

## Appendix C

“Updated Maximum Incremental Reactivity Scale and Hydrocarbon Bin  
Reactivities for Regulatory Applications,”  
Final Report to California Air Resources Board  
September 10, 2009

# Updated Maximum Incremental Reactivity Scale and Hydrocarbon Bin Reactivities for Regulatory Applications

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## **SUMMARY**

The table of maximum incremental reactivity (MIR) values for quantifying relative ground-level ozone impacts of volatile organic compounds (VOCs), and its associated uncertainty classifications, have been updated. The updates incorporate an update of the chemical mechanism used to calculate the ozone impacts from SAPRC-99 to the newly developed SAPRC-07 mechanism, and the addition of a number of VOCs and mixtures to the MIR tabulation. The revised MIR scale and uncertainty classifications are presented in this report, and their derivation and changes relative to the previous MIR tabulation are briefly summarized. A more complete discussion of the derivation of the scale and the underlying chemical mechanism is given in the recently updated SAPRC-07 mechanism documentation report (Carter, 2009a), which is incorporated by reference into this report.

As part of this update, the method used to derive MIR values for complex hydrocarbon solvents using the "bin" method as defined by Kwok et al. (2000) for the CARB's aerosol coatings regulations (CARB, 2000) was revised. Instead of assigning bin reactivities based on correlations between boiling points and MIR values as done previously, we derive a chemical composition for each hydrocarbon bin, and then use this, and the MIR's for the constituents, to calculate the MIR for each bin. The two methods are compared with each other and with explicitly calculated MIRs for representative solvents for which analytical data are available. It is concluded that the revised method gives better estimates of MIR values for the solvents for which data are available.

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# MAXIMUM INCREMENTAL REACTIVITY SCALE UPDATE

## Introduction

In recent years, the California Air Resources Board (CARB) has adopted regulations of volatile organic compounds (VOCs) based on calculations of their relative ground-level ozone impacts (e.g., CARB, 2000, 2003). For the purposes of these regulations, these impacts are quantified using the Maximum Incremental Reactivity (MIR) scale. This scale was developed by Carter (1994a) and is based on model calculations of effects of additions of the VOCs on ozone formation in one-day box model scenarios representing conditions where ambient ozone is most sensitive to changes in VOC emissions. These calculations require a model or models for airshed conditions, a method for quantifying ozone impacts, and a chemical mechanism to calculate the effects of the VOCs' reactions on ozone formation in the atmosphere. The original MIR scale of Carter (1994a) was calculated using the SAPRC-90 chemical mechanism (Carter, 1990), but it has since been updated to SAPRC-99 (Carter, 2000) and most recently SAPRC-07 (Carter, 2009a). However, the version of the MIR scale used in current CARB reactivity-based regulations (CARB, 2003) was calculated using the SAPRC-99 mechanism, so the current regulatory scale does not reflect the latest version of the chemical mechanism. This report gives the update of the MIR scale to the current version of the chemical mechanism, which is SAPRC-07.

## Methods of Procedure

The methods and procedure used to derive the MIR scale presented in this report are comprehensively documented by Carter (2009a) and references therein, and those reports should be consulted for details. Briefly, the reactivity scale is based on calculations of relative ozone impacts, expressed as mass of additional ozone formed per mass of VOC added to the emissions, for various compounds under various atmospheric conditions, given a chemical mechanism for the compounds and other relevant atmospheric species, models for various atmospheric conditions, and a modeling and reactivity assessment procedure. The methods, atmospheric scenarios, and modeling and reactivity assessment procedures were the same as employed in previous calculations of the MIR scale (Carter, 1994a, 2000, 2003), including the MIR scale currently used in CARB regulations (CARB, 2003), and are based on those first developed by Carter (1994a,b), with a few modifications as described by Carter (2000). The only difference between this updated scale and the previous MIR scales of Carter (2000) and used in the CARB regulations (CARB, 2003) concerns the chemical mechanism used and the number and types of VOCs whose ozone impacts are calculated.

