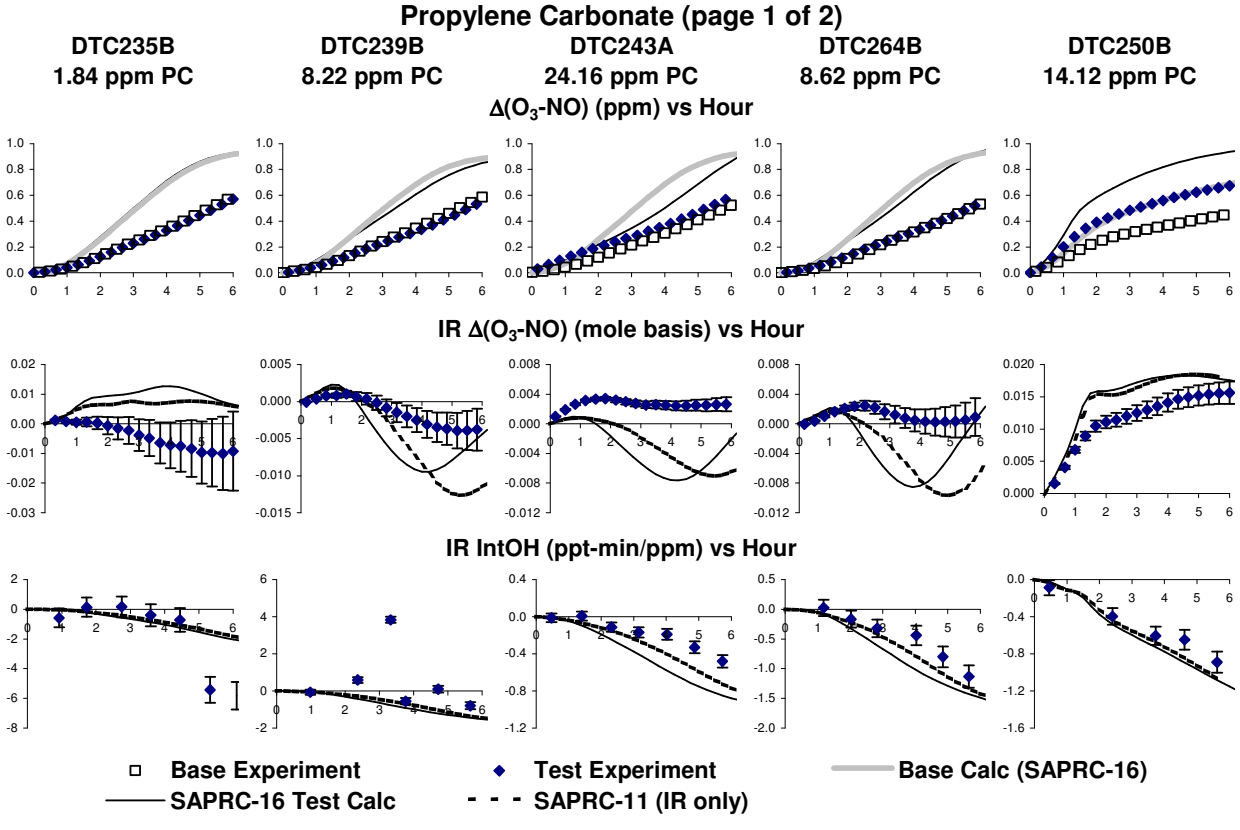
SAPRC-16 Test Calc | SAPRC-11 (IR only)


Dimethyl Glutarate
CTC201A
7.90 ppm DBE-5
CTC209B
4.25 ppm DBE-5
CTC204A
4.52 ppm DBE-5
CTC212B
4.35 ppm DBE-5
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Dimethyl Glutarate
CTC205B
4.52 ppm DBE-5
CTC215A
6.67 ppm DBE-5
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)

Dimethyl Carbonate



Propylene Carbonate (page 1 of 2)



