

APPENDIX D

ESTIMATION OF UPPER LIMIT MAXIMUM INCREMENTAL REACTIVITIES

A. Abstract

A procedure is presented for estimating upper limit Maximum Incremental ozone Reactivities (MIR's) for volatile organic compounds (VOCs) whose atmospheric ozone impacts are uncertain. This might be applicable for including compounds of unknown reactivity in reactivity-based regulations which employ the MIR scale for quantifying ozone impacts. The procedure is based on deriving upper limits for the two factors that determine the ozone impact of a compound in pollution episode. These are the fraction of emitted VOC that reacts during the episode (the kinetic reactivity), and the amount of ozone formed per molecule of VOC that reacts (the mechanistic reactivity). Upper limit kinetic reactivities are derived from the rate constants for the atmospheric reactions of the VOCs if they are known, otherwise a maximum kinetic reactivity of unity is assumed. Upper limit mechanistic reactivities are obtained from calculated relative mechanistic reactivities for a variety of VOCs for MIR scenarios, with lower upper limits being obtained for compounds known not to photolyze, or for alkanes or saturated compounds containing only alcohol, ether or ester groups. The information needed for making such estimates is discussed, and examples are given for representative VOCs whose reactivities are reasonably well known.

B. Introduction

In recognition of the fact that volatile organic compounds (VOCs) differ in their impacts on photochemical ozone formation, The California Air Resources Board (CARB) has implemented ozone reactivity adjustments in vehicle emissions regulations (CARB, 1993), and is now considering use or reactivity adjustments in regulations of VOCs from consumer products. The reactivity adjustments currently used in the CARB vehicle regulations are based on the Maximum Incremental Reactivity (MIR) scale (Carter, 1994a), and an updated version of this scale would likely be used in any consumer product reactivity-based regulations. Although ozone impacts of VOCs depend on atmospheric conditions (Carter and Atkinson; 1989; Carter, 1994a; Jeffries and Crouse, 1991), the MIR scale was chosen for this purpose because it reflects ozone impacts under conditions where ozone is most sensitive to VOC emissions. In addition, the MIR scale has been shown to correlate reasonably well to effects of VOCs on integrated ozone and ozone exposure (Carter, 1994a; McNair et al 1992, 1994; CARB, 1993).

One problem with implementing reactivity adjustments in VOC regulations for consumer products and other stationary sources is that a wide variety of VOCs are involved, including many whose ozone impacts are highly uncertain or unknown. Some means is necessary to incorporate such compounds in reactivity-based regulations which provides incentives for using compounds of known low reactivity, but which is not unduly burdensome to the producers and users of compounds of unknown reactivity, some of which may also turn out to be beneficial. One approach is to use "default" reactivity factors for compounds whose reactivities are unknown, which would be the upper limit of their actual likely ozone impact. This approach allows regulations to cover compounds of both known and unknown reactivity in a relatively simple and consistent manner, and provides incentives for producers or users to reduce the uncertainties concerning the environmental effects of the emissions they cause. For this

approach to be acceptable, the default reactivity factors must not be so high that they cause an unfair burden to producers and users of new or unstudied compounds, which may turn out to have relatively low reactivity. Ideally, they should incorporate, to the maximum extent possible, any knowledge we have concerning the likely upper limit ozone impacts of the compounds, so they will not be higher than absolutely necessary given the limitations in our knowledge. In addition, the procedures for deriving them should not be so complex that they cannot be applied to large numbers of unstudied compounds that might be covered by reactivity-based regulations.

Given below is a suggested set of procedures that can be employed to estimate upper limit MIR's for VOCs for which limited kinetic or mechanistic information is available. The procedures take into account our current knowledge concerning the general factors that affect ozone reactivities of all VOCs. This provides a means for appropriate upper limit values to be derived for compounds whose atmospheric reaction rate constants are known, or which belongs to classes of compounds where the range of possible oxidation products and mechanisms are reasonably well understood.

C. Methods

1. Factors Affecting Reactivity

a. Kinetic and Mechanistic Reactivities

For regulatory applications, the appropriate quantification of ozone impact is the *incremental reactivity*, which is the amount of additional ozone formation caused by adding a small amount of the compound to the emissions, divided by the amount emitted (Carter and Atkinson, 1989; Carter, 1994a). For upper limit estimation purposes, it is useful to think of incremental reactivities as being a product of three factors, as follows (Carter and Atkinson, 1989):

$$\begin{array}{ccccccc} \text{Incremental} & & \text{Kinetic} & & \text{Mechanistic} & & \text{Mass Conv-} \\ \text{Reactivity} & = & \text{Reactivity} & = & \text{Reactivity} & \cdot & \text{ersion Factor} & \text{(I)} \\ \text{(Ozone per} & & \text{(VOC reacted} & & \text{(moles O}_3 & & \text{(moles VOC} & \\ \text{mass VOC} & & \text{/VOC emitted)} & & \text{/mole VOC} & & \text{/mass VOC)} & \\ \text{emitted)} & & & & \text{reacted)} & & & \end{array}$$

The *kinetic reactivity* is the fraction of the emitted VOC which undergoes chemical reaction in the atmosphere during the time period being considered. It depends primarily on the rate constants for the VOCs atmospheric reactions, but also on the overall levels of OH radicals, ozone, or light in the scenario, depending on how the VOC reacts. Being a fraction, it is a unitless number. Note that kinetic reactivity is *not* the same as the atmospheric reaction rate, which is the speed at which it reacts. Although they are approximately proportional for slowly reacting compounds, for rapidly reacting compounds the kinetic reactivity is approximately unity, and thus almost independent of the reaction rate. Therefore, if insufficient information is available to derive upper limit atmospherically relevant rate constants for a compound, then kinetic reactivities of unity can be used for upper limit estimation purposes.

The *mechanistic reactivity* is the number of molecules of ozone formed for each molecule of VOC that reacts. It reflects both the nature of the VOCs reaction mechanism and also the efficiency of ozone formation from the reactions of VOCs in the particular scenario. Although the mechanistic reactivity factor can be given in other units besides molecules of ozone per molecule VOC, molecular

units are more meaningful chemically and therefore are more straightforward to use for estimation purposes. Upper limits for mechanistic reactivities can be estimated based on the range of mechanistic reactivities of compounds with known mechanisms or ozone impacts, as discussed below. In some cases, structural information and knowledge of the general features of atmospheric chemistry may permit limiting the range of possible mechanisms and products, allowing for lower upper limit estimates for mechanistic reactivities for certain types of compounds.

The product of the kinetic and mechanistic reactivities is incremental reactivities in units of molecules of ozone formed per molecule of VOC emitted. Since emissions of VOCs are quantified and regulated on a mass basis, the appropriate incremental reactivity units for regulatory applications is ozone formed per unit mass of VOC emitted. Therefore, a *mass conversion factor* is applied to place the incremental reactivities on a mass VOC basis. It is inversely proportional to the VOC's molecular weight.

b. Environmental Conditions

Both kinetic and mechanistic reactivities depend on the conditions of the environment where the VOC reacts. For example, the OH radical levels in the environment determine the fraction reacted for a VOC which reacts primarily with OH radicals, and the NO_x levels significantly affect the efficiency for O₃ formation once a VOC reacts, which determines its mechanistic reactivity (see, for example, Carter and Atkinson, 1989). However, if the VOCs with known reactivities are to be regulated according to their MIR's, then we need only be concerned with estimates of kinetic and mechanistic reactivities for MIR conditions. Therefore, in this work we are concerned only with a single set of environmental conditions, which is that used to derive the MIR scale.

MIR conditions consist of scenarios where the NO_x inputs have been adjusted so that the peak ozone levels are the most sensitive to changes in total reactive VOC emissions. The MIR scale developed by Carter (1994a) is based on averages of incremental reactivities calculated for 39 different single-day EKMA model scenarios (Baugues, 1990) where NO_x inputs have been adjusted in this way. However, it was also found that incremental reactivities calculated using a single "Averaged Conditions" MIR scenario were essentially the same, to within a few percent for all positively reactive VOCs, as average reactivities calculated from the 39 MIR scenarios. Therefore, for the purpose of estimating approximate upper limit kinetic and mechanistic reactivities for upper limit MIR determinations, it is sufficient to limit our consideration to the Averaged Conditions MIR scenario. The detailed input data and derivation of this scenario are given elsewhere (Carter, 1994a,b).

2. Upper Limit Kinetic Reactivities for MIR

a. Information Required

Most VOCs react in the atmosphere with OH radicals, and many also react to non-negligible extents with O₃, NO₃ radicals, or by photolysis. If insufficient information is available concerning the rate constants for these processes (or their upper limits) under atmospheric conditions, then an upper limit kinetic reactivity of unity should be used when deriving upper limit MIR values. However, for many if not most VOCs, sufficient information is available to permit more precise kinetic reactivity estimates. The minimum information for making kinetic reactivity estimates is summarized in the following section.

OH Radical Rate Constant. Because VOCs react in the atmosphere with OH radicals, the rate constant for this reaction, or its upper limit, must be determined, or its upper limit must be estimated. Some VOCs can be concluded not to react significantly with OH radicals based on the lack of modes for which OH to react, such as a lack of abstractable hydrogens or double bonds. Only if a VOC contains only functional groups which have been shown in other molecules not to react with OH radicals, or if there are no thermodynamically feasible means for OH radicals to react with the compound, it is safe to conclude that it does not react with OH radicals without the benefit of carrying out a direct experimental measurement. (Because of possible interactions, functional groups that are immediately adjacent to another functional group should be considered to be different from those that are isolated. This is applicable for all reactions discussed here.) Available information concerning OH + VOC rate constants is summarized by Atkinson (1989, 1994).

Methods exist for estimating OH radical rate constants for many compounds that are usually accurate to within a factor of 2 or better (Kwok and Atkinson, 1995). Therefore, if no measurements are available concerning the OH radical rate constant of the compound, but the rate constant can be measured using the methods of Kwok and Atkinson (1995), then a rate constant which is two times the estimated value can be used for the purpose of making upper limit kinetic reactivity estimates. The factor of two increase is necessary to take into account the uncertainty of the estimation methods when making upper limit determinations.

Ozone Rate Constant. Some VOCs, usually (but not always) those with C=C double bonds, can react with ozone at significant rates, and these reactions often have a net positive effect on ozone because of the subsequent reactions of the radicals formed. Only if a VOC contains only functional groups that have been shown in other molecules not to react with ozone, or if there are no thermodynamically feasible means for such a reaction to occur, is it safe to conclude that the reaction with ozone will be negligible in the absence of direct experimental measurement. Available information concerning ozone + VOC rate constants is given by Atkinson and Carter (1984), and is updated by Atkinson (1994).

Although Atkinson and Carter (1984) discuss possible approaches for estimating O₃ rate constants, no comprehensive approach has been developed which performs very reliably for estimation purposes. Therefore, if the compound contains groups which might possibly react with O₃ (e.g. C=C, C=N, or N-N bonds), and its O₃ rate constant has not been measured or its upper limit determined, then a kinetic reactivity of unity must be assumed when making upper limit reactivity estimates.

NO₃ Radical Rate Constant. Some VOCs, usually (but not always) those with C=C double bonds, can react with NO₃ radicals at sufficiently high rates to affect their ozone impact. Only if a VOC contains only functional groups which have been shown in other molecules not to react with NO₃ radicals, or if there are no thermodynamically feasible means for such a reaction to occur, is it safe to conclude that this reaction with ozone will be negligible in the absence of direct experimental measurement. Available information concerning NO₃ + VOC rate constants is given by Atkinson (1991, 1994). Atkinson (1991, 1994) also gives methods for estimating these rate constants. As with the OH radical rate constant, if the rate constant has to be estimated, then the estimate should be increased by a factor of two for upper limit reactivity estimates.

Photolysis Rates. Some VOCs can react in the atmosphere by direct photolysis, and if photodecomposition is sufficiently rapid and involves radical formation, then their reactions can result in

high ozone impacts. Upper limit atmospheric photolysis rates can be estimated given the compound's UV-visible absorption spectrum for wavelengths ≈ 290 nm, and the actinic fluxes for direct overhead sunlight for clear-sky conditions, assuming unit quantum yields. The actinic fluxes given by Peterson (1976) should be sufficient for this purpose. Only if the VOC contains only functional groups which have no absorption at $\lambda \approx 290$ nm, or has no decomposition pathway with a heat of reaction of less than the energy of a 290 nm photon, is it safe to conclude that the compound will not photolyze in the absence of absorption cross section data. If the compound has non-negligible absorption cross sections in the $\lambda \approx 290$ nm region, then unit quantum yields should be assumed for making upper limit photolysis rate estimates, unless there is information justifying the use of lower quantum yields for this purpose. Information concerning absorption cross sections and quantum yields for photolyses of smaller molecules of atmospheric significance are given in the most recent NASA (1994) and IUPAC (Atkinson et al, 1997, 1999) evaluations, though for higher molecular weight VOCs, and organics in general, there does not appear to be a more current or comprehensive review of absorption cross section data than that of Calvert and Pitts (1966).

b. Estimation of MIR Kinetic Reactivities from Rate Constants

Most VOCs react significantly only with OH radicals. In this case, the fraction reacted in given scenario can be estimated by

$$\text{Kinetic Reactivity} \approx (1 - e^{-k_{\text{OH}} \cdot \text{EffIntOH}}) \quad (\text{II})$$

or

$$\text{Kinetic Reactivity} \approx k_{\text{OH}} \cdot \text{EffIntOH} \quad (\text{III})$$

(if $k_{\text{OH}} \cdot \text{IntOH} \ll 1$). Here, k_{OH} is the VOC's OH radical rate constant, and EffIntOH is a scenario-dependent "Effective Integrated OH" parameter which is related to, but is not exactly the same as, the integrated OH radical levels (Carter and Atkinson, 1989). Note that for slowly reacting compounds, Equation (III) predicts that the kinetic reactivities are approximately proportional to the integrated reaction rates, while for rapidly reacting compounds the kinetic reactivity approaches the upper limit value of unity. For the Averaged Conditions MIR scenario, a value of

$$\text{EffIntOH}^{\text{MIR}} = 1.8 \times 10^{11} \text{ molec cm}^3 \text{ s}$$

is appropriate for use in upper limit kinetic reactivity estimates. This gives good fits to kinetic reactivities for VOCs with $k_{\text{OH}} < 5 \times 10^{-12} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$, while slightly overestimating (by no more than ~5%) kinetic reactivities for faster reacting compounds.