As indicated above, the previous MIR scales used in the current CARB regulations (CARB, 2003) were calculated using the SAPRC-99 chemical mechanism, which is documented by Carter (2000). Since then, this has undergone a comprehensive update to the SAPRC-07 mechanism, which is documented by Carter (2009a). This mechanism incorporates a complete update of the base mechanism used to represent the reactions of the inorganics and the common organic products, and of the mechanisms for the many classes of emitted VOCs that are represented. This new mechanism has been comprehensively evaluated against available environmental chamber data, including results of many experiments carried out since SAPRC-99 was developed. The results of the evaluation are included in the documentation report of Carter (2009a). In general the model performance is comparable to that of SAPRC-99 except that a larger number of compounds are evaluated.

Additional types of VOCs have also been added to the mechanism as a result of requests from the CARB, industry groups and others, and as a result of analyses of emissions speciation data. The current

updated MIR tabulation includes reactivity estimates for a total of 1061 types of compounds or simple mixtures, of which 760 are represented using mechanisms explicitly derived for the compound, with the MIRs of the remainder being estimated based on ozone impacts derived for other compounds. In addition, ozone impacts for a total of 55 mixtures are included in the tabulation, based on assumed compositions in terms of compounds whose mechanisms have been derived. Note that MIRs for other mixtures can be derived as linear summations of those for its components, so it is not necessary to tabulate MIR values for all possible mixtures that may be of interest.

Among the mixtures added to the current MIR tabulation are the 24 hydrocarbon "bins" used in the current CARB aerosol coatings regulation (CARB, 2000, Kwok et al, 2000). These "bins" represent various types of complex hydrocarbon mixtures, defined by composition type and boiling point range, for which MIR estimates are needed for regulatory applications. For this purpose, Kwok et al (2000) derived MIR estimates for these bins based on correlations between boiling points for various types of compounds and their SAPRC-99 MIR values. To avoid the need to re-do this analysis for each reactivity scale update, we derived an alternative method to derive the MIR values for the bin, based on deriving compositions for each of these bins in terms of individual compounds for which MIR values are available. The changes to the hydrocarbon bin calculation methodology, and their effects on the hydrocarbon bin MIR calculations, are discussed separately in the "Hydrocarbon Bin MIR Calculation" section of this report.

Because of its proposed use in regulatory applications, the CARB funded a peer review of the SAPRC-07 mechanism as originally documented by Carter (2008a). This resulted in the peer reviews of Derwent et al. (2008), Azzi et al. (2008), Harley (2009) and Stockwell (2009). These reviews have been considered, and responses to each have been prepared (Carter, 2009b). Although in general these reviews were favorable, some problems were noted, and these are discussed in our response (Carter, 2009b). In most cases we concluded that although the comments have merit, changes to the mechanism are not indicated at this time. However, the review of Stockwell (2009) revealed an error in the base mechanism, and we independently found errors concerning organic hydroperoxide species that needed to be corrected. The SAPRC-07 mechanism was therefore revised, its evaluation and documentation updated, and its reactivity scales were recalculated (Carter, 2009a). The revisions to the mechanism are discussed by Carter (2009b) and summarized in a new Appendix E of the mechanism documentation report (Carter, 2009a). The MIR tabulation given in this report reflects these revisions. However, the changes affect only reactions that become non-negligible under low NO<sub>x</sub> conditions that are not important in MIR calculations, and because of this none of the current MIR values differ from the values previously tabulated by Carter (2008a) by more than 4%.

## **Results and Discussion**

The updated table of MIR values for all the types of VOCs that are currently represented is given in Table A-1 in Appendix A to this report. Footnotes to the table give various uncertainty classifications for the various types of VOCs, based on considerations noted in the footnotes. For comparison, Table A-1 also gives MIR values that are incorporated in current CARB regulations (CARB, 2003), or derived for the hydrocarbon bins by Kwok et al (2000), and shows the percentage change in the MIR resulting from the update. If there is no value given in the "old" column of Table A-1, then the compound or mixture is new to this tabulation.

The uncertainty and bias estimates shown on Table A-1 are intended to serve as a qualitative indication of the level of uncertainty of the MIR values and other factors that may be useful to consider when using these values for regulatory applications. However, it is important to recognize that the uncertainty and bias estimates are entirely subjective, and not based on any comprehensive sensitivity and uncertainty analysis. This also does not take into the account that reactivities of some VOCs may be sensitive to environmental conditions or changes in the base mechanism, and may change if the base

mechanism or scenarios are updated even if the mechanism for the VOC itself is unchanged. An analysis of such would clearly be useful, but was beyond the scope of the mechanism update projects.