Propylene Carbonate (page 2 of 2)

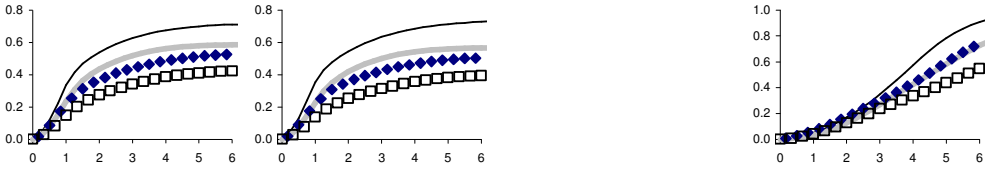
Methyl Isopropyl Carbonate

DTC260B
7.50 ppm PC

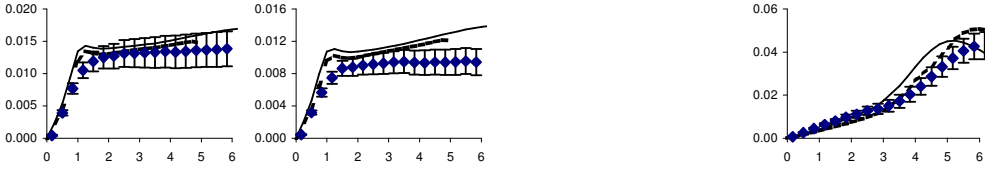
DTC266A
11.78 ppm PC

DTC750B
4.49 ppm MIPR-CB

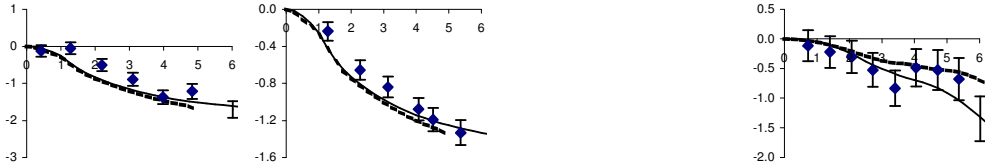
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