Equation (II) obviously will not work if the VOC reacts significantly with O_3 or NO_3 radicals or undergoes photolysis. For the purpose of estimating kinetic reactivities for such compounds, we assume that Equation (II) can be generalized to

$$\text{Kinetic Reactivity} \approx (1 - e^{-\text{Integrated Reaction Rate}}) \quad (\text{IV})$$

where

$$\text{Integrated Reaction Rate} \approx k_{\text{OH}}^{\text{VOC}} \cdot \text{IntOH} + k_{\text{O}_3}^{\text{VOC}} \cdot \text{IntO}_3 + k_{\text{NO}_3}^{\text{VOC}} \cdot \text{IntNO}_3 + \int k_{\text{Phot}}^{\text{VOC}} dt \quad (\text{V})$$

and IntOH, IntO₃, and IntNO₃ are the integrated levels of OH radicals, O₃, and NO₃ radicals, respectively, and $\int k_{\text{Phot}}^{\text{VOC}} dt$ is the integrated photolysis rate. (Note that IntOH, the actual integrated OH radical levels, is not the same as EffIntOH, which depends on when the VOC is emitted in the scenario as well as the integrated OH radical levels.) For the Averaged Conditions MIR scenario, the integrated OH, O₃, and NO₃ are

$$\text{IntOH}^{\text{MIR}} = 1.8 \times 10^{11} \text{ molec cm}^{-3} \text{ s}$$

$$\text{IntO}_3^{\text{MIR}} = 8.0 \times 10^{16} \text{ molec cm}^{-3} \text{ s},$$

and

$$\text{IntNO}_3^{\text{MIR}} = 8.5 \times 10^{11} \text{ molec cm}^{-3} \text{ s}.$$

An estimate of the upper limit $\int k_{\text{Phot}}^{\text{VOC}} dt$ can be obtained using the measured cross sections, the measured or upper limit quantum yields, and the clear-sky, direct overhead sun actinic flux data (such as those given by Peterson, 1976) to calculate the maximum photolysis rate, kPhot. If there is no information available concerning the quantum yield for the photodecomposition of the compound (as usually is the case), then unit quantum yields at all wavelengths should be assumed. For the Averaged Conditions MIR scenario, the integrated photolysis rate can then be approximated from kPhot using:

$$\int k_{\text{Phot}}^{\text{VOC}} dt \approx 3.6 \times 10^4 \text{ s} \cdot 0.7 \cdot k_{\text{Phot}} \approx 2.5 \times 10^4 \text{ sec} \cdot k_{\text{Phot}} \quad (\text{VI})$$

where 3.6×10^4 seconds is the length of time in the scenario [10 hours for all EKMA scenarios used by Carter (1994a,b)], and the 0.7 factor is the ratio of the average to the maximum photolysis rate, and was derived for the photolysis of NO₂ in the Averaged Conditions MIR scenario. Most photolysis reactions are more sensitive to shorter wavelength UV than is NO₂ photolysis, and would have a lower average-to-maximum ratio because their photolysis rates would vary more with solar zenith angle. Therefore, the 0.7 factor is considered appropriate for upper limit estimates. To be consistent with the units shown above, the units of kPhot should be s⁻¹.

Equations (IV) and (V) can be combined to yield

$$\text{Kinetic Reactivity} \approx (1 - e^{-\text{Effective } k_{\text{OH}} \cdot \text{EffIntOH}}) \quad (\text{VII})$$

where

$$\text{Effective } k_{\text{OH}}^{\text{VOC}} = k_{\text{OH}}^{\text{VOC}} + \frac{\text{IntO}_3}{\text{IntOH}} k_{\text{O}_3}^{\text{VOC}} + \frac{\text{IntNO}_3}{\text{IntOH}} k_{\text{NO}_3}^{\text{VOC}} + \frac{3.0 \times 10^4}{\text{IntOH}} k_{\text{Phot}_{\text{max}}}^{\text{VOC}} \quad (\text{VIII})$$

Using the IntOH, IntO₃, IntNO₃, and $\int k_{\text{Phot}}^{\text{VOC}} dt/k_{\text{Phot}}$ for the Averaged Conditions MIR scenario (see above), we then obtain

$$\text{Effective } k_{\text{OH}}^{\text{VOC}} \approx k_{\text{OH}}^{\text{VOC}} + 4.4 \times 10^5 k_{\text{O}_3}^{\text{VOC}} + 4.6 k_{\text{NO}_3}^{\text{VOC}} + 1.3 \times 10^{-7} k_{\text{Phot}}. \quad (\text{IX})$$

where the units of the bimolecular rate constants are cm³ molec⁻¹ s⁻¹, and the units of kPhot is s⁻¹. This in effect amounts to a correction to the OH radical rate constant for the other reaction pathways for the purpose of estimating kinetic reactivities.

3. Estimation of Upper Limit MIR Maximum Mechanistic Reactivities

Upper limit estimates for mechanistic reactivities can be obtained from examining the mechanistic reactivities for a sufficiently wide variety of VOCs under MIR conditions. Incremental reactivities calculated using the SAPRC-99 mechanism (Carter, 2000) were used for this purpose. This mechanism contains separate representations for the atmospheric reactions of approximately 400 different types of VOCs, though only a fraction of these have been experimentally evaluated. Although some of these mechanisms are uncertain, they can be considered to represent a sufficiently wide variety of ways that VOCs can react for the purpose of establishing upper limit mechanistic reactivity estimates.

Figure C-1 and Figure C-2 show the mechanistic reactivities for the Averaged Conditions MIR scenario calculated for a variety of VOCs. Note that the mechanistic reactivities shown will be different than those calculated by Carter (1994a), who used the SAPRC-90 (Carter, 1990) mechanism. Figure C-1 shows the mechanistic reactivities in units of moles O₃ per mole VOC reacted, and Figure C-2 shows the values as moles O₃ per mole carbon reacted. The highest molar MIR mechanistic reactivities is in the ~30-40 range, which are calculated for methyl methacrolate, 1,3,5- and 1,2,3-trimethyl benzene, and biacetyl. The highest per-carbon MIR mechanistic reactivities are for biacetyl, methyl glyoxal and glyoxal, which are in the range of ~8-10. However, if photoreactive compounds are excluded, then no compound has per-carbon MIR mechanistic reactivities which are significantly greater than ~7, with values in the 4-5 range being observed for methane and a variety of olefins and aromatics.

These data suggest that the upper limit per molecule MIR mechanistic reactivities can be estimated by

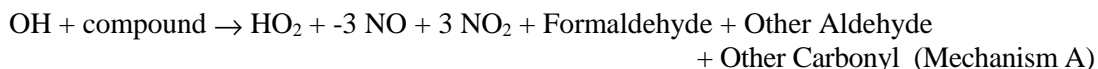
$$\text{Mechanistic Reactivity} \approx \text{MIN}(7 \cdot n_c, 35) \quad (\text{X})$$

for compounds which are known to be non-photoreactive, and by

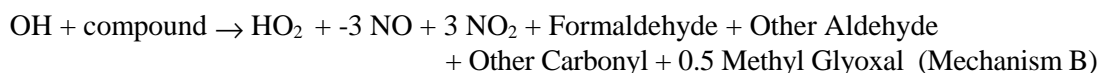
$$\text{Mechanistic Reactivity} \approx \text{MIN}(10 \cdot n_c, 40) \quad (\text{XI})$$

for photoreactive compounds or compounds for which photodecomposition cannot be ruled out. The units are moles of ozone per mole carbon VOC that reacts, and n_c is the number of carbons in the molecule.

For some compounds, specifically saturated hydrocarbons or non-photoreactive compounds containing only alcohol, ether, or ester groups, our knowledge of atmospheric reaction mechanisms, and how various types of reactions affects reactivity, can permit somewhat lower upper limit estimates to be made. Compounds such as these will react significantly only with OH radicals, would probably convert no more than 3-4 molecules of NO to NO₂, and the most reactive products they are likely to form are higher aldehydes or, in the case of esters, possibly some α -dicarbonyls such as methyl glyoxal (Carter, 2000). Probably the most reactive reasonable mechanism for such compounds would be:



if the compound did not have a carbonyl group (i.e., not an ester), or



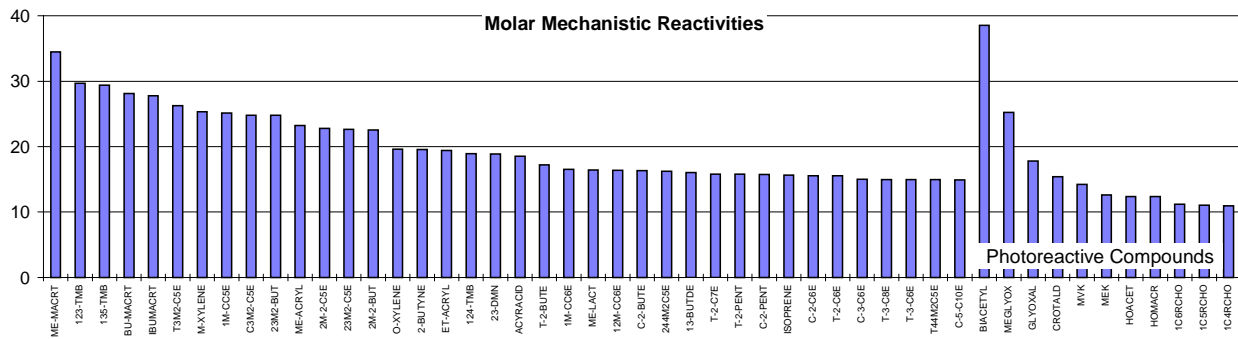


Figure D-1. Plots of calculated mechanistic reactivities, in units of moles ozone formed per mole VOC reacted, for selected compounds in the averaged conditions MIR scenario.

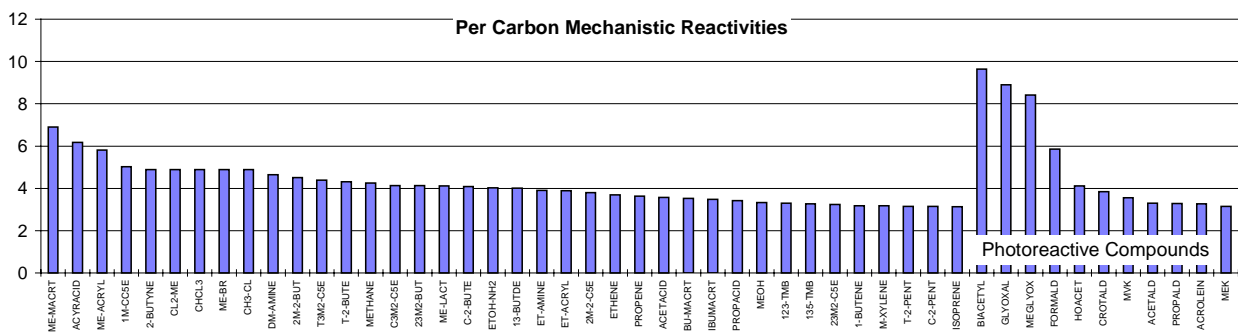


Figure D-2. Plots of calculated mechanistic reactivities, in units of moles ozone formed per mole carbon VOC reacted, for selected compounds in the averaged conditions MIR scenario.

otherwise. These are based on the observations that mechanisms with more than three NO to NO₂ conversions have not been observed for such compounds, that aldehydes are the most reactive products expected to be formed from compounds not containing carbonyl groups but formation of more than two moles of aldehydes rarely occurs, and that although some carbonyl-containing compounds may form α -dicarbonyls (e.g., see Carter et al, 1997d), it is probably not the dominant reaction route since carbonyl substitution tends to deactivate OH reaction at groups next to it (Kwok and Atkinson, 1995).

As discussed by Carter and Atkinson (1989), mechanistic reactivities of compounds that react only with OH radicals can be expressed in terms of sums of mechanistic reactivities of "pure mechanism species", which reflect specific aspects of the VOC's mechanism, such as the numbers of NO to NO₂ conversions, and yields of various types of reactive products. Table D-1 gives MIR mechanistic reactivities calculated for the major pure mechanism species likely to be involved in atmospheric reaction mechanisms of saturated hydrocarbons, alcohols, ethers or esters, and the corresponding mechanistic reactivities calculated for Mechanisms A and B, above. Note that the high mechanistic reactivities of the α -dicarbonyls make it appropriate to consider upper-limit reactivity mechanisms of carbonyl-containing compounds, whose reactions might result in formation of α -dicarbonyls, separately from upper limit mechanisms for compounds where these products cannot be formed.

Table D-1. Mechanistic reactivities of the major pure mechanism species affecting reactivities of non-photoreactive saturated hydrocarbons or oxygenates, and mechanistic reactivities of the mechanisms used for upper limit reactivity estimates for such compounds.

Pure Mechanism	Yields in Upper Limit Mechanisms		MIR Mechanistic Reactivity (Mol O ₃ / Mol Pure Mechanism Species)		
	A	B			
OH Rate Constant (cm ³ molec ⁻¹ s ⁻¹)			2.0e-12	2.0e-11	6.8e-11
Methyl Glyoxal Formation		0.5	9.7	14.9	20.3
Higher Aldehyde Formation	1.0	1.0	3.7	6.1	8.4
Acetaldehyde Formation			2.6	4.2	5.6
Formaldehyde Formation	1.0	1.0	2.3	3.5	4.8
Higher Ketone Formation	1.0	1.0	2.6	4.1	5.6
Acetone Formation			0.2	0.3	0.4
Organic Nitrates (radical termination)			-2.8	-3.8	-5.6
HO ₂ Radicals (radical propagation)	1.0	1.0	1.0	1.2	1.4
Extra NO to NO ₂ Conversions	3.0	3.0	1.1	1.3	1.4
Mechanism A Upper Limit Mechanistic Reactivities (no carbonyl group)			13.0	18.8	24.3
Mechanism B Upper Limit Mechanistic Reactivities (with carbonyl group)			17.8	26.3	34.4

Table D-1 shows that mechanistic reactivities of some of the pure model species, and thus of the upper limit mechanisms A and B, are not independent of the OH radical rate constant, particularly at higher rate constants. In particular, although the mechanistic reactivity contribution of NO to NO₂ conversions is relatively unaffected by the reaction rate, the mechanistic reactivity contribution of reactive products tends to increase as the rate constant increases. For Mechanisms A and B, the Averaged Conditions MIR mechanistic reactivities shown on Table D-1 can be fit by the following empirical equations:

$$\text{MIR Mechanistic Reactivity A} = 25.4 - 13.2 \exp(-3.3 \times 10^{10} \cdot \text{kOH}) \quad (\text{XII})$$

$$\text{MIR Mechanistic Reactivity B} = 36.3 - 19.5 \exp(-3.2 \times 10^{10} \cdot \text{kOH}) \quad (\text{XIII})$$

where the units of the mechanistic reactivities are mole O₃ per mole VOC, and the kOH is the OH radical rate constants in units of cm³ molec⁻¹ s⁻¹.