Plots of the new MIR values against those in the current CARB (2003) regulation are shown in Figure 1. The 1:1 and  $\pm 30\%$  lines are also shown. The average change (excluding the 16 outliers where the change was greater than 60%) in the MIR's was -14%, and the average absolute magnitude of the change (again excluding the outliers) was 16%. The MIR for the base ROG mixture, which is used as the standard for relative reactivity scales, decreased by about 5%. If this is taken into account, the average change in relative MIR values would be approximately -7%, excluding the outliers. Table 1 summarizes the numbers and fractions of compounds whose MIR values changed by more than various amounts, and includes a distribution plot of the relative changes. Figure 1 also gives the average MIR changes for various chemical types of VOCs.

The reason that MIRs for most compounds were lower has not been fully assessed. For some compounds this may be due in part for the lower reactivity calculated for the PROD2 model species used to represent the higher ketone products for many compounds such as higher alkanes, because of its assumed lower photolysis rate. However changes in the base mechanism may also be contributing to this general reduction in MIR values. The average maximum O<sub>3</sub> concentration in the MIR scenarios was about ~5% lower in the SAPRC-07 mechanism than SAPRC-07, and this is consistent with the ~5% lower MIR of the base ROG mixture (Carter, 2009a). Sensitivity calculations or more analyses are needed to assess the reasons for this change in more detail.

The compounds whose incremental reactivities in the MIR scale changed by more than 30% are listed in Table 2. The table also indicates the probable reasons for the changes for those with the greatest changes. Excluding the compounds where the CARB (2003) regulation used upper limit MIR values and

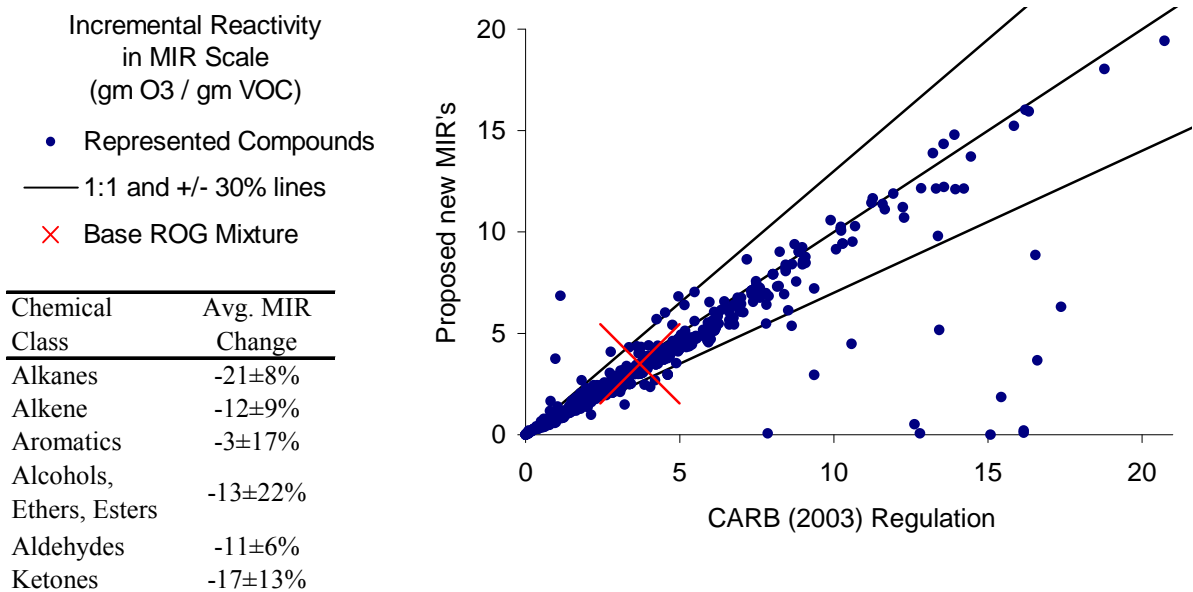
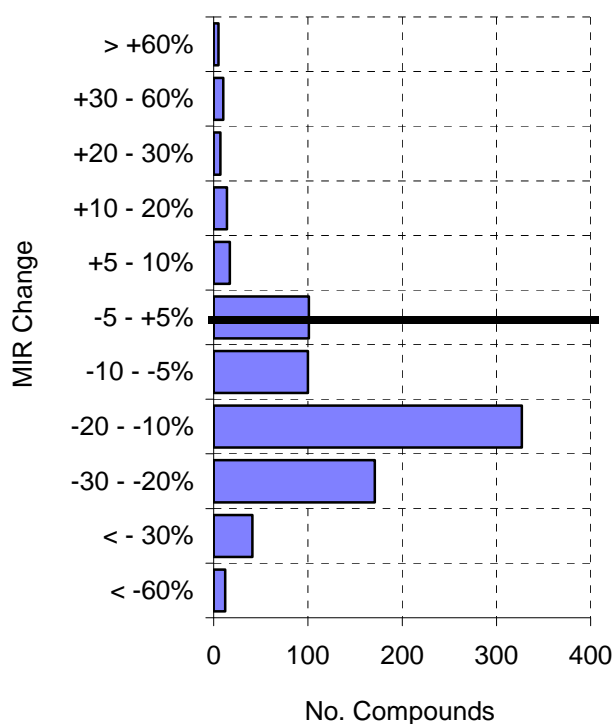