IR IntOH (ppt-min/ppm) vs Hour



Methyl Isopropyl Carbonate

DTC759A
3.81 ppm MIPR-CB

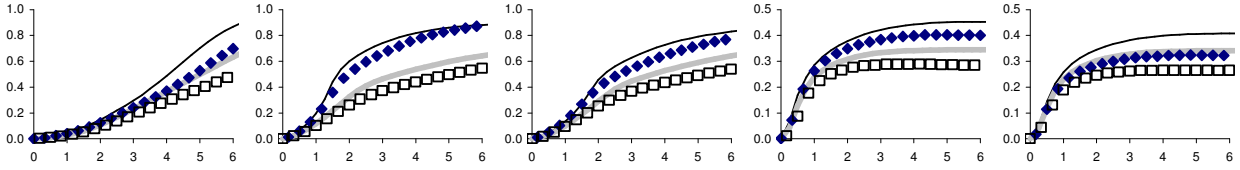
DTC755A
3.08 ppm MIPR-CB

DTC762A
1.66 ppm MIPR-CB

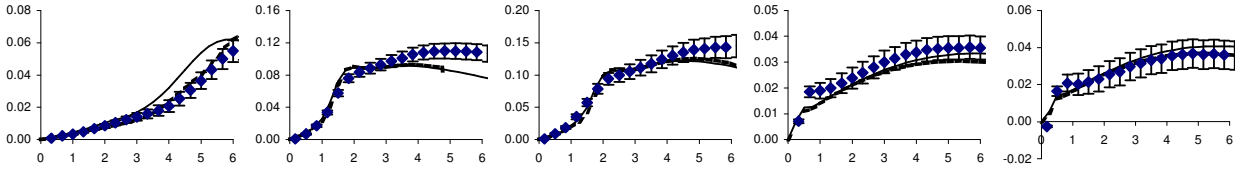
DTC758B
3.27 ppm MIPR-CB

DTC763B
1.63 ppm MIPR-CB

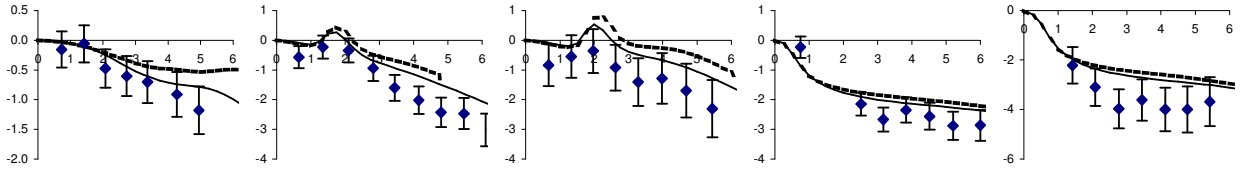
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



IR IntOH (ppt-min/ppm) vs Hour

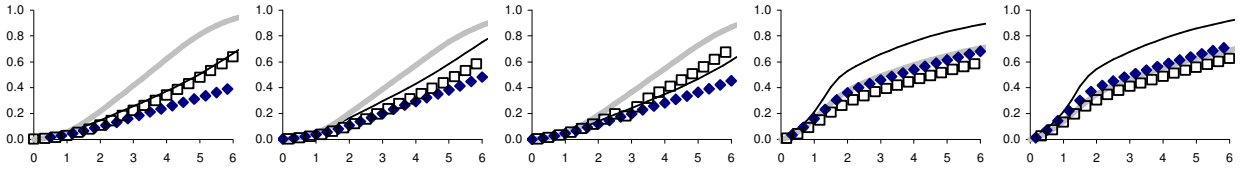


□ Base Experiment ◆ Test Experiment Base Calc (SAPRC-16)
SAPRC-16 Test Calc - - - SAPRC-11 (IR only)

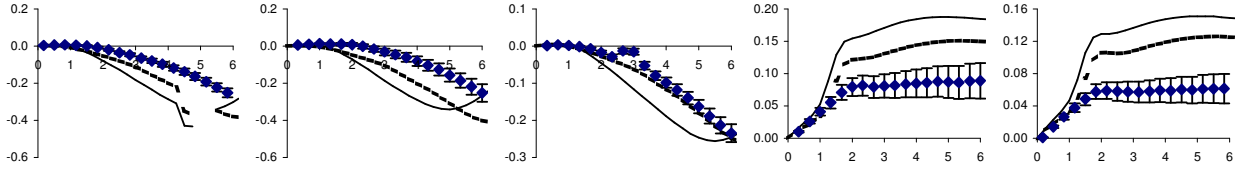
1-Methoxy-2-Propyl Acetate

DTC532B	DTC537A	DTC549B	DTC538B	DTC547B
0.88 ppm PGME-ACT	0.50 ppm PGME-ACT	1.05 ppm PGME-ACT	0.99 ppm PGME-ACT	1.53 ppm PGME-ACT

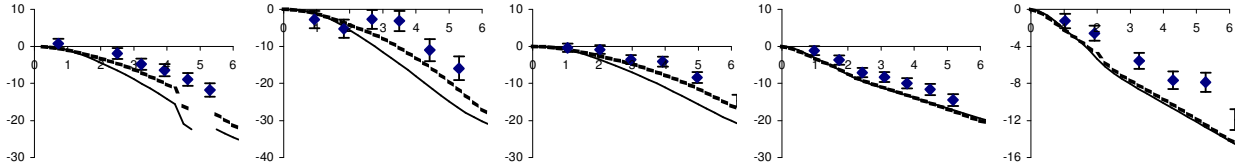
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