Based on these considerations, we conclude that for alkanes or saturated compounds containing no groups other than alcohols and ethers, and no atoms other than H, C, or O, then the upper limit mechanistic reactivity can be given by either Equation (X) or (XII), whichever gives the lower value. Likewise, if the compound contains a carbonyl group but no other groups besides alcohol or ether and no atoms other than N, C, or O, then the upper limit mechanistic reactivity can be given by either Equation

(XI) or (XIII), whichever is lower. For any other compound, only Equations (X) or (XI) can be used, depending on whether the compound is or may be photoreactive.

4. Upper Limit MIR Estimates

The upper limit kinetic and mechanistic reactivities derived as discussed above can then be combined, according to Equation (II) to obtain an estimate of the *incremental reactivity* in the MIR scale, which is the quantity of interest. The incremental reactivities obtained by multiplying the kinetic and mechanistic reactivities derived as discussed above will be in units of moles of ozone formed per mole VOC emitted, but for regulatory applications the appropriate units are grams of O₃ per gram VOC. This conversion is done by multiplying by the ratio of the molecular weight of O₃ to the molecular weight of the VOC. Therefore,

$$\text{Upper Limit MIR (gm O}_3\text{ / gm VOC)} = \frac{\text{Upper Limit Kinetic Reactivity (mol O}_3\text{ / mol VOC)} \cdot \text{Upper Limit Mech. React'y (mol O}_3\text{ / mol VOC)} \cdot \frac{48 \text{ (gm O}_3\text{ / gm VOC)}}{\text{Mwt}^{\text{VOC}} \text{ (gm / mol)}}}{1}$$

(XIV)

D. Results and Discussion

1. Kinetic Reactivities

Table D-2 gives the rate constants and the corresponding estimated MIR kinetic reactivities for all the VOCs that can be separately represented in the SAPRC-99 mechanism (Carter, 2000). The table also indicates which rate constants were estimated and which are based on measurement data. Note that a factor of 2 uncertainty factor was applied to all estimated rate constants, but measured rate constants (no matter how uncertain) were used without any uncertainty adjustments. The $k_{\text{Phot}}^{\text{MAX}}$ values were calculated using the absorption cross sections in the mechanism, but assuming unit quantum yields. This is based on the assumption that quantum yields are not known for most photoreactive VOCs for which upper limit reactivity estimates have to be made, and thus upper limit quantum yields of unity would have to be used.

2. Mechanistic Reactivities

Table D-2 gives the both the directly calculated ("best estimate") and the upper limit MIR mechanistic reactivities for all the compounds in the current mechanism. The "MR Tp." column on the table shows how the compounds were classified for the purpose of estimating upper limit mechanistic reactivities, and shows how the upper limit values were obtained. The upper limits are close to the directly calculated values for the most mechanistically reactive compounds such as methane some of the alkyl benzenes, but are up to a factor of ~5-10 for compounds with low mechanistic reactivity. The latter include compounds such as naphthalenes or high molecular weight esters, where the relatively low upper limit mechanism A cannot be used. On the average, the upper limit mechanistic reactivities are higher than the directly calculated values a factor of ~3. Given the large variability and many factors that affect mechanistic reactivities, this is probably as close an estimate that can reasonably be obtained.

3. Upper Limit MIR's

The upper limit MIR's for all the for all the separately represented VOCs in the mechanism are shown on Table D-2, where they can be compared with their directly calculated ("best estimate") values. The table also shows the ratio of the upper limit to the directly calculated MIRs, which is in effect the margin of error involved in making the upper limit estimates. For most compounds, whose rate constants have been measured or which react sufficiently rapidly that the kinetic reactivity is not highly sensitive to the rate constant, the difference between upper limit and best estimate MIRs reflect primarily the differences for the mechanistic reactivities. Obviously the differences between upper limit and best estimate would be greater if the rate constants were unknown or significantly uncertain, and unit kinetic reactivities had to be used.

4. Discussion

The recommendations for estimating upper limit reactivities were developed to assist the application of reactivity-based regulations to compounds of uncertain reactivity. The objective to derive upper limit MIR estimates for compounds of uncertain reactivity such that it is unlikely that the actual ozone impacts of the compounds would be higher than the upper limit, but which are as low as possible given our limited knowledge. It is also important that the procedure be as objective and straightforward as possible, so that it can be applied to the full variety of compounds which might be subject to reactivity based regulations. The procedures discussed above should adequately address these objectives.

The recommendations given in this work are based on reactivity calculations for a wide variety of compounds. However, it should be pointed out that the upper limit mechanistic reactivities for compounds with unknown mechanisms are driven primarily by calculated reactivities for aromatic hydrocarbons, methyl glyoxal, and methane. The other classes of compounds which were considered were primarily alkanes, olefins, and various relatively low molecular weight oxygenates (see Carter, 2000). If a compound is expected to possibly have a significantly different mechanism than any compound in this group, then the possibility that the ozone impacts may actually be higher than estimated using these procedures cannot be totally ruled out. In this case, the upper limit estimates would need to be modified accordingly. However, given our current knowledge of atmospheric chemistry and the variety of compounds studied, we think that the probability of any given compound having a greater ozone impact the upper limit estimate is relatively low.

It is important to recognize the limitations of this work. The procedure is intended only for estimating upper limits for Maximum Incremental Reactivities calculated using the approach and one-day EKMA model airshed scenarios employed by Carter (1990), and using the SAPRC-99 mechanisms as described by Carter (2000). The upper limit mechanistic reactivities are particularly sensitive to the type of scenario employed, and are also subject to change as the chemical mechanism is updated. Therefore, these upper limit estimates should not be considered as independent of the reactivity scale upon which it is based, but rather as an extension of it, which would be updated and modified as the scale is updated in the process of ongoing research.

In particular, the upper limits given here are *not* to be compared with MIR values used in the current CARB vehicle regulations (CARB, 1993), or those given by Carter (1994a), since they were calculated using an earlier chemical mechanism, which generally gives lower MIR values. The upper

limit MIRs given on Table D-2 should be compared *only* with the best estimate MIRs given on the same table [or by Carter (2000)], and not with those given in any previously published or distributed tabulation, or with any updated scale that may be developed in the future. However, the general approach discussed here can be used to update the upper limit estimates if any changes are made to the chemical mechanism or scenarios used to derive the underlying reactivity scale upon which this is based.

It is also important to recognize that the general procedures discussed here are only applicable to regulatory or other applications where, by their nature, the ozone impacts must be quantified using a single scale. Examples would include the CARB clean-fuel/low emissions vehicle regulations (CARB, 1993), or the reactivity adjustments to VOC content limits being considered for CARB consumer product regulations. This procedure is *not* applicable to applications such as deciding whether to exempt a VOC from regulation on the basis of having negligible ozone impact, which can be based on a VOC's impact under a full variety of atmospheric conditions. A set of procedures considered more appropriate for upper limit reactivity estimates for making VOC exemption decisions is described in a separate document (Carter, 1997).

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Table D-2. Summary of upper limit MIR estimates for the SAPRC-99 mechanism, and comparison with directly calculated MIRs.

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
CO	Carbon Monoxide	1	28.0	2.1e-13	2.1e-13				0.04	A	7	0.45	1	0.06	7.8
METHANE	Methane	1	16.0	6.6e-15	6.6e-15				0.00	A	7	0.03	1	0.01	1.8
ETHANE	Ethane	2	30.1	2.6e-13	2.6e-13				0.05	A	12	0.92	1	0.31	3.0
PROPANE	Propane	3	44.1	1.1e-12	1.1e-12				0.19	A	13	2.61	1	0.56	4.7
N-C4	n-Butane	4	58.1	2.5e-12	2.5e-12				0.36	A	13	3.99	1	1.33	3.0
N-C5	n-Pentane	5	72.2	4.0e-12	4.0e-12				0.52	A	14	4.83	1	1.54	3.1
N-C6	n-Hexane	6	86.2	5.5e-12	5.5e-12				0.63	A	14	5.09	2	1.45	3.5
N-C7	n-Heptane	7	100.2	7.0e-12	7.0e-12				0.73	A	15	5.20	2	1.28	4.1
N-C8	n-Octane	8	114.2	8.8e-12	8.8e-12				0.80	A	16	5.22	2	1.11	4.7
N-C9	n-Nonane	9	128.3	1.0e-11	1.0e-11				0.84	A	16	5.02	3	0.95	5.3
N-C10	n-Decane	10	142.3	1.1e-11	1.1e-11				0.87	A	16	4.81	3	0.83	5.8
N-C11	n-Undecane	11	156.3	1.3e-11	1.3e-11				0.91	A	17	4.68	3	0.74	6.3
N-C12	n-Dodecane	12	170.3	1.4e-11	1.4e-11				0.92	A	17	4.44	3	0.66	6.8
N-C13	n-Tridecane	13	184.4	1.6e-11	1.6e-11				0.95	A	18	4.35	3	0.62	7.0
N-C14	n-Tetradecane	14	198.4	1.8e-11	1.8e-11				0.96	A	18	4.23	3	0.58	7.3
N-C15	n-Pentadecane	15	212.4	2.1e-11	2.1e-11				0.98	A	19	4.17	3	0.56	7.5
N-C16	n-C16	16	226.5	2.3e-11	2.3e-11				0.99	A	19	4.02	3	0.52	7.7
2-ME-C3	Isobutane	4	58.1	2.2e-12	2.2e-12				0.33	A	13	3.62	1	1.35	2.7
2-ME-C4	Iso-Pentane	5	72.2	3.7e-12	3.7e-12				0.49	A	14	4.51	2	1.68	2.7
22-DM-C3	Neopentane	5	72.2	8.6e-13	8.6e-13				0.15	A	13	1.23	2	0.69	1.8
22-DM-C4	2,2-Dimethyl Butane	6	86.2	2.4e-12	2.4e-12				0.35	A	13	2.61	2	1.33	2.0
23-DM-C4	2,3-Dimethyl Butane	6	86.2	5.8e-12	5.8e-12				0.65	A	15	5.30	2	1.14	4.7
2-ME-C5	2-Methyl Pentane	6	86.2	5.3e-12	5.3e-12				0.62	A	14	4.97	2	1.80	2.8
3-ME-C5	3-Methylpentane	6	86.2	5.4e-12	5.4e-12				0.63	A	14	5.04	2	2.07	2.4
223TM-C4	2,2,3-Trimethyl Butane	7	100.2	4.3e-12	4.3e-12				0.54	A	14	3.62	2	1.32	2.7
22-DM-C5	2,2-Dimethyl Pentane	7	100.2	3.4e-12	3.4e-12				0.46	A	14	3.03	2	1.22	2.5
23-DM-C5	2,3-Dimethyl Pentane	7	100.2	1.4e-11	7.2e-12	*			0.93	A	17	7.64	2	1.55	4.9
24-DM-C5	2,4-Dimethyl Pentane	7	100.2	5.0e-12	5.0e-12				0.60	A	14	4.10	2	1.65	2.5
2-ME-C6	2-Methyl Hexane	7	100.2	1.4e-11	6.9e-12	*			0.92	A	17	7.52	2	1.37	5.5
33-DM-C5	3,3-Dimethyl Pentane	7	100.2	6.0e-12	3.0e-12	*			0.67	A	15	4.67	2	1.32	3.5

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
3-ME-C6	3-Methyl Hexane	7	100.2	1.4e-11	7.2e-12	*			0.93	A	17	7.65	2	1.86	4.1
2233M-C4	2,2,3,3-Tetramethyl Butane	8	114.2	1.1e-12	1.1e-12				0.18	A	13	0.94	3	0.44	2.1
224TM-C5	2,2,4-Trimethyl Pentane	8	114.2	3.6e-12	3.6e-12				0.48	A	14	2.78	2	1.44	1.9
22-DM-C6	2,2-Dimethyl Hexane	8	114.2	4.8e-12	4.8e-12				0.59	A	14	3.49	3	1.13	3.1
234TM-C5	2,3,4-Trimethyl Pentane	8	114.2	7.1e-12	7.1e-12				0.73	A	15	4.59	3	1.23	3.7
23-DM-C6	2,3-Dimethyl Hexane	8	114.2	1.7e-11	8.6e-12	*			0.96	A	18	7.22	3	1.34	5.4
24-DM-C6	2,4-Dimethyl Hexane	8	114.2	1.7e-11	8.6e-12	*			0.96	A	18	7.22	3	1.80	4.0
25-DM-C6	2,5-Dimethyl Hexane	8	114.2	1.7e-11	8.3e-12	*			0.95	A	18	7.12	3	1.68	4.2
2-ME-C7	2-Methyl Heptane	8	114.2	1.7e-11	8.3e-12	*			0.95	A	18	7.13	3	1.20	5.9
3-ME-C7	3-Methyl Heptane	8	114.2	1.7e-11	8.6e-12	*			0.96	A	18	7.22	3	1.35	5.4
4-ME-C7	4-Methyl Heptane	8	114.2	1.7e-11	8.6e-12	*			0.96	A	18	7.22	3	1.48	4.9
225TM-C6	2,2,5-Trimethyl Hexane	9	128.3	1.2e-11	6.1e-12	*			0.89	A	17	5.55	3	1.33	4.2
235TM-C6	2,3,5-Trimethyl Hexane	9	128.3	7.9e-12	7.9e-12				0.77	A	15	4.37	3	1.33	3.3
24-DM-C7	2,4-Dimethyl Heptane	9	128.3	2.0e-11	1.0e-11	*			0.97	A	19	6.79	3	1.48	4.6
2-ME-C8	2-Methyl Octane	9	128.3	1.0e-11	1.0e-11				0.84	A	16	5.04	3	0.96	5.3
33-DE-C5	3,3-Diethyl Pentane	9	128.3	4.9e-12	4.9e-12				0.59	A	14	3.15	3	1.35	2.3
35-DM-C7	3,5-Dimethyl Heptane	9	128.3	2.1e-11	1.0e-11	*			0.98	A	19	6.86	3	1.63	4.2
4-ET-C7	4-Ethyl Heptane	9	128.3	2.1e-11	1.0e-11	*			0.98	A	19	6.88	3	1.44	4.8
4-ME-C8	4-Methyl Octane	9	128.3	9.7e-12	9.7e-12				0.83	A	16	4.93	3	1.08	4.6
24-DM-C8	2,4-Dimethyl Octane	10	142.3	2.3e-11	1.1e-11	*			0.98	A	19	6.39	3	1.09	5.8
26DM-C8	2,6-Dimethyl Octane	10	142.3	1.3e-11	1.3e-11				0.91	A	17	5.15	3	1.27	4.1
2-ME-C9	2-Methyl Nonane	10	142.3	1.3e-11	1.3e-11				0.90	A	17	5.12	3	0.86	6.0
34-DE-C6	3,4-Diethyl Hexane	10	142.3	7.4e-12	7.4e-12				0.74	A	15	3.78	3	1.20	3.2
3-ME-C9	3-Methyl Nonane	10	142.3	2.3e-11	1.1e-11	*			0.98	A	19	6.39	3	0.89	7.2
4-ME-C9	4-Methyl Nonane	10	142.3	2.3e-11	1.1e-11	*			0.98	A	19	6.39	3	0.99	6.5
4-PR-C7	4-Propyl Heptane	10	142.3	2.4e-11	1.2e-11	*			0.99	A	19	6.45	3	1.24	5.2
26DM-C9	2,6-Dimethyl Nonane	11	156.3	2.6e-11	1.3e-11	*			0.99	A	20	6.02	3	0.95	6.3
35-DE-C7	3,5-Diethyl Heptane	11	156.3	2.8e-11	1.4e-11	*			0.99	A	20	6.16	3	1.21	5.1
3-ME-C10	3-Methyl Decane	11	156.3	2.6e-11	1.3e-11	*			0.99	A	20	6.03	3	0.77	7.9