Figure 1. Plots of incremental reactivities in the MIR scale computed using the updated mechanism against those used in the current CARB (2003) regulation. Negative MIR values are shown as zero on the plot. Average MIR changes for different chemical classes are also shown. (The erroneous SAPRC-99 value for 3-methoxy-1-butanol excluded from the averages for the alcohols, ethers, and esters.)

Table 1. Summary of numbers of compounds and mixtures whose MIR values changed by various amounts.

MIR Change	Compounds or mixtures [a]	Fraction [b]
< -60%	12	1.5%
< -30%	41	5%
-30 - -20%	171	21%
-20 - -10%	327	41%
-10 - -5%	100	12%
-5 - +5%	101	13%
+5 - 10%	17	2%
+10 - 20%	14	2%
+20 - 30%	7	1%
+30 - 60%	10	1%
> +60%	5	1%
Abs Chg < 30%	737	92%
New MIRs	380	33%



[a] Based on the CARB (2003) and SAPRC-07 MIR values listed in Table A-1.

[b] Fractions for changes are relative to number of MIRs in the SAPRC-99 tabulation. Fractions for new MIRs are relative to the number in the updated tabulation.

3-methoxy-1-butanol, where the SAPRC-99 mechanism had a factor of 10 error in the OH rate constant, the greatest changes were for amines, for which new mechanisms were derived based on new chamber data by Carter (2008b), and for halogenated compounds because of the higher estimated photolysis rates for the chloroaldehyde and chloroketone products predicted to be formed. It is interesting to note that except for the compound where upper limit MIRs were used or with the erroneous mechanism that was corrected, all the changes are less than about 110%. This suggests the probable upper limit for changes that might occur in future updates for compounds with very uncertain mechanisms for which mechanistic estimates have been made.

### Revised Upper Limit MIR Estimates for VOCs with Unknown Mechanisms

The current CARB regulatory MIR scale (CARB, 2003) includes a number of VOCs for which mechanisms have not been derived and where upper limit MIR (ULMIR) estimates are used. Mechanisms for many of these have now been derived for SAPRC-07, allowing actual best estimate MIR values to be used in place of ULMIR estimates (see Footnote 1 to Table 2). However, there remain six VOCs on the CARB (2003) regulatory for which no mechanism or MIR estimate has yet been derived, and for which ULMIR values still need to be used. These are listed on Table 3.

Since the mechanism used to derive the regulatory MIR values has been updated, it is also appropriate to update the corresponding ULMIR estimates. The current ULMIR estimates are based on a procedure developed by Carter (2000), based on considerations of the type of compound being



Table 2. List of compounds and mixtures whose reactivities in the MIR scale changed by more than 30%.