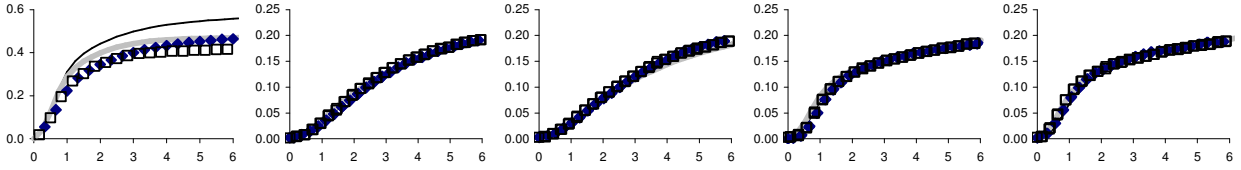
IR IntOH (ppt-min/ppm) vs Hour



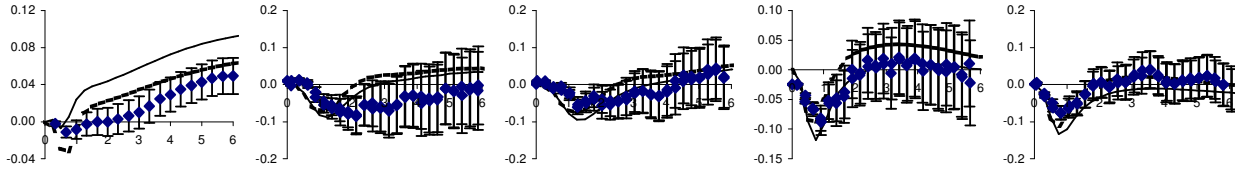
(continued) Texanol® isomers

DTC540B	EPA229A	EPA230B	EPA231B	EPA232A
0.96 ppm PGME-ACT	0.08 ppm TEXANOL	0.09 ppm TEXANOL	0.11 ppm TEXANOL	0.14 ppm TEXANOL