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
4-ME-C10	4-Methyl Decane	11	156.3	2.6e-11	1.3e-11	*			0.99	A	20	6.03	3	0.80	7.5
36-DE-C8	2,6-Diethyl Octane	12	170.3	3.1e-11	1.5e-11	*			1.00	A	21	5.79	3	1.09	5.3
36DM-C10	3,6-Dimethyl Decane	12	170.3	2.9e-11	1.5e-11	*			1.00	A	20	5.71	3	0.88	6.5
3-ME-C11	3-Methyl Undecane	12	170.3	2.9e-11	1.4e-11	*			0.99	A	20	5.69	3	0.70	8.1
5-ME-C11	5-Methyl Undecane	12	170.3	2.9e-11	1.4e-11	*			0.99	A	20	5.69	3	0.72	7.9
36DM-C11	3,6-Dimethyl Undecane	13	184.4	3.2e-11	1.6e-11	*			1.00	A	21	5.41	3	0.82	6.6
37-DE-C9	3,7-Diethyl Nonane	13	184.4	3.4e-11	1.7e-11	*			1.00	A	21	5.48	3	1.08	5.1
3-ME-C12	3-Methyl Dodecane	13	184.4	3.1e-11	1.6e-11	*			1.00	A	21	5.39	3	0.64	8.4
5-ME-C12	5-Methyl Dodecane	13	184.4	3.1e-11	1.6e-11	*			1.00	A	21	5.39	3	0.64	8.4
37DM-C12	3,7-Dimethyl Dodecane	14	198.4	3.5e-11	1.7e-11	*			1.00	A	21	5.13	3	0.74	6.9
38DE-C10	3,8-Diethyl Decane	14	198.4	3.6e-11	1.8e-11	*			1.00	A	21	5.19	3	0.68	7.6
3-ME-C13	3-Methyl Tridecane	14	198.4	3.4e-11	1.7e-11	*			1.00	A	21	5.11	3	0.57	9.0
6-ME-C13	6-Methyl Tridecane	14	198.4	3.4e-11	1.7e-11	*			1.00	A	21	5.11	3	0.62	8.3
37DM-C13	3,7-Dimethyl Tridecane	15	212.4	3.8e-11	1.9e-11	*			1.00	A	22	4.88	3	0.64	7.6
39DE-C11	3,9-Diethyl Undecane	15	212.4	3.9e-11	2.0e-11	*			1.00	A	22	4.93	3	0.62	7.9
3-ME-C14	3-Methyl Tetradecane	15	212.4	3.7e-11	1.9e-11	*			1.00	A	22	4.86	3	0.53	9.1
6-ME-C14	6-Methyl Tetradecane	15	212.4	3.7e-11	1.9e-11	*			1.00	A	22	4.86	3	0.57	8.5
3-ME-C15	3-Methyl Pentadecane	16	226.5	4.0e-11	2.0e-11	*			1.00	A	22	4.64	3	0.50	9.2
48DM-C14	4,8-Dimethyl Tetradecane	16	226.5	4.0e-11	2.0e-11	*			1.00	A	22	4.65	3	0.58	8.1
7-ME-C15	7-Methyl Pentadecane	16	226.5	4.0e-11	2.0e-11	*			1.00	A	22	4.64	3	0.51	9.0
CYCC3	Cyclopropane	3	42.1	8.4e-14	8.4e-14				0.02	A	12	0.21	3	0.10	2.1
CYCC4	Cyclobutane	4	56.1	1.5e-12	1.5e-12				0.24	A	13	2.65	3	1.05	2.5
CYCC5	Cyclopentane	5	70.1	5.1e-12	5.1e-12				0.61	A	14	5.91	2	2.69	2.2
CYCC6	Cyclohexane	6	84.2	7.3e-12	7.3e-12				0.74	A	15	6.32	2	1.46	4.3
IPR-CC3	Isopropyl Cyclopropane	6	84.2	2.7e-12	2.7e-12				0.39	A	13	2.98	3	1.52	2.0
ME-CYCC5	Methylcyclopentane	6	84.2	1.1e-11	5.7e-12	*			0.88	A	16	8.17	3	2.42	3.4
13DMCYC5	1,3-Dimeth. Cyclopentane	7	98.2	1.4e-11	6.8e-12	*			0.92	A	17	7.64	3	2.15	3.6
CYCC7	Cycloheptane	7	98.2	1.3e-11	1.3e-11				0.91	A	17	7.48	3	2.26	3.3
ET-CYCC5	Ethyl Cyclopentane	7	98.2	1.5e-11	7.3e-12	*			0.93	A	17	7.86	3	2.27	3.5

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
ME-CYCC6	Methylcyclohexane	7	98.2	1.0e-11	1.0e-11				0.84	A	16	6.55	3	1.99	3.3
13DMCYC6	1,3-Dimethyl Cyclohexane	8	112.2	2.4e-11	1.2e-11	*			0.99	A	19	8.20	3	1.72	4.8
CYCC8	Cyclooctane	8	112.2	1.4e-11	1.4e-11				0.92	A	17	6.76	3	1.73	3.9
ET-CYCC6	Ethylcyclohexane	8	112.2	2.4e-11	1.2e-11	*			0.99	A	19	8.22	3	1.75	4.7
PR-CYCC5	Propyl Cyclopentane	8	112.2	1.7e-11	8.7e-12	*			0.96	A	18	7.38	3	1.91	3.9
113MCYC6	1,1,3-Trimethyl Cyclohex.	9	126.2	8.7e-12	8.7e-12				0.80	A	16	4.71	3	1.37	3.4
1E4MCYC6	1-Eth.-4-Meth. Cyclohex.	9	126.2	2.7e-11	1.4e-11	*			0.99	A	20	7.59	3	1.62	4.7
C3-CYCC6	Propyl Cyclohexane	9	126.2	2.7e-11	1.3e-11	*			0.99	A	20	7.55	3	1.47	5.1
13DECYC6	1,3-Diethyl-Cyclohexane	10	140.3	3.1e-11	1.6e-11	*			1.00	A	21	7.06	3	1.34	5.3
14DECYC6	1,4-Diethyl-Cyclohexane	10	140.3	3.1e-11	1.6e-11	*			1.00	A	21	7.06	3	1.49	4.7
1M3IPCY6	1-Meth.-3-Isopr. Cyclohex.	10	140.3	3.0e-11	1.5e-11	*			1.00	A	21	7.01	3	1.26	5.6
C4-CYCC6	Butyl Cyclohexane	10	140.3	3.0e-11	1.5e-11	*			1.00	A	21	6.99	3	1.07	6.5
13E5MCC6	13-Dieth-5-Me. Cyclohex.	11	154.3	3.4e-11	1.7e-11	*			1.00	A	21	6.58	3	1.11	5.9
1E2PCYC6	1-Ethyl-2-Propyl Cyclohex.	11	154.3	3.4e-11	1.7e-11	*			1.00	A	21	6.56	3	0.95	6.9
C5-CYCC6	Pentyl Cyclohexane	11	154.3	3.3e-11	1.6e-11	*			1.00	A	21	6.50	3	0.91	7.1
135ECYC6	1,3,5-Triethyl Cyclohex.	12	168.3	3.8e-11	1.9e-11	*			1.00	A	22	6.17	3	1.06	5.8
1M4C5CY6	1-Meth.-4-Pentyl Cyclohex.	12	168.3	3.6e-11	1.8e-11	*			1.00	A	21	6.10	3	0.81	7.6
C6-CYCC6	Hexyl Cyclohexane	12	168.3	1.8e-11	1.8e-11				0.96	A	18	4.97	2	0.75	6.6
13E5PCC6	13-Dieth-5-Pent Cyclohx.	13	182.4	4.1e-11	2.1e-11	*			1.00	A	22	5.80	3	0.99	5.8
1M2C6CC6	1-Meth.-2-Hexyl-Cyclohex.	13	182.4	3.9e-11	1.9e-11	*			1.00	A	22	5.73	3	0.70	8.2
C7-CYCC6	Heptyl Cyclohexane	13	182.4	3.8e-11	1.9e-11	*			1.00	A	22	5.71	3	0.66	8.6
13P5ECC6	13-Diprop-5-Eth Cyclohx.	14	196.4	4.4e-11	2.2e-11	*			1.00	A	22	5.46	3	0.94	5.8
1M4C7CC6	1-Meth.-4-Heptyl Cyclohex.	14	196.4	4.2e-11	2.1e-11	*			1.00	A	22	5.40	3	0.58	9.3
C8-CYCC6	Octyl Cyclohexane	14	196.4	4.1e-11	2.1e-11	*			1.00	A	22	5.38	2	0.60	8.9
135PCYC6	135-Tripropyl Cyclohex.	15	210.4	4.7e-11	2.3e-11	*			1.00	A	23	5.16	3	0.90	5.7
1M2C8CC6	1-Methyl-2-Octyl Cyclohex.	15	210.4	4.4e-11	2.2e-11	*			1.00	A	22	5.11	3	0.60	8.5
C9-CYCC6	Nonyl Cyclohexane	15	210.4	4.4e-11	2.2e-11	*			1.00	A	22	5.10	3	0.54	9.4
13P5BCC6	1,3-Prop.-5-Butyl Cyclohex.	16	224.4	4.9e-11	2.5e-11	*			1.00	A	23	4.89	3	0.77	6.3
1M4C9CY6	1-Methyl-4-Nonyl Cyclohex.	16	224.4	4.7e-11	2.4e-11	*			1.00	A	23	4.85	3	0.55	8.8

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct		
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)			
C10CYCC6	Decyl Cyclohexane	16	224.4	4.7e-11	2.3e-11	*			1.00	A	23	4.84	3	0.50	9.6		
ETHENE	Ethene	2	28.1	9.2e-12	8.4e-12		1.7e-18	2.2e-16	0.81	NP	14	19.51	1	9.08	2.1		
PROPENE	Propene	3	42.1	3.1e-11	2.6e-11		1.1e-17	9.7e-15	1.00	NP	21	23.87	1	11.58	2.1		
1-BUTENE	1-Butene	4	56.1	3.6e-11	3.1e-11		1.0e-17	1.4e-14	1.00	NP	28	23.92	2	10.29	2.3		
1-PENTEN	1-Pentene	5	70.1	3.6e-11	3.1e-11		1.0e-17	1.4e-14	*	1.00	NP	35	23.92	2	7.79	3.1	
3M-1-BUT	3-Methyl-1-Butene	5	70.1	3.7e-11	3.1e-11		1.1e-17	1.4e-14	*	1.00	NP	35	23.92	3	6.99	3.4	
1-HEXENE	1-Hexene	6	84.2	4.2e-11	3.7e-11		1.1e-17	1.4e-14	*	1.00	NP	35	19.95	2	6.17	3.2	
33M1-BUT	3,3-Dimethyl-1-Butene	6	84.2	3.0e-11	2.8e-11		5.4e-18	1.4e-14	*	1.00	NP	35	19.88	3	6.06	3.3	
3M1-C5E	3-Methyl-1-Pentene	6	84.2	6.6e-11	3.2e-11	*	5.1e-18	1.4e-14	*	1.00	NP	35	19.96	3	6.22	3.2	
4M1-C5E	4-Methyl-1-Pentene	6	84.2	6.8e-11	3.2e-11	*	9.6e-18	1.4e-14	*	1.00	NP	35	19.96	3	6.26	3.2	
1-HEPTEN	1-Heptene	7	98.2	4.5e-11	4.0e-11		1.2e-17	1.4e-14	*	1.00	NP	35	17.11	3	4.56	3.8	
1-OCTENE	1-Octene	8	112.2	7.0e-11	3.2e-11	*	1.5e-17	1.4e-14	*	1.00	NP	35	14.97	4	3.45	4.3	
1-C9E	1-Nonene	9	126.2	7.2e-11	3.2e-11	*	1.0e-17	*	1.4e-14	*	1.00	NP	35	13.31	4	2.76	4.8
1-C10E	1-Decene	10	140.3	6.8e-11	3.2e-11	*	9.7e-18	1.4e-14	*	1.00	NP	35	11.98	4	2.28	5.2	
1-C11E	1-Undecene	11	154.3	7.2e-11	3.2e-11	*	1.0e-17	*	1.4e-14	*	1.00	NP	35	10.89	4	1.95	5.6
1-C12E	1-Dodecene	12	168.3	7.2e-11	3.2e-11	*	1.0e-17	*	1.4e-14	*	1.00	NP	35	9.98	4	1.72	5.8
1-C13E	1-Tridecene	13	182.4	7.2e-11	3.2e-11	*	1.0e-17	*	1.4e-14	*	1.00	NP	35	9.21	4	1.55	6.0
1-C14E	1-Tetradecene	14	196.4	7.2e-11	3.2e-11	*	1.0e-17	*	1.4e-14	*	1.00	NP	35	8.55	4	1.48	5.8
1-C15E	1-Pentadecene	15	210.4	7.2e-11	3.2e-11	*	1.0e-17	*	1.4e-14	*	1.00	NP	35	7.98	4	1.30	6.2
ISOBUTEN	Isobutene	4	56.1	5.8e-11	5.1e-11		1.2e-17	3.3e-13		1.00	NP	28	23.95	1	6.35	3.8	
2M-1-BUT	2-Methyl-1-Butene	5	70.1	7.1e-11	6.0e-11		1.7e-17	3.3e-13	*	1.00	NP	35	23.95	3	6.51	3.7	
23M1-BUT	23-Dimethyl-1-Butene	6	84.2	1.2e-10	5.8e-11	*	1.3e-17	3.3e-13	*	1.00	NP	35	19.96	3	4.77	4.2	
2E1-BUT	2-Ethyl-1-Butene	6	84.2	1.2e-10	5.8e-11	*	1.3e-17	3.3e-13	*	1.00	NP	35	19.96	3	5.04	4.0	
2M1-C5E	2-Methyl-1-Pentene	6	84.2	7.2e-11	6.2e-11		1.6e-17	3.3e-13	*	1.00	NP	35	19.96	3	5.18	3.9	
233M1BUT	2,3,3-trimethyl-1-Butene	7	98.2	1.2e-10	5.8e-11	*	8.6e-18	3.3e-13	*	1.00	NP	35	17.11	3	4.62	3.7	
3M2I1C4E	3-Methyl-2-Isopropyl-1-Butene	8	112.2	1.2e-10	5.8e-11	*	3.5e-18	3.3e-13	*	1.00	NP	35	14.97	4	3.29	4.6	
C-2-BUTE	cis-2-Butene	4	56.1	1.1e-10	5.6e-11		1.3e-16	3.5e-13		1.00	NP	28	23.95	2	13.22	1.8	
T-2-BUTE	trans-2-Butene	4	56.1	1.5e-10	6.3e-11		1.9e-16	3.9e-13		1.00	NP	28	23.95	1	13.91	1.7	