Compound	MIR (gm O <sub>3</sub> / gm VOC)			Probable Reasons
	Old	New	Change	
2-Amino-2-methyl-1-propanol	15.08	-2.57		1, 2
2-(chloromethyl)-3-chloropropene	1.13	6.85	506%	3, 4
3-Methoxy-1-butanol	0.97	3.75	287%	5
1,2-Dichloroethane	0.10	0.21	107%	4
trans-1,2-Dichloroethene	0.81	1.65	103%	4
nitroethane	12.79	0.06	-100%	1
2-nitropropane	16.16	0.10	-99%	1
nitromethane	7.86	0.06	-99%	1
1-nitropropane	16.16	0.20	-99%	1
peroxyacetic acid	12.62	0.52	-96%	1
1,2-Dibromoethane	0.05	0.10	96%	6
methyl ethyl ketoxime	22.04	1.52	-93%	1
morpholine	15.43	1.85	-88%	1
triethyl amine	16.60	3.66	-78%	1, 2
Dimethyl amine	9.37	2.95	-69%	2
Mesityl oxide (2-methyl-2-penten-4-one)	17.37	6.31	-64%	7
1-amino-2-propanol	13.42	5.17	-61%	1, 2
3,5,5-trimethyl-2-cyclohexenone	10.58	4.48	-58%	7
Indene	3.21	1.48	-54%	
Unspeciated C9 Alkanes	2.13	0.99	-54%	
Propionic acid	0.79	1.17	49%	
Triethanolamine	2.76	4.08	48%	2
Phenol	1.82	2.69	48%	8
Furan	16.54	8.86	-46%	9
Dichloromethane	0.07	0.04	-45%	
CARB Hydrocarbon Bin 5	2.56	1.47	-43%	10
Diethanol amine	4.05	2.36	-42%	2
CARB Hydrocarbon Bin 20	1.49	0.89	-41%	10
CARB Hydrocarbon Bin 3	2.52	1.53	-39%	10
1,3-diethyl-5-pentyl cyclohexane	0.99	0.61	-39%	
1,2-Propylene glycol diacetate	0.94	0.58	-39%	
CARB Hydrocarbon Bin 4	2.24	1.37	-39%	10
isobornyl methacrylate	8.64	5.37	-38%	1
methane	0.01	0.01	38%	
Unspeciated C11 aromatics	4.96	6.82	38%	11
1,1,2-Trichloroethane	0.06	0.08	37%	4
2-Methyl 3,5-diisopropyl heptane	0.78	0.49	-37%	
CARB Hydrocarbon Bin 1	2.08	1.33	-36%	10
6-Methyl tridecane	0.62	0.40	-36%	
C13 monosubstituted naphthalene	3.86	2.47	-36%	
C12 monosubstituted naphthalene	4.20	2.69	-36%	
6-Methyl tetradecane	0.57	0.37	-36%	
Methyl naphthalenes	4.61	2.96	-36%	
1-methyl naphthalene	4.61	2.96	-36%	
2-methyl naphthalene	4.61	2.96	-36%	

Table 2 (continued)

Compound	MIR (gm O <sub>3</sub> / gm VOC)			Probable Reasons
	Old	New	Change	
5-Methyl dodecane	0.64	0.41	-36%	
1,1-Dichloroethane	0.10	0.07	-35%	
4,5-Dimethylheptyl acetate	0.96	0.63	-35%	
2-Methyl-2,4-pentanediol	1.04	1.39	34%	
p-Xylene	4.25	5.69	34%	
Chloroform	0.03	0.02	-33%	
Unspeciated C12 Aromatics	4.53	6.02	33%	11
1-Octanol	2.01	1.35	-33%	
2,7-Dimethyl 3,5-diisopropyl heptane	0.69	0.47	-33%	
5-methyl undecane	0.72	0.49	-32%	
Acetic acid	0.50	0.66	32%	
4,7,9-Trimethyldecyl acetate	0.55	0.37	-32%	
CARB Hydrocarbon Bin 12	0.81	0.55	-32%	10
5-Methylhexyl acetate	0.79	0.54	-32%	
4-Octanol	3.07	2.10	-32%	
3-Isopropylheptyl acetate	0.71	0.49	-31%	
2,3,6-Trimethyl 4-isopropyl heptane	1.24	0.85	-31%	
CARB Hydrocarbon Bin 19	0.88	0.61	-31%	10
3,4-diethyl hexane	1.20	0.83	-31%	
CARB Hydrocarbon Bin 11	0.91	0.63	-31%	10
3,4-Dimethylhexyl acetate	1.16	0.81	-30%	
2,2,3,3-Tetramethyl butane	0.44	0.31	-30%	