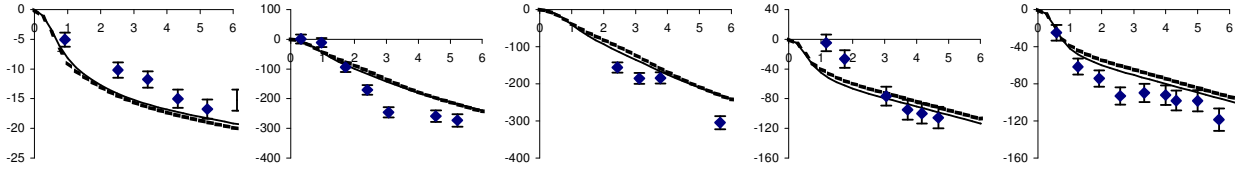
$\Delta(O_3\text{-NO})$ (ppm) vs Hour



IR $\Delta(O_3\text{-NO})$ (mole basis) vs Hour



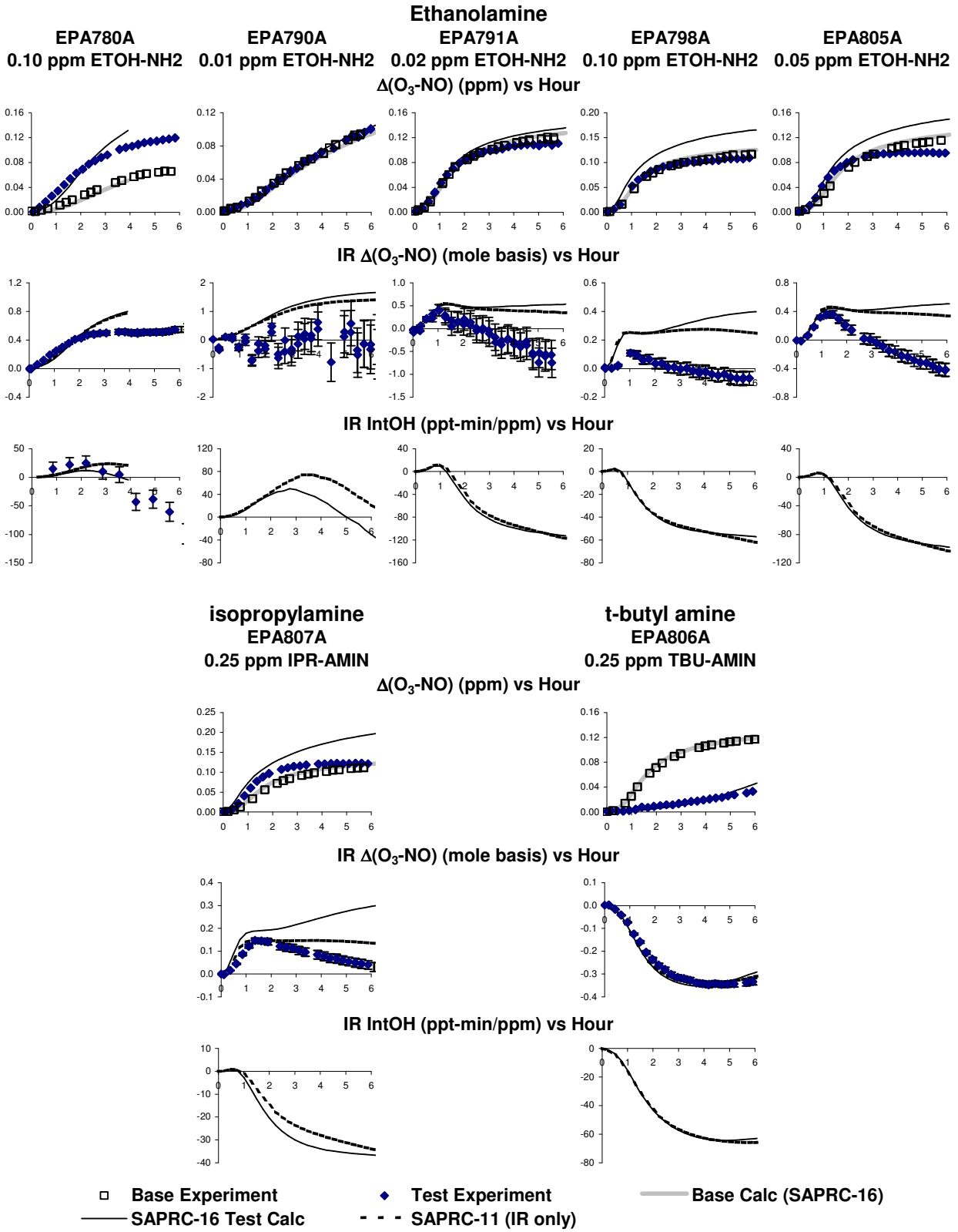
IR IntOH (ppt-min/ppm) vs Hour

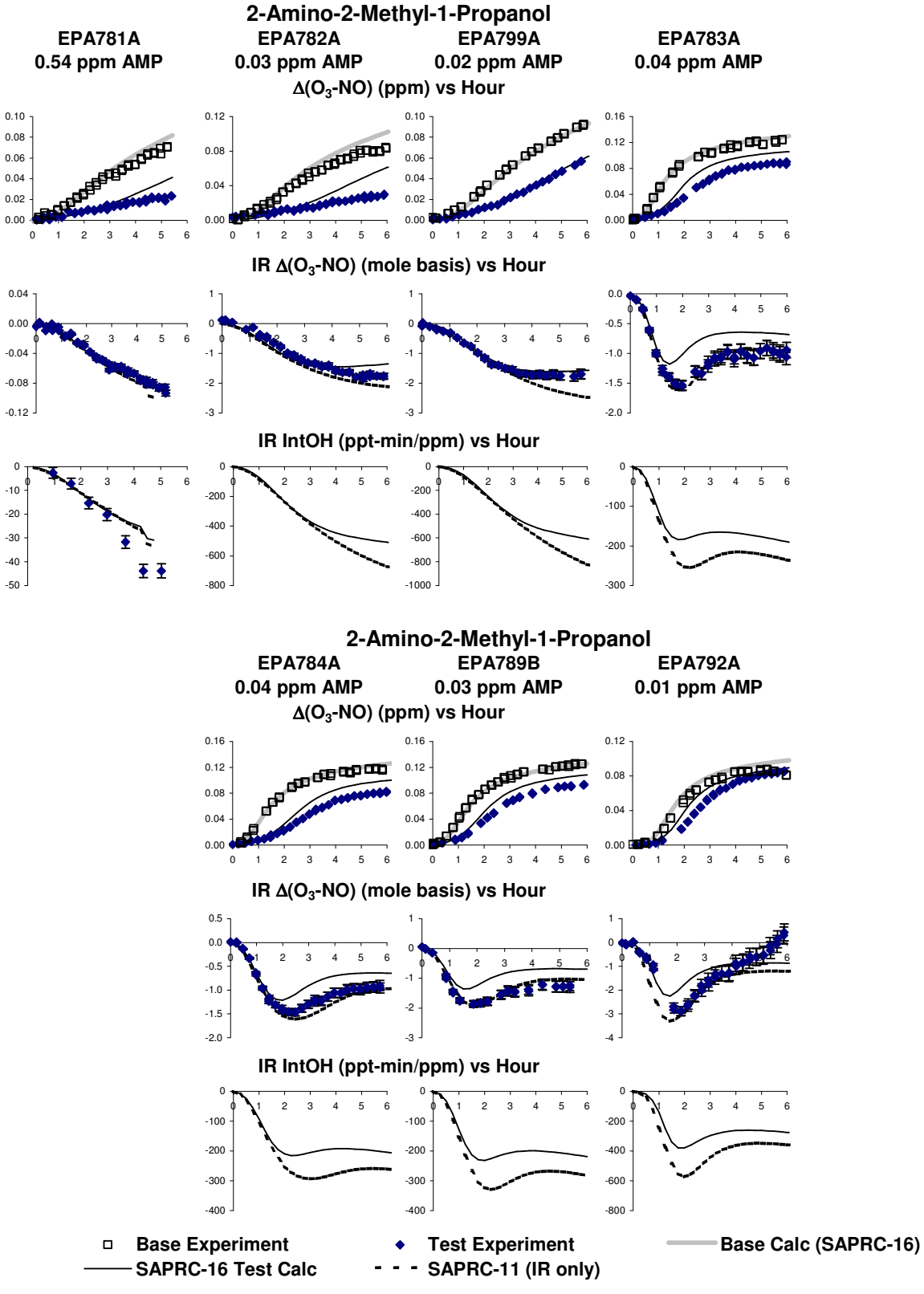


Base Experiment ◆ Test Experiment Base Calc (SAPRC-16)

SAPRC-16 Test Calc - - - SAPRC-11 (IR only)

Figure B-6. Plots of selected experimental and model calculation results for the incremental reactivity experiments with various amines.




2-Amino-2-Methyl-1-Propanol
EPA781A
0.54 ppm AMP
EPA782A
0.03 ppm AMP
EPA799A
0.02 ppm AMP
EPA783A
0.04 ppm AMP
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
2-Amino-2-Methyl-1-Propanol
EPA784A
0.04 ppm AMP
EPA789B
0.03 ppm AMP
EPA792A
0.01 ppm AMP
Δ(O3-NO) (ppm) vs Hour
IR Δ(O3-NO) (mole basis) vs Hour
IR IntOH (ppt-min/ppm) vs Hour
Base Experiment
Test Experiment
Base Calc (SAPRC-16)
SAPRC-16 Test Calc
SAPRC-11 (IR only)