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
2M-2-BUT	2-Methyl-2-Butene	5	70.1	3.1e-10	8.6e-11	4.1e-16	9.4e-12		1.00	NP	35	23.95	3	14.45	1.7
C-2-PENT	cis-2-Pentene	5	70.1	1.7e-10	6.4e-11	1.2e-16	* 3.7e-13	*	1.00	NP	35	23.95	3	10.24	2.3
T-2-PENT	trans-2-Pentene	5	70.1	1.7e-10	6.6e-11	1.2e-16	* 3.7e-13	*	1.00	NP	35	23.95	3	10.23	2.3
23M2-BUT	2,3-Dimethyl-2-Butene	6	84.2	8.7e-10	1.1e-10	1.1e-15	5.7e-11		1.00	NP	35	19.96	3	13.32	1.5
2M-2-C5E	2-Methyl-2-Pentene	6	84.2	4.8e-10	8.8e-11	3.5e-16	* 9.4e-12	*	1.00	NP	35	19.96	3	12.28	1.6
C-2-C6E	Cis-2-Hexene	6	84.2	2.3e-10	6.3e-11	* 1.2e-16	* 3.7e-13	*	1.00	NP	35	19.96	3	8.44	2.4
C-3-C6E	Cis-3-Hexene	6	84.2	2.0e-10	6.3e-11	* 1.5e-16	3.7e-13	*	1.00	NP	35	19.96	3	8.22	2.4
C3M2-C5E	Cis-3-Methyl-2-Hexene	6	84.2	4.6e-10	8.7e-11	* 4.6e-16	9.4e-12	*	1.00	NP	35	19.96	3	13.38	1.5
T3M2-C5E	Trans 3-Methyl-2-Hexene	6	84.2	5.1e-10	8.7e-11	* 5.7e-16	9.4e-12	*	1.00	NP	35	19.96	3	14.17	1.4
T4M2-C5E	Trans 4-Methyl-2-Hexene	6	84.2	1.6e-10	6.0e-11	1.2e-16	* 3.7e-13	*	1.00	NP	35	19.96	3	7.88	2.5
T-2-C6E	Trans-2-Hexene	6	84.2	2.3e-10	6.3e-11	* 1.2e-16	* 3.7e-13	*	1.00	NP	35	19.96	3	8.44	2.4
T-3-C6E	Trans-3-Hexene	6	84.2	2.1e-10	6.3e-11	* 1.7e-16	3.7e-13	*	1.00	NP	35	19.96	3	8.16	2.4
23M2-C5E	2,3-Dimethyl-2-Hexene	7	98.2	1.2e-9	1.0e-10	6.7e-16	* 5.7e-11	*	1.00	NP	35	17.11	4	10.41	1.6
C-3-C7E	Cis-3-Heptene	7	98.2	2.3e-10	6.3e-11	* 1.2e-16	* 3.7e-13	*	1.00	NP	35	17.11	4	6.96	2.5
T44M2C5E	Trans 4,4-dimethyl-2-Pentene	7	98.2	1.6e-10	5.4e-11	1.2e-16	* 3.7e-13	*	1.00	NP	35	17.11	4	6.99	2.4
T-2-C7E	Trans-2-Heptene	7	98.2	1.7e-10	6.7e-11	1.2e-16	* 3.7e-13	*	1.00	NP	35	17.11	4	7.33	2.3
T-3-C7E	Trans-3-Heptene	7	98.2	2.3e-10	6.3e-11	* 1.2e-16	* 3.7e-13	*	1.00	NP	35	17.11	4	6.96	2.5
C-4-C8E	Cis-4-Octene	8	112.2	1.7e-10	6.3e-11	* 9.7e-17	3.7e-13	*	1.00	NP	35	14.97	4	5.94	2.5
T22M3C6E	Trans 2,2-Dimethyl 3-Hexene	8	112.2	1.5e-10	6.3e-11	* 4.3e-17	3.7e-13	*	1.00	NP	35	14.97	4	5.97	2.5
T25M3C6E	Trans 2,5-Dimethyl 3-Hexene	8	112.2	1.5e-10	6.3e-11	* 4.2e-17	3.7e-13	*	1.00	NP	35	14.97	4	5.44	2.8
T-3-C8E	Trans-3-Octene	8	112.2	2.3e-10	6.3e-11	* 1.2e-16	* 3.7e-13	*	1.00	NP	35	14.97	4	6.13	2.4
T-4-C8E	Trans-4-Octene	8	112.2	1.3e-10	6.8e-11	1.4e-16	3.7e-13	*	1.00	NP	35	14.97	4	5.90	2.5
244M2C5E	2,4,4-trimethyl-2-Pentene	8	126.2	3.2e-10	8.7e-11	* 1.4e-16	9.4e-12	*	1.00	NP	35	13.31	4	5.85	2.3
T-4-C9E	Trans-4-Nonene	9	128.3	2.3e-10	6.3e-11	* 1.2e-16	* 3.7e-13	*	1.00	NP	35	13.10	4	5.23	2.5
34E2-C6E	3,4-Diethyl-2-Hexene	10	140.3	2.6e-10	8.7e-11	* 4.4e-18	9.4e-12	*	1.00	NP	35	11.98	4	3.95	3.0
C-5-C10E	Cis-5-Decene	10	140.3	1.8e-10	6.3e-11	* 1.2e-16	3.7e-13	*	1.00	NP	35	11.98	4	4.89	2.5
T-4-C10E	Trans-4-Decene	10	140.3	2.3e-10	6.3e-11	* 1.2e-16	* 3.7e-13	*	1.00	NP	35	11.98	4	4.50	2.7
T-5-C11E	Trans-5-Undecene	11	154.3	2.3e-10	6.3e-11	* 1.2e-16	* 3.7e-13	*	1.00	NP	35	10.89	4	4.23	2.6
T-5-C12E	Trans-5-Dodecene	12	168.3	2.3e-10	6.3e-11	* 1.2e-16	* 3.7e-13	*	1.00	NP	35	9.98	4	3.74	2.7

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct		
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)			
T-5-C13E	Trans-5-Tridecene	13	182.4	2.3e-10	6.3e-11	*	1.2e-16	*	3.7e-13	*	1.00	NP	35	9.21	4	3.38	2.7
T-5-C14E	Trans-5-Tetradecene	14	196.4	2.3e-10	6.3e-11	*	1.2e-16	*	3.7e-13	*	1.00	NP	35	8.55	4	3.08	2.8
T-5-C15E	Trans-5-Pentadecene	15	210.4	2.3e-10	6.3e-11	*	1.2e-16	*	3.7e-13	*	1.00	NP	35	7.98	4	2.82	2.8
CYC-PNTE	Cyclopentene	5	68.1	3.1e-10	6.6e-11		5.6e-16		5.3e-13		1.00	NP	35	24.66	4	7.38	3.3
1M-CC5E	1-Methyl cyclopentene	5	82.2	5.6e-10	8.7e-11	*	6.8e-16		9.4e-12	*	1.00	NP	35	20.45	4	13.95	1.5
CYC-HEXE	Cyclohexene	6	82.2	1.1e-10	6.7e-11		8.3e-17		5.9e-13		1.00	NP	35	20.45	4	5.45	3.8
1M-CC6E	1-Methyl Cyclohexene	7	96.2	3.3e-10	8.7e-11	*	1.7e-16		9.4e-12	*	1.00	NP	35	17.47	4	7.81	2.2
4M-CC6E	4-Methyl Cyclohexene	7	96.2	1.7e-10	6.3e-11	*	8.4e-17		3.7e-13	*	1.00	NP	35	17.47	4	4.48	3.9
12M-CC6E	1,2-Dimethyl Cyclohexene	8	110.2	8.3e-10	1.1e-10	*	2.1e-16		5.7e-11	*	1.00	NP	35	15.25	4	6.77	2.3
13-BUTDE	1,3-Butadiene	4	54.1	6.9e-11	6.6e-11		6.6e-18		1.0e-13		1.00	NP	28	24.85	3	13.58	1.8
ISOPRENE	Isoprene	5	68.1	1.1e-10	1.0e-10		1.3e-17		6.9e-13		1.00	NP	35	24.66	1	10.69	2.3
3-CARENE	3-Carene	10	136.2	1.5e-10	8.7e-11		3.8e-17		9.1e-12		1.00	NP	35	12.33	2	3.21	3.8
A-PINENE	a-Pinene	10	136.2	1.2e-10	5.3e-11		8.8e-17		6.1e-12		1.00	NP	35	12.33	2	4.29	2.9
B-PINENE	b-Pinene	10	136.2	9.7e-11	7.8e-11		1.5e-17		2.5e-12		1.00	NP	35	12.33	3	3.28	3.8
D-LIMONE	d-Limonene	10	136.2	3.1e-10	1.7e-10		2.0e-16		1.2e-11		1.00	NP	35	12.33	2	3.99	3.1
SABINENE	Sabinene	10	136.2	2.0e-10	1.2e-10		8.7e-17		1.0e-11		1.00	NP	35	12.33	2	3.67	3.4
STYRENE	Styrene	8	104.2	6.6e-11	5.8e-11		1.7e-17		1.5e-13		1.00	NP	35	16.13	2	1.95	8.3
BENZENE	Benzene	6	78.1	1.2e-12	1.2e-12						0.20	NP	35	4.38	3	0.81	5.4
TOLUENE	Toluene	7	92.1	5.9e-12	5.9e-12						0.66	NP	35	12.07	2	3.97	3.0
C2-BENZ	Ethyl Benzene	8	106.2	7.1e-12	7.1e-12						0.73	NP	35	11.53	2	2.79	4.1
I-C3-BEN	Isopropyl Benzene (cumene)	9	120.2	6.5e-12	6.5e-12						0.70	NP	35	9.74	3	2.32	4.2
N-C3-BEN	n-Propyl Benzene	9	120.2	6.0e-12	6.0e-12						0.67	NP	35	9.33	3	2.20	4.2
S-C4-BEN	s-Butyl Benzene	10	134.2	6.0e-12	6.0e-12						0.67	NP	35	8.36	3	1.97	4.2
M-XYLENE	m-Xylene	8	106.2	2.4e-11	2.4e-11						0.99	NP	35	15.62	2	10.61	1.5
O-XYLENE	o-Xylene	8	106.2	1.4e-11	1.4e-11						0.92	NP	35	14.55	2	7.49	1.9
P-XYLENE	p-Xylene	8	106.2	1.4e-11	1.4e-11						0.93	NP	35	14.68	2	4.25	3.5
123-TMB	1,2,3-Trimethyl Benzene	9	120.2	3.3e-11	3.3e-11						1.00	NP	35	13.94	2	11.26	1.2
124-TMB	1,2,4-Trimethyl Benzene	9	120.2	3.3e-11	3.3e-11						1.00	NP	35	13.94	2	7.18	1.9
135-TMB	1,3,5-Trimethyl Benzene	9	120.2	5.8e-11	5.8e-11						1.00	NP	35	13.98	2	11.22	1.2