## Discussion of probable reasons for MIR changes:

- 1 The CARB (2003) list had an upper limit MIR. A best estimate MIR value is now available, and this should replace the upper limit value. In some cases the change was very large.
- 2 New amine mechanisms were developed. Note that amines without hydrogens on groups adjacent to amino groups are now estimated to be inhibitors.
- 3 The CARB (2003) value disagrees with the latest SAPRC-99 MIR value, which is 3.13.
- 4 Chlorinated aldehyde and ketone products are now assumed to be much more photoreactive.
- 5 The OH radical rate constant used in SAPRC-99 was found to be low by a factor of 10.
- 6 The approximate method used to represent bromine-containing compounds was changed. SAPRC-07 represents them using the mechanism for the corresponding Cl-containing compound.
- 7 The estimated mechanisms used in SAPRC-99 for these compounds is considered to be unreliable. They are now represented by the model species used to represent the lumped C5 isoprene products.
- 8 Phenol is lumped with Cresols in SAPRC-07 but was represented explicitly in SAPRC-99. However, the change in MIR is well within the relatively large uncertainty of the mechanism.
- 9 Furan is now represented explicitly. Previously it was represented using the lumped molecule method.
- 10 See the "Hydrocarbon Bin MIR Calculation" section for a discussion of the MIR calculations for the CARB hydrocarbon bin categories. The "old" values are those derived by Kwok et al (2000) based on correlations between boiling points and SAPRC-99 MIRs for various types of hydrocarbons. The "new" values are calculated using SAPRC-07 and the chemical compositions derived for each bin. The changes in MIR values reflect both a change in mechanism and a change in methodology.
- 11 The compounds assigned to this mixture were changed and more classes of higher aromatics were added to take into account isomeric differences.

considered, its atmospheric reaction rates (if known), and the SAPRC-99 MIRs for the most reactive compounds of the various types. However, this is probably a more complex procedure than is needed for this application, especially since there are no atmospheric reaction rate data for most compounds where ULMIR estimates are needed. Therefore, as part of this update we have derived a revised ULMIR estimation procedure that depends primarily on the molecular weight of the compound.

Figure 2 shows a plot of the SAPRC-07 MIRs of all the compounds that have positive MIR values against their molecular weight. It can be seen that while the MIRs vary widely depending on the compound, the highest values tend to have a fairly good correlation with molecular weight, at least for molecular weights greater than about 80. The line shows a reasonable upper limit curve based on these data. It was derived by fitting the MIRs for compound with the highest MIRs in various molecular weight ranges, and adding a 5% margin to prevent underestimation of MIRs for any of those compounds. Since there is no clear relationship between molecular weight and MIR for compounds with lower molecular weight than 86.09 (that of biacetyl), the ULMIR is assumed to be constant for lower molecular weights than that. The ULMIR estimate derived in this way is given by

$$\text{ULMIR} = \text{Min} \{19.63, 1.05 \times [ (859.61 / \text{Mwt}) + (255.80 / \text{Mwt})^2 ]\} \quad (\text{I})$$

where Mwt is the molecular weight of the compound and ULMIR is in units of grams O<sub>3</sub> per gram VOC. Equation (I) is the new recommendation for deriving ULMIRs for compounds for which kinetic and mechanistic data are not available.

If atmospheric reaction rate data are available but no other mechanistic estimates, then the recommended ULMIR value is

$$\text{ULMIR} = \text{Kinetic Reactivity} \times \text{ULMIR (Equation I)} \quad (\text{II})$$

where the “Kinetic Reactivity” is the estimated fraction of the compound that reacts in the atmosphere in 1 day, which is derived as discussed in the upper limit estimation method given by Carter (2000). This would be appropriate to use to derive ULMIR estimates for compounds known to react relatively slowly but whose mechanisms are not otherwise known. The kinetic reactivity approaches 100% for compounds that react sufficiently rapidly, and thus Equation (I) is appropriate for rapidly reacting compounds, as well as for compounds whose atmospheric reaction rates are unknown.