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
NAPHTHAL	Naphthalene	10	128.2	2.1e-11	2.1e-11				0.98	NP	35	12.84	3	3.26	3.9
TETRALIN	Tetralin	10	132.2	3.4e-11	3.4e-11				1.00	NP	35	12.68	3	2.83	4.5
ME-NAPH	Methyl Naphthalenes	11	142.2	5.2e-11	5.2e-11				1.00	NP	35	11.81	3	4.61	2.6
23-DMN	2,3-Dimethyl Naphth.	12	156.2	7.7e-11	7.7e-11				1.00	NP	35	10.75	3	5.54	1.9
ACETYLEN	Acetylene	2	26.0	9.2e-13	9.1e-13	8.6e-21			0.15	NP	14	3.99	2	1.25	3.2
ME-ACTYL	Methyl Acetylene	3	40.1	5.9e-12	5.9e-12	1.6e-20			0.66	NP	21	16.65	4	6.45	2.6
2-BUTYNE	2-Butyne	4	54.1	2.7e-11	2.7e-11	2.1e-20			0.99	NP	28	24.68	4	16.33	1.5
ET-ACTYL	Ethyl Acetylene	4	54.1	8.0e-12	8.0e-12	2.1e-20			0.77	NP	28	19.14	4	6.20	3.1
MEOH	Methanol	1	32.0	9.3e-13	9.3e-13				0.16	A	7	1.65	1	0.71	2.3
ETOH	Ethanol	2	46.1	3.3e-12	3.3e-12				0.45	A	14	6.39	1	1.69	3.8
I-C3-OH	Isopropyl Alcohol	3	60.1	5.3e-12	5.3e-12				0.62	A	14	7.14	1	0.71	10.0
N-C3-OH	n-Propyl Alcohol	3	60.1	5.5e-12	5.5e-12				0.64	A	14	7.35	2	2.74	2.7
I-C4-OH	Isobutyl Alcohol	4	74.1	1.4e-11	6.9e-12	*			0.92	A	17	10.18	3	2.24	4.5
N-C4-OH	n-Butyl Alcohol	4	74.1	8.6e-12	8.6e-12				0.79	A	15	7.95	3	3.34	2.4
S-C4-OH	s-Butyl Alcohol	4	74.1	2.0e-11	1.0e-11	*			0.97	A	19	11.73	3	1.60	7.4
T-C4-OH	t-Butyl Alcohol	4	74.1	1.1e-12	1.1e-12				0.19	A	13	1.54	3	0.45	3.4
CC5-OH	Cyclopentanol	5	86.1	1.1e-11	1.1e-11				0.86	A	16	7.74	3	1.96	4.0
2-C5OH	2-Pentanol	5	88.2	1.2e-11	1.2e-11				0.89	A	16	7.95	3	1.74	4.6
3-C5OH	3-Pentanol	5	88.2	1.2e-11	1.2e-11				0.89	A	17	8.08	3	1.73	4.7
C5OH	Pentyl Alcohol	5	88.2	1.1e-11	1.1e-11				0.87	A	16	7.71	3	3.35	2.3
CC6-OH	Cyclohexanol	6	100.2	3.5e-11	1.7e-11	*			1.00	A	21	10.17	3	2.25	4.5
1-C6OH	1-Hexanol	6	102.2	1.3e-11	1.3e-11				0.90	A	17	7.05	3	2.74	2.6
2-C6OH	2-Hexanol	6	102.2	1.2e-11	1.2e-11				0.89	A	17	6.94	3	2.46	2.8
1-C7OH	1-Heptanol	7	116.2	1.4e-11	1.4e-11				0.92	A	17	6.47	3	2.21	2.9
1-C8-OH	1-Octanol	8	130.2	2.0e-11	2.0e-11				0.98	A	19	6.71	2	2.01	3.3
2-ETC6OH	2-Ethyl-1-Hexanol	8	130.2	2.7e-11	1.3e-11	*			0.99	A	20	7.30	3	2.20	3.3
2-C8-OH	2-Octanol	8	130.2	2.5e-11	2.5e-11				0.99	A	20	7.19	2	2.16	3.3
3-C8-OH	3-Octanol	8	130.2	3.1e-11	3.1e-11				1.00	A	21	7.63	2	2.57	3.0
4-C8-OH	4-Octanol	8	130.2	2.9e-11	2.9e-11				0.99	A	20	7.45	3	3.07	2.4

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
I-C10-OH	8-Methyl-1-Nonanol (Isodecyl Alcohol)	10	158.3	3.1e-11	1.5e-11	*			1.00	A	21	6.24	3	1.18	5.3
ET-GLYCL	Ethylene Glycol	2	62.1	1.5e-11	1.5e-11				0.93	A	14	10.10	2	3.36	3.0
PR-GLYCL	Propylene Glycol	3	76.1	2.2e-11	2.2e-11				0.98	A	19	11.72	1	2.75	4.3
12-C4OH2	1,2-Butandiol	4	90.1	3.2e-11	1.6e-11	*			1.00	A	21	11.06	2	2.21	5.0
GLYCERL	Glycerol	3	92.1	3.7e-11	1.9e-11	*			1.00	A	21	10.93	2	3.27	3.3
C6-GLYCL	1,2-Dihydroxy Hexane	6	118.2	3.7e-11	1.9e-11	*			1.00	A	22	8.76	3	2.75	3.2
2M24C5OH	2-Methyl-2,4-Pentanediol	6	118.2	1.1e-11	1.1e-11				0.86	A	16	5.62	3	1.04	5.4
ME-O-ME	Dimethyl Ether	2	46.1	3.0e-12	3.0e-12				0.42	A	13	5.96	1	0.93	6.4
TME-OX	Trimethylene Oxide	3	58.1	1.0e-11	1.0e-11				0.85	A	16	11.25	3	5.22	2.2
THF	Tetrahydrofuran	4	72.1	1.6e-11	1.6e-11				0.95	A	18	11.16	3	4.95	2.3
ET-O-ET	Diethyl Ether	4	74.1	1.3e-11	1.3e-11				0.91	A	17	9.92	2	4.01	2.5
METHYLAL	Dimethoxy methane	3	76.1	4.9e-12	4.9e-12				0.59	A	14	5.31	1	1.04	5.1
AM-THF	Alpha-Methyltetrahydrofuran	5	86.1	2.2e-11	2.2e-11				0.98	A	19	10.43	3	4.62	2.3
THP	Tetrahydropyran	5	86.1	1.4e-11	1.4e-11				0.92	A	17	8.76	3	3.81	2.3
ET-O-IPR	Ethyl Isopropyl Ether	5	88.2	4.9e-11	2.4e-11	*			1.00	A	23	12.41	3	3.86	3.2
MNBE	Methyl n-Butyl Ether	5	88.2	1.5e-11	1.5e-11				0.93	A	17	8.82	3	3.66	2.4
MTBE	Methyl t-Butyl Ether	5	88.2	2.9e-12	2.9e-12				0.42	A	13	3.06	1	0.78	3.9
PR-O-PR	Di n-Propyl Ether	6	102.2	1.8e-11	1.8e-11				0.97	A	18	8.29	3	3.24	2.6
ENBE	Ethyl n-Butyl Ether	6	102.2	2.1e-11	2.1e-11				0.98	A	19	8.70	3	3.86	2.3
ETBE	Ethyl t-Butyl Ether	6	102.2	8.8e-12	8.8e-12				0.80	A	16	5.87	3	2.11	2.8
MTAE	Methyl t-Amyl Ether	6	102.2	7.9e-12	7.9e-12				0.77	A	15	5.49	3	2.14	2.6
2BU-THF	2-Butyl Tetrahydrofuran	8	128.2	5.5e-11	2.8e-11	*			1.00	A	23	8.72	3	2.53	3.5
IBU2-O	Di-Isobutyl Ether	8	130.2	2.6e-11	2.6e-11				0.99	A	20	7.25	3	1.29	5.6
BU-O-BU	Di-n-butyl Ether	8	130.2	2.9e-11	2.9e-11				0.99	A	20	7.46	3	3.17	2.4
C5-O-C5	Di-n-Pentyl Ether	10	158.3	3.5e-11	3.5e-11				1.00	A	21	6.43	3	2.64	2.4
MEO-ETOH	2-Methoxyethanol	3	76.1	1.3e-11	1.3e-11				0.91	A	17	9.75	3	2.98	3.3
MEOC3OH	1-Methoxy-2-Propanol	4	90.1	2.0e-11	2.0e-11				0.97	A	19	9.66	1	2.62	3.7
ETO-ETOH	2-Ethoxyethanol	4	90.1	1.9e-11	1.9e-11				0.97	A	18	9.44	2	3.78	2.5

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
2MEOC3OH	2-Methoxy-1-Propanol	4	90.1	5.1e-11	2.5e-11	*			1.00	A	23	12.22	3	3.01	4.1
ETOC3OH	1-Ethoxy-2-Propanol	5	104.2	5.2e-11	2.6e-11	*			1.00	A	23	10.64	3	3.25	3.3
2PROETOH	2-Propoxyethanol	5	104.2	4.9e-11	2.5e-11	*			1.00	A	23	10.53	3	3.52	3.0
3ETOC3OH	3-Ethoxy-1-Propanol	5	104.2	2.2e-11	2.2e-11				0.98	A	19	8.63	3	4.24	2.0
3MEOC4OH	3-Methoxy-1-Butanol	5	104.2	2.4e-11	2.4e-11				0.99	A	19	8.82	3	0.97	9.1
DET-GLCL	Diethylene Glycol	4	106.1	5.5e-11	2.8e-11	*			1.00	A	23	10.53	3	3.55	3.0
PROXC3OH	1-Propoxy-2-Propanol	6	118.2	2.9e-11	2.9e-11				1.00	A	20	8.24	3	2.86	2.9
BUO-ETOH	2-Butoxyethanol	6	118.2	2.6e-11	2.6e-11				0.99	A	20	7.96	1	2.90	2.7
3MOMC4OH	3 methoxy -3 methyl-Butanol	6	118.2	1.4e-11	7.1e-12	*			0.93	A	17	6.46	3	1.74	3.7
MOEOETOH	2-(2-Methoxyethoxy) Ethanol	5	120.2	6.8e-11	3.4e-11	*			1.00	A	24	9.60	3	2.90	3.3
PG-1TB-E	1-tert-Butoxy-2-Propanol	7	132.2	3.7e-11	1.9e-11	*			1.00	A	22	7.83	3	1.71	4.6
PG-2TB-E	2-tert-Butoxy-1-Propanol	7	132.2	4.9e-11	2.5e-11	*			1.00	A	23	8.29	3	1.81	4.6
BUOC3OH	n-Butoxy-2-Propanol	7	132.2	6.1e-11	3.1e-11	*			1.00	A	24	8.59	3	2.70	3.2
CARBITOL	2-(2-Ethoxyethoxy) EtOH	6	134.2	5.1e-11	5.1e-11				1.00	A	23	8.22	2	3.19	2.6
DPR-GLCL	Dipropylene Glycol	6	134.2	7.3e-11	3.6e-11	*			1.00	A	24	8.67	3	2.48	3.5
EGHE	2-Hexyloxyethanol	8	146.2	5.8e-11	2.9e-11	*			1.00	A	23	7.71	3	2.45	3.1
DGPE	2-(2-Propoxyethoxy) ethanol	7	148.2	8.8e-11	4.4e-11	*			1.00	A	25	8.00	3	3.00	2.7
DPRGOME	Dipropylene Glycol Methyl Ether	7	148.2	9.8e-11	4.9e-11	*			1.00	A	25	8.06	3	2.21	3.7
C8-CELSV	2-(2-Butoxyethoxy)-EtOH	8	162.2	9.0e-11	4.5e-11	*			1.00	A	25	7.32	3	2.70	2.7
TGME	2-[2-(2-Methoxyethoxy) ethoxy] ethanol	7	164.2	1.1e-10	5.3e-11	*			1.00	A	25	7.32	3	2.62	2.8
EGEHE	2-(2-Ethylhexyloxy) ethanol	10	174.3	6.5e-11	3.2e-11	*			1.00	A	24	6.58	3	1.71	3.8
TGEE	2-[2-(2-Ethoxyethoxy) ethoxy] ethanol	8	178.2	1.2e-10	6.0e-11	*			1.00	A	25	6.78	3	2.66	2.5
DGHE	2-(2-Hexyloxyethoxy) ethanol	10	190.3	9.6e-11	4.8e-11	*			1.00	A	25	6.27	3	2.03	3.1
TGPE	2-[2-(2-Propoxyethoxy) ethoxy] ethanol	9	192.3	1.3e-10	6.3e-11	*			1.00	A	25	6.29	3	2.46	2.6

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3 (* = Estimated k)	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
TGBE	2-[2-(2-Butoxyethoxy) ethoxy] ethanol	10	206.3	1.3e-10	6.4e-11	*			1.00	A	25	5.87	3	2.24	2.6
TPRGOME	Tripropylene Monomethyl Ether	Glycol	10	206.3	1.6e-10	7.8e-11	*		1.00	A	25	5.90	3	1.90	3.1
TETRAGME	2,5,8,11-Tetraoxatridecan- 13-ol	9	208.3	1.4e-10	7.2e-11	*			1.00	A	25	5.83	3	2.15	2.7
TETRAGBE	3,6,9,12-Tetraoxahexadecan- 1-ol	12	250.3	1.7e-10	8.4e-11	*			1.00	A	25	4.86	3	1.90	2.6
ME-FORM	Methyl Formate	2	60.1	2.3e-13	2.3e-13				0.04	B	14	0.46	3	0.07	6.9
ET-FORM	Ethyl Formate	3	74.1	1.0e-12	1.0e-12				0.17	B	17	1.93	3	0.52	3.7
ME-ACET	Methyl Acetate	3	74.1	3.5e-13	3.5e-13				0.06	B	17	0.68	1	0.07	9.4
ET-ACET	Ethyl Acetate	4	88.1	1.6e-12	1.6e-12				0.25	B	18	2.46	1	0.64	3.8
ME-PRAT	Methyl Propionate	4	88.1	1.0e-12	1.0e-12				0.17	B	17	1.63	3	0.71	2.3
C3-FORM	n-Propyl Formate	4	88.1	2.4e-12	2.4e-12				0.35	B	18	3.51	3	0.93	3.8
ET-PRAT	Ethyl Propionate	5	102.1	2.1e-12	2.1e-12				0.32	B	18	2.76	3	0.79	3.5
IPR-ACET	Isopropyl Acetate	5	102.1	3.4e-12	3.4e-12				0.46	B	19	4.10	2	1.24	3.3
ME-BUAT	Methyl Butyrate	5	102.1	3.0e-12	3.0e-12				0.43	B	19	3.73	3	1.18	3.2
ME-IBUAT	Methyl Isobutyrate	5	102.1	1.7e-12	1.7e-12				0.27	B	18	2.28	2	0.70	3.2
C4-FORM	n-Butyl Formate	5	102.1	3.1e-12	3.1e-12				0.44	B	19	3.82	3	0.95	4.0
PR-ACET	Propyl Acetate	5	102.1	3.4e-12	3.4e-12				0.46	B	19	4.10	3	0.87	4.7
ET-BUAT	Ethyl Butyrate	6	116.2	4.9e-12	4.9e-12				0.60	B	20	4.83	3	1.25	3.9
IBU-ACET	Isobutyl Acetate	6	116.2	9.2e-12	4.6e-12	*			0.82	B	22	7.33	3	0.67	10.9
ME-PVAT	Methyl Pivalate	6	116.2	1.3e-12	1.3e-12				0.21	B	18	1.51	2	0.41	3.7
BU-ACET	n-Butyl Acetate	6	116.2	4.2e-12	4.2e-12				0.54	B	19	4.27	2	0.89	4.8
PR-PRAT	n-Propyl Propionate	6	116.2	4.0e-12	4.0e-12				0.52	B	19	4.12	3	0.93	4.4
SBU-ACET	s-Butyl Acetate	6	116.2	5.5e-12	5.5e-12				0.64	B	20	5.23	3	1.43	3.6
TBU-ACET	t-Butyl Acetate	6	116.2	4.3e-13	4.3e-13				0.08	B	17	0.53	2	0.22	2.4
BU-PRAT	Butyl Propionate	7	130.2	1.0e-11	5.1e-12	*			0.84	B	22	6.89	3	0.89	7.8
AM-ACET	Amyl Acetate	7	130.2	1.2e-11	6.1e-12	*			0.89	B	23	7.56	3	0.96	7.9

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
PR-BUAT	n-Propyl Butyrate	7	130.2	7.4e-12	7.4e-12				0.74	B	21	5.72	3	1.17	4.9
23MC4ACT	2,3-Dimethylbutyl Acetate	8	144.2	1.5e-11	7.7e-12	*			0.94	NP	35	10.96	3	0.84	13.1
2MC5-ACT	2-Methylpentyl Acetate	8	144.2	1.5e-11	7.7e-12	*			0.94	NP	35	10.97	3	1.11	9.9
3MC5-ACT	3-Methylpentyl Acetate	8	144.2	1.5e-11	7.7e-12	*			0.94	NP	35	10.97	3	1.31	8.4
4MC5-ACT	4-Methylpentyl Acetate	8	144.2	1.5e-11	7.5e-12	*			0.94	NP	35	10.89	3	0.92	11.9
IBU-IBTR	Isobutyl Isobutyrate	8	144.2	1.1e-11	5.5e-12	*			0.87	B	23	6.51	3	0.64	10.2
BU-BUAT	n-Butyl Butyrate	8	144.2	1.1e-11	1.1e-11				0.86	B	22	6.38	3	1.12	5.7
NC6-ACET	n-Hexyl Acetate	8	144.2	1.5e-11	7.5e-12	*			0.94	NP	35	10.90	3	0.87	12.5
E3EOC3OH	Ethyl 3-Ethoxy Propionate	7	146.2	3.9e-11	2.0e-11	*			1.00	B	31	10.06	3	3.61	2.8
24MC5ACT	2,4-Dimethylpentyl Acetate	9	158.2	1.8e-11	9.1e-12	*			0.97	NP	35	10.25	3	0.98	10.5
2MC6-ACT	2-Methylhexyl Acetate	9	158.2	1.8e-11	9.2e-12	*			0.97	NP	35	10.25	3	0.89	11.5
3EC5-ACT	3-Ethylpentyl Acetate	9	158.2	1.9e-11	9.6e-12	*			0.97	NP	35	10.30	3	1.24	8.3
3MC6-ACT	3-Methylhexyl Acetate	9	158.2	1.8e-11	9.2e-12	*			0.97	NP	35	10.25	3	1.01	10.2
4MC6-ACT	4-Methylhexyl Acetate	9	158.2	1.8e-11	9.2e-12	*			0.97	NP	35	10.25	3	0.91	11.3
5MC6-ACT	5-Methylhexyl Acetate	9	158.2	1.8e-11	8.9e-12	*			0.96	NP	35	10.21	3	0.79	12.9
IC5IBUAT	Isoamyl Isobutyrate	9	158.2	1.4e-11	6.9e-12	*			0.92	B	24	6.63	3	0.89	7.4
NC7-ACET	n-Heptyl Acetate	9	158.2	1.8e-11	8.9e-12	*			0.96	NP	35	10.21	3	0.73	14.0
24MC6ACT	2,4-Dimethylhexyl Acetate	10	172.3	2.2e-11	1.1e-11	*			0.98	NP	35	9.57	3	0.93	10.3
2ETHXACT	2-Ethyl-Hexyl Acetate	10	172.3	2.2e-11	1.1e-11	*			0.98	B	27	7.28	3	0.79	9.3
34MC6ACT	3,4-Dimethylhexyl Acetate	10	172.3	2.2e-11	1.1e-11	*			0.98	NP	35	9.57	3	1.16	8.2
35MC6ACT	3,5-Dimethylhexyl Acetate	10	172.3	2.1e-11	1.1e-11	*			0.98	NP	35	9.55	3	1.09	8.8
3EC6-ACT	3-Ethylhexyl Acetate	10	172.3	2.2e-11	1.1e-11	*			0.98	NP	35	9.58	3	1.03	9.3
3MC7-ACT	3-Methylheptyl Aceate	10	172.3	2.1e-11	1.1e-11	*			0.98	NP	35	9.55	3	0.76	12.6
45MC6ACT	4,5-Dimethylhexyl Acetate	10	172.3	2.1e-11	1.1e-11	*			0.98	NP	35	9.55	3	0.86	11.1
4MC7-ACT	4-Methylheptyl Acetate	10	172.3	2.1e-11	1.1e-11	*			0.98	NP	35	9.55	3	0.72	13.2
5MC7-ACT	5-Methylheptyl Aceate	10	172.3	2.1e-11	1.1e-11	*			0.98	NP	35	9.55	3	0.73	13.1
NC8-ACET	n-Octyl Acetate	10	172.3	2.1e-11	1.0e-11	*			0.98	NP	35	9.53	3	0.64	14.8
235M6ACT	2,3,5-Teimethylhexyl Acetate	11	186.3	2.4e-11	1.2e-11	*			0.99	NP	35	8.92	3	0.86	10.3
23MC7ACT	2,3-Dimethylheptyl Acetate	11	186.3	2.5e-11	1.2e-11	*			0.99	NP	35	8.92	3	0.84	10.6

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
24MC7ACT	2,4-Dimethylheptyl Acetate	11	186.3	2.5e-11	1.2e-11	*			0.99	NP	35	8.92	3	0.88	10.2
25MC7ACT	2,5-Dimethylheptyl Acetate	11	186.3	2.5e-11	1.2e-11	*			0.99	NP	35	8.92	3	0.86	10.3
2MC8-ACT	2-Methyloctyl Acetate	11	186.3	2.4e-11	1.2e-11	*			0.99	NP	35	8.91	3	0.63	14.2
35MC7ACT	3,5-Dimethylheptyl Acetate	11	186.3	2.5e-11	1.2e-11	*			0.99	NP	35	8.92	3	1.01	8.8
36MC7ACT	3,6-Dimethylheptyl Acetate	11	186.3	2.4e-11	1.2e-11	*			0.99	NP	35	8.91	3	0.87	10.2
3EC7-ACT	3-Ethylheptyl Acetate	11	186.3	2.5e-11	1.2e-11	*			0.99	NP	35	8.92	3	0.71	12.6
45MC7ACT	4,5-Dimethylheptyl Acetate	11	186.3	2.5e-11	1.2e-11	*			0.99	NP	35	8.92	3	0.96	9.3
46MC7ACT	4,6-Dimethylheptyl Acetate	11	186.3	2.4e-11	1.2e-11	*			0.99	NP	35	8.91	3	0.83	10.7
4MC8-ACT	4-Methyloctyl Acetate	11	186.3	2.4e-11	1.2e-11	*			0.99	NP	35	8.91	3	0.68	13.1
5MC8-ACT	5-Methyloctyl Acetate	11	186.3	2.4e-11	1.2e-11	*			0.99	NP	35	8.91	3	0.67	13.3
NC9-ACET	n-Nonyl Acetate	11	186.3	2.3e-11	1.2e-11	*			0.99	NP	35	8.89	3	0.58	15.3
36MC8ACT	3,6-Dimethyloctyl Acetate	12	200.3	2.7e-11	1.4e-11	*			0.99	NP	35	8.33	3	0.88	9.5
3IPC7ACT	3-Isopropylheptyl Acetate	12	200.3	2.8e-11	1.4e-11	*			0.99	NP	35	8.33	3	0.71	11.7
46MC8ACT	4,6-Dimethyloctyl Acetate	12	200.3	2.7e-11	1.4e-11	*			0.99	NP	35	8.33	3	0.85	9.8
357M8ACT	3,5,7-Trimethyloctyl Acetate	13	214.4	3.0e-11	1.5e-11	*			1.00	NP	35	7.81	3	0.83	9.4
3E6M8ACT	3-Ethyl-6-Methyloctyl Acetate	13	214.4	3.1e-11	1.6e-11	*			1.00	NP	35	7.81	3	0.80	9.8
47MC9ACT	4,7-Dimethylnonyl Acetate	13	214.4	3.0e-11	1.5e-11	*			1.00	NP	35	7.81	3	0.64	12.3
2357M8AC	2,3,5,7-Tetramethyloctyl Acetate	14	228.4	3.4e-11	1.7e-11	*			1.00	NP	35	7.34	3	0.74	10.0
357M9ACT	3,5,7-Trimethylnonyl Acetate	14	228.4	3.4e-11	1.7e-11	*			1.00	NP	35	7.34	3	0.76	9.7
368M9ACT	3,6,8-Trimethylnonyl Acetate	14	228.4	3.3e-11	1.7e-11	*			1.00	NP	35	7.34	3	0.72	10.2
2468M8AC	2,4,6,8-Tetramethylnonyl Acetate	15	242.4	3.6e-11	1.8e-11	*			1.00	NP	35	6.92	3	0.63	11.1
3E67M9AC	3-Ethyl-6,7-Dimethylnonyl Acetate	15	242.4	3.7e-11	1.9e-11	*			1.00	NP	35	6.92	3	0.76	9.1
479M10AC	4,7,9-Trimethyldecyl Acetate	15	242.4	3.6e-11	1.8e-11	*			1.00	NP	35	6.92	3	0.55	12.6
23568M9A	2,3,5,6,8-Pentaamethylnonyl Acetate	16	256.4	4.0e-11	2.0e-11	*			1.00	NP	35	6.55	3	0.74	8.8

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
3579M10A	3,5,7,9-Tetramethyldecyl Acetate	16	256.4	3.9e-11	2.0e-11	*			1.00	NP	35	6.55	3	0.58	11.2
5E368M9A	5-Ethyl-3,6,8-Trimethylnonyl Acetate	16	256.4	4.0e-11	2.0e-11	*			1.00	NP	35	6.55	3	0.77	8.5
DMC	Dimethyl Carbonate	3	90.1	3.3e-13	3.3e-13				0.06	B	17	0.53	2	0.06	9.0
PC	Propylene Carbonate	4	102.1	6.9e-13	6.9e-13				0.12	B	17	0.96	2	0.25	3.8
ME-LACT	Methyl Lactate	4	104.1	2.8e-12	2.8e-12				0.40	B	18	3.37	3	2.75	1.2
MCSVACET	2-Methoxyethyl Acetate	5	118.1	2.5e-11	1.3e-11	*			0.99	B	28	11.07	3	1.18	9.4
ET-LACT	Ethyl Lactate	5	118.1	3.9e-12	3.9e-12				0.51	B	19	3.97	3	2.71	1.5
MIPR-CB	Methyl Isopropyl Carbonate	5	118.1	2.6e-12	2.6e-12				0.37	B	18	2.78	2	0.69	4.0
PGME-ACT	1-Methoxy-2-Propyl Acetate	6	132.2	1.4e-11	1.4e-11				0.93	B	24	8.08	2	1.71	4.7
CSV-ACET	2-Ethoxyethyl Acetate	6	132.2	3.9e-11	1.9e-11	*			1.00	B	31	11.10	3	1.90	5.8
2PGMEACT	2-Methoxy-1-propyl Acetate	6	132.2	4.6e-11	2.3e-11	*			1.00	B	32	11.53	3	1.12	10.3
DBE-4	Dimethyl Succinate	6	146.1	1.5e-12	1.5e-12				0.24	B	18	1.40	3	0.25	5.6
ETGLDACT	Ethylene Glycol Diacetate	6	146.1	7.6e-12	3.8e-12	*			0.75	B	21	5.16	3	0.72	7.2
DIPR-CB	Diisopropyl Carbonate	7	146.2	1.4e-11	6.9e-12	*			0.92	B	24	7.15	3	1.04	6.9
DBE-5	Dimethyl Glutarate	7	160.2	3.5e-12	3.5e-12				0.47	B	19	2.67	3	0.49	5.4
2BUETACT	2-Butoxyethyl Acetate	8	160.2	4.8e-11	2.4e-11	*			1.00	B	32	9.58	3	1.67	5.7
DBE-6	Dimethyl Adipate	8	174.2	8.8e-12	8.8e-12				0.80	B	22	4.75	3	1.95	2.4
DGEEA	2-(2-Ethoxyethoxy) acetate	ethyl	8	176.2	7.7e-11	3.9e-11	*		1.00	B	35	9.42	3	1.50	6.3
DGBEA	2-(2-Butoxyethoxy) acetate	ethyl	10	204.3	8.6e-11	4.3e-11	*		1.00	B	35	8.22	3	1.38	6.0
TEXANOL2	1-Hydroxy-2,2,4- Trimethylpentyl-3- Isobutyrate	12	216.3	2.6e-11	1.3e-11	*			0.99	B	28	6.09	3	0.92	6.6
TEXANOL1	3-Hydroxy-2,2,4- Trimethylpentyl-1- Isobutyrate	12	216.3	3.2e-11	1.6e-11	*			1.00	B	29	6.49	3	0.88	7.4
ETOX	Ethylene Oxide	2	44.1	7.6e-14	7.6e-14				0.01	A	12	0.18	3	0.05	4.1