Table 3 includes the revised ULMIR estimates for the compounds in the current CARB (2003) regulation for which mechanisms have not yet been derived. Since the reaction rates for these compounds are not known and most are expected to react relatively rapidly, the new ULMIR values were been derived using Equation (I). In general the change is small, especially considering the large uncertainty in ULMIR estimates in the first case. But it is recommended that the new values be used if these compounds are to be used in the updated regulatory MIR list, and that Equation (I) or (II) (as applicable) be used to estimate ULMIRs if new compounds without mechanistic estimates are added to the list.

## Conclusions and Recommendations

The table of MIR values has been updated to the current version of the SAPRC mechanism, which is believed to represent the current state of the science. It is recommended that the regulatory MIR values derived using the SAPRC-99 or earlier versions of the SAPRC mechanism be replaced by the values in Table A-1. This update also includes an update of the methodology to calculate MIRs for hydrocarbon bins that we recommend to be adopted; as discussed in the following section of this report. Although the change in MIR values was less than 20% for a majority of the VOCs, a similar majority of

the VOCs also had changes that were over 10%. Therefore, we recommend replacing the regulatory MIR table entirely with the new values, and not just changing those that change by more than a certain amount.

Table 3. List of VOCs on the CARB (2003) regulatory MIR list for which MIR estimates are still not available.

Compound	Mwt	ULMIR (gm O <sub>3</sub> / gm VOC)		
		New	2003	Change
N-methyl acetamide	73.09	19.6	19.7	0%
diethylenetriamine	103.17	15.1	13.0	-12%
hydroxyethylethylene urea	130.15	10.9	14.8	-26%
cumene hydroperoxide; 1-methyl-1-phenylethylhydroperoxide	152.19	8.8	12.6	-30%
dexpanthenol (pantothenylol)	205.25	6.0	9.4	-36%

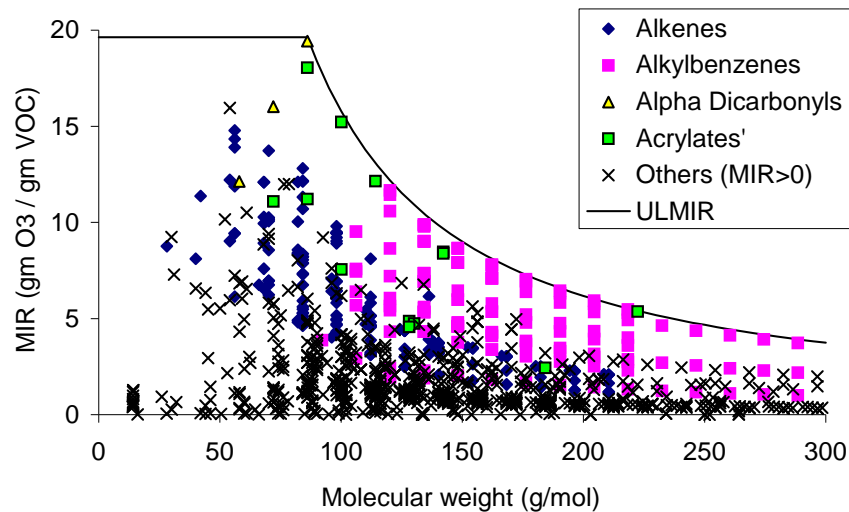


Figure 2. Plots of SAPRC-07 MIRs for all compounds with positive MIRs against molecular weight, and upper limit MIR estimates based on molecular weight.

## HYDROCARBON BIN MIR CALCULATION

### Summary

This revised method to estimate maximum incremental reactivity (MIR) values for hydrocarbon solvents using the "bin" method as defined by Kwok et al. (2000) for the CARB's aerosol coatings regulations (CARB, 2000) is described. Instead of assigning bin reactivities based on correlations between boiling points and MIR values for various types of compounds as done by Kwok et al (2000), this method derives a chemical composition for each hydrocarbon bin, and then uses this, and the MIR's for the constituents, to calculate the MIR for each bin. The two methods are compared with each other and with explicitly calculated MIRs for representative solvents for which analytical data are available. The two methods give similar results except for the four lighter hydrocarbon bins containing cycloalkanes and for some of the heavy aromatic bins. The light hydrocarbon bins with cycloalkanes changed because the previous method may be biased high because it overestimates the MIR for cyclohexane. The heavy aromatic bins changed because new compositional data suggest that these may contain more naphthalene constituents than previously estimated. The revised method is then used to update the MIRs for the bins to the newly-developed SAPRC-07 mechanism.

### Introduction

In recent years, the California Air Resources Board (CARB) has adopted regulations of volatile organic compounds (VOCs) based on calculations of their relative ground-level ozone impacts (e.g., CARB, 2000). Hydrocarbon solvents used in coatings and other applications (e.g., "mineral spirits", "naphtha", etc.) are covered by such regulations, but calculation of their ozone impacts is more difficult because they are generally complex mixtures of alkanes, and in some cases aromatics, whose exact compositions are usually unknown. Reactivity estimates for complex hydrocarbon mixtures can be made, provided sufficient compositional information is available, and the SAPRC-99 (Carter, 2000) and SAPRC-07 mechanisms (Carter, 2009) were found to usually give predictions that are reasonably consistent with environmental chamber data for most of the types of complex hydrocarbon solvents that have been studied to date. However, the type of compositional analysis required for a comprehensive reactivity evaluation requires extensive analytical information that is expensive to obtain and is not generally available for most hydrocarbon solvent products.

Because of the need to derive reactivity estimates for such materials in its aerosol coatings regulations (CARB, 2000), the CARB developed a general "Binning" procedure to estimating MIRs for hydrocarbon solvents based on their boiling point ranges, aromatic fractions, and types of alkanes primarily present (Kwok et al, 2000). The bin specifications and their corresponding SAPRC-99 MIR assignments are shown on Table 4. (The table also shows the updated bin reactivity assignments derived in this work, as discussed below.) The work of Kwok et al (2000) is an important contribution towards reducing uncertainties in reactivity estimates for these important types of VOCs. Unfortunately, the speciation data they used to derive the MIR assignments for the bins was not provided because the data used were proprietary, and the available documentation does not provide information necessary to revise the assignments should the underlying reactivity scale be modified or updated. This is a problem now because the SAPRC-99 mechanism used for the MIR scale used in the current regulations has been updated to SAPRC-07 (Carter, 2009), and the regulatory MIR scale needs to be updated.

Table 4. Definition of the CARB hydrocarbon bins and MIR values assigned by Kwok et al (2000). Updated MIR assignments and uncertainty codes are also shown.

Bin	Boiling Range [a]	Composition Range	MIR [b]		
			SAPRC-99	SAPRC-07	Unc
1	80-205	Alkanes (< 2% Aromatics)	2.08	1.33	7
2	80-205	N- & Iso-Alkanes (≥ 90% and < 2% Aromatics)	1.59	1.23	7
3	80-205	Cyclo-Alkanes (≥ 90% and < 2% Aromatics)	2.52	1.53	7
4	80-205	Alkanes (2 to < 8% Aromatics)	2.24	1.37	7
5	80-205	Alkanes (8 to 22% Aromatics)	2.56	1.47	7
6	>205-340	Alkanes (< 2% Aromatics)	1.41	1.08	7
7	>205-340	N- & Iso-Alkanes (≥ 90% and < 2% Aromatics)	1.17	0.95	7
8	>205-340	Cyclo-Alkanes (≥ 90% and < 2% Aromatics)	1.65	1.34	7
9	>205-340	Alkanes (2 to < 8% Aromatics)	1.62	1.35	7
10	>205-340	Alkanes (8 to 22% Aromatics)	2.03	1.88	7
11	>340-460	Alkanes (< 2% Aromatics)	0.91	0.63	8
12	>340-460	N- & Iso-Alkanes (≥ 90% and < 2% Aromatics)	0.81	0.55	8
13	>340-460	Cyclo-Alkanes (≥ 90% and < 2% Aromatics)	1.01	0.79	8
14	>340-460	Alkanes (2 to < 8% Aromatics)	1.21	0.91	8
15	>340-460	Alkanes (8 to 22% Aromatics)	1.82	1.48	8
16	>460-580	Alkanes (< 2% Aromatics)	0.57	0.47	8
17	>460-580	N- & Iso-Alkanes (≥ 90