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
PROX	Propylene Oxide	3	58.1	5.2e-13	5.2e-13				0.09	A	12	0.94	3	0.32	2.9
12BUOX	1,2-Epoxybutane	4	72.1	1.9e-12	1.9e-12				0.30	A	13	2.56	3	1.02	2.5
FORMACID	Formic Acid	1	46.0	4.5e-13	4.5e-13				0.08	A	7	0.58	3	0.08	7.6
ACETACID	Acetic Acid	2	60.1	8.0e-13	8.0e-13				0.14	A	13	1.37	3	0.71	1.9
ACYRACID	Acrylic Acid	3	72.1	3.7e-11	2.8e-11	1.0e-17	* 2.8e-18	*	1.00	NP	21	13.97	5	11.66	1.2
PROPACID	Propionic Acid	3	74.1	1.2e-12	1.2e-12				0.19	A	13	1.58	3	1.16	1.4
ME-ACRYL	Methyl Acrylate	4	86.1	6.6e-11	2.8e-11	* 1.0e-17	* 2.8e-18	*	1.00	NP	28	15.61	5	12.24	1.3
VIN-ACET	Vinyl Acetate	4	86.1	7.2e-11	3.2e-11	* 1.0e-17	* 1.4e-14	*	1.00	NP	28	15.61	5	3.26	4.8
MBUTENOL	2-Methyl-2-Butene-3-ol	4	86.1	6.7e-11	6.3e-11	9.3e-18	1.2e-14		1.00	NP	28	15.60	3	4.12	3.8
ET-ACRYL	Ethyl Acrylate	5	100.1	6.6e-11	2.8e-11	* 1.0e-17	* 2.8e-18	*	1.00	NP	35	16.78	5	8.78	1.9
ME-MACRT	Methyl Methacrylate	5	100.1	6.2e-11	5.2e-11	1.2e-17	* 6.6e-17	*	1.00	NP	35	16.78	5	15.84	1.1
BU-MACRT	Butyl Methacrylate	8	142.2	6.2e-11	5.2e-11	1.2e-17	* 6.6e-17	*	1.00	NP	35	11.81	5	9.09	1.3
IBUMACRT	Isobutyl Methacrylate	8	142.2	6.2e-11	5.2e-11	1.2e-17	* 6.6e-17	*	1.00	NP	35	11.81	5	8.99	1.3
FORMALD	Formaldehyde	1	30.0	2.5e-11	9.2e-12			1.2e-4	0.99	P	10	15.81	2	8.97	1.8
ACETALD	Acetaldehyde	2	44.1	2.1e-11	1.6e-11		2.8e-15	4.3e-5	0.98	P	20	21.36	1	6.84	3.1
PROPALD	Propionaldehyde	3	58.1	2.8e-11	2.0e-11		3.8e-15	* 5.8e-5	0.99	P	30	24.64	2	7.89	3.1
2MEC3AL	2-Methylpropanal	4	72.1	3.4e-11	2.6e-11		3.8e-15	* 5.8e-5	1.00	P	40	26.57	3	5.87	4.5
1C4RCHO	Butanal	4	72.1	3.1e-11	2.3e-11		3.8e-15	* 5.8e-5	1.00	P	40	26.53	3	6.74	3.9
22DMC3AL	2,2-Dimethylpropanal (pivaldehyde)	5	86.1	3.4e-11	2.6e-11		3.8e-15	* 5.8e-5	1.00	P	40	22.25	3	5.40	4.1
3MC4RCHO	3-Methylbutanal (Isovaleraldehyde)	5	86.1	3.5e-11	2.7e-11		3.8e-15	* 5.8e-5	1.00	P	40	22.26	3	5.52	4.0
1C5RCHO	Pentanal (Valeraldehyde)	5	86.1	3.6e-11	2.8e-11		3.8e-15	* 5.8e-5	1.00	P	40	22.26	3	5.76	3.9
GLTRALD	Glutaraldehyde	5	100.1	9.1e-11	4.2e-11	*	7.6e-15	* 5.8e-5	1.00	P	40	19.18	3	4.79	4.0
1C6RCHO	Hexanal	6	100.2	5.6e-11	2.4e-11	*	3.8e-15	* 5.8e-5	1.00	P	40	19.17	3	4.98	3.8
1C7RCHO	Heptanal	7	114.2	5.9e-11	2.6e-11	*	3.8e-15	* 5.8e-5	1.00	P	40	16.81	3	4.23	4.0
1C8RCHO	Octanal	8	128.2	6.2e-11	2.7e-11	*	3.8e-15	* 5.8e-5	1.00	P	40	14.97	3	3.65	4.1
GLYOXAL	Glyoxal	2	58.0	4.0e-10	1.1e-11			3.0e-3	1.00	P	20	16.54	3	14.22	1.2
MEGLYOX	Methyl Glyoxal	3	72.1	1.8e-10	1.5e-11			1.3e-3	1.00	P	30	19.98	3	16.21	1.2

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
ACROLEIN	Acrolein	3	56.1	9.2e-11	2.0e-11	3.1e-19	9.7e-17 *	5.5e-4	1.00	P	30	25.69	3	7.60	3.4
CROTALD	Crotonaldehyde	4	70.1	1.1e-10	3.6e-11	9.0e-19	5.1e-15	5.5e-4	1.00	P	40	27.39	3	10.07	2.7
METHACRO	Methacrolein	4	70.1	1.1e-10	3.3e-11	1.2e-18	4.8e-15	5.5e-4	1.00	P	40	27.39	1	6.23	4.4
HOMACR	Hydroxy Methacrolein	4	86.1	1.2e-10	4.3e-11	1.2e-18	4.8e-15	5.5e-4	1.00	P	40	22.30	3	6.61	3.4
BENZALD	Benzaldehyde	7	106.1	1.5e-10	1.3e-11			1.0e-3	1.00	P	40	18.09	2	-0.61	-29.7
ACETONE	Acetone	3	58.1	2.2e-12	2.2e-13			1.5e-5	0.33	P	30	8.28	1	0.43	19.4
CC4-KET	Cyclobutanone	4	70.1	2.9e-12	8.7e-13			1.6e-5	0.42	P	40	11.39	4	0.68	16.7
MEK	Methyl Ethyl Ketone	4	72.1	3.3e-12	1.2e-12			1.6e-5	0.45	P	40	11.97	1	1.49	8.0
CC5-KET	Cyclopentanone	5	84.1	5.0e-12	2.9e-12			1.6e-5	0.60	P	40	13.70	4	1.43	9.6
MPK	2-Pentanone	5	86.1	6.6e-12	4.6e-12			1.6e-5	0.70	P	40	15.68	2	3.07	5.1
DEK	3-Pentanone	5	86.1	4.1e-12	2.0e-12			1.6e-5	0.53	P	40	11.71	3	1.45	8.1
CC6-KET	Cyclohexanone	6	98.2	8.4e-12	6.4e-12			1.6e-5	0.79	P	40	15.41	3	1.61	9.6
MIBK	4-Methyl-2-Pentanone	6	100.2	1.6e-11	1.4e-11			1.6e-5	0.95	P	40	18.18	2	4.31	4.2
MNBK	Methyl n-Butyl Ketone	6	100.2	1.1e-11	9.1e-12			1.6e-5	0.87	P	40	16.70	3	3.55	4.7
MTBK	Methyl t-Butyl Ketone	6	100.2	3.3e-12	1.2e-12			1.6e-5	0.45	P	40	8.65	3	0.78	11.0
C7-KET-2	2-Heptanone	7	114.2	1.4e-11	1.2e-11			1.6e-5	0.92	P	40	15.47	2	2.80	5.5
2M-3-HXO	2-Methyl-3-Hexanone	7	114.2	1.6e-11	7.2e-12 *			1.6e-5	0.95	P	40	16.00	3	1.79	9.0
DIPK	Di-Isopropyl Ketone	7	114.2	7.4e-12	5.4e-12			1.6e-5	0.74	P	40	12.52	3	1.63	7.7
C8-KET-2	2-Octanone	8	128.2	1.3e-11	1.1e-11			1.6e-5	0.91	P	40	13.61	3	1.66	8.2
C9-KET-2	2-Nonanone	9	142.2	1.4e-11	1.2e-11			1.6e-5	0.93	P	40	12.51	3	1.30	9.6
DIBK	Di-isobutyl ketone (2,6-dimethyl-4-heptanone)	9	142.2	3.0e-11	2.8e-11			1.6e-5	1.00	P	40	13.44	3	2.94	4.6
C10-K-2	2-Decanone	10	156.3	1.5e-11	1.3e-11			1.6e-5	0.94	P	40	11.54	3	1.06	10.9
BIACETYL	Biacetyl	4	86.1	2.8e-10				2.2e-3	1.00	P	40	22.30	3	20.73	1.1
MVK	Methylvinyl ketone	4	70.1	9.3e-11	1.9e-11	4.7e-18		5.5e-4	1.00	P	40	27.39	1	8.73	3.1
HOACET	Hydroxy Acetone	3	74.1	5.1e-12	3.0e-12			1.6e-5	0.61	P	30	11.78	3	3.08	3.8
MEOACET	Methoxy Acetone	4	88.1	8.8e-12	6.8e-12			1.6e-5	0.80	P	40	17.48	3	2.14	8.2
DIACETALC	Diacetone Alcohol	6	116.2	5.0e-12	1.5e-12 *			1.6e-5	0.60	P	40	9.97	3	0.68	14.6
PHENOL	Phenol	6	94.1	2.6e-11	2.6e-11				0.99	NP	35	17.71	4	1.82	9.7

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
O-CRESOL	o-Cresol	7	108.1	4.2e-11	4.2e-11				1.00	NP	35	15.53	3	2.34	6.6
NO2-BENZ	Nitrobenzene	6	123.1	1.5e-13	1.5e-13				0.03	NP	35	0.37	6	0.07	5.5
P-TI	Para Toluene Isocyanate	7	134.2	5.9e-12	5.9e-12				0.66	NP	35	8.29	2	0.93	8.9
TDI	Toluene Diisocyanate	9	174.2	7.4e-12	7.4e-12				0.74	NP	35	7.17	2	-0.13	-54.3
MDI	Methylene Diphenylene Diisocyanate	15	250.3	1.2e-11	1.2e-11				0.89	NP	35	5.94	3	0.79	7.5
DM-AMINE	Dimethyl Amine	2	45.1	6.6e-11	6.6e-11				1.00	NP	14	14.91	6	9.37	1.6
ET-AMINE	Ethyl Amine	2	45.1	2.8e-11	2.8e-11				0.99	NP	14	14.81	6	7.80	1.9
TM-AMINE	Trimethyl Amine	3	59.1	6.1e-11	6.1e-11				1.00	NP	21	17.05	6	7.06	2.4
ETOH-NH2	Ethanolamine	2	61.1	3.2e-11	3.2e-11				1.00	NP	14	10.97	6	5.97	1.8
DMAE	Dimethylaminoethanol	4	89.1	9.0e-11	9.0e-11				1.00	A	25	13.33	6	4.76	2.8
ETOH2-NH	Diethanol Amine	4	105.1	9.4e-11	9.4e-11				1.00	NP	28	12.78	6	4.05	3.2
ETOH3-N	Triethanolamine	6	149.2	1.2e-10	1.2e-10				1.00	NP	35	11.26	6	2.76	4.1
NMP	N-Methyl-2-Pyrrolidone	5	99.1	2.2e-11	2.2e-11		1.3e-13		0.98	NP	35	16.65	2	2.56	6.5
CH3-CL	Methyl Chloride	1	50.5	4.5e-14	4.5e-14				0.01	NP	7	0.05	6	0.03	1.6
CL-ETHE	Vinyl Chloride	2	62.5	6.9e-12	6.9e-12				0.72	NP	14	7.72	6	2.92	2.6
C2-CL	Ethyl Chloride	2	64.5	4.2e-13	4.2e-13				0.07	NP	14	0.77	6	0.25	3.1
CL2-ME	Dichloromethane	1	84.9	1.5e-13	1.5e-13				0.03	NP	7	0.10	6	0.07	1.6
ME-BR	Methyl Bromide	1	95.0	4.1e-14	4.1e-14				0.01	NP	7	0.03	6	0.02	1.6
11CL2-C2	1,1-Dichloroethane	2	99.0	2.6e-13	2.6e-13				0.05	NP	14	0.32	6	0.10	3.1
12CL2-C2	1,2-Dichloroethane	2	99.0	2.5e-13	2.5e-13				0.05	NP	14	0.31	6	0.10	3.1
C2-BR	Ethyl Bromide	2	109.0	3.1e-13	3.1e-13				0.06	NP	14	0.34	6	0.11	3.1
CHCL3	Chloroform	1	119.4	1.1e-13	1.1e-13				0.02	NP	7	0.05	6	0.03	1.6
C3-BR	n-Propyl Bromide	3	123.0	1.2e-12	1.2e-12				0.19	NP	21	1.60	6	0.35	4.6
111-TCE	1,1,1-Trichloroethane	2	133.4	1.2e-14	1.2e-14				0.00	NP	14	0.01	6	0.00	3.2
112CL3C2	1,1,2-Trichloroethane	2	133.4	2.0e-13	2.0e-13				0.04	NP	14	0.18	6	0.06	3.1
C4-BR	n-Butyl Bromide	4	137.0	2.5e-12	2.5e-12				0.36	NP	28	3.57	6	0.60	5.9
11BR2-C2	1,2-Dibromoethane	2	187.9	2.3e-13	2.3e-13				0.04	NP	14	0.15	6	0.05	3.1
T-12-DCE	Trans-1,2-Dichloroethene	2	97.0	2.3e-12	2.3e-12				0.35	NP	14	2.41	6	0.81	3.0

Table D-2 (continued)

Name	Description	Cs	MWt	Effective kOH (cm ³ molec ⁻¹ s ⁻¹)	kOH	kO3	kNO3	kPhot Max (s ⁻¹)	Upper Limit Est. (U.L.)				Direct Calc		U.L. / Direct
									KR	MR Tp.	MR Max	MIR (g/g)	Unc	MIR (g/g)	
CL2IBUTE	2-(Cl-methyl)-3-Cl-Propene	4	125.0	3.2e-11	3.2e-11	3.9e-19	1.0e-15		1.00	NP	28	10.72	6	1.13	9.5
CL3-ETHE	Trichloroethylene	2	131.4	2.3e-12	2.3e-12				0.35	NP	14	1.78	6	0.60	3.0
CL4-ETHE	Perchloroethylene	2	165.9	1.7e-13	1.7e-13				0.03	NP	14	0.13	6	0.04	3.2
CL-BEN	Monochlorobenzene	6	112.6	7.7e-13	7.7e-13				0.13	NP	35	1.97	6	0.36	5.4
CF3-BEN	Benzotrifluoride	7	146.1	4.6e-13	4.6e-13				0.08	NP	35	0.93	6	0.26	3.5
CL2-BEN	p-Dichlorobenzene	6	147.0	5.6e-13	5.6e-13				0.10	NP	35	1.11	6	0.20	5.5
PCBTF	p-Trifluoromethyl-Cl-Benzene	7	180.6	2.4e-13	2.4e-13				0.04	NP	35	0.40	6	0.11	3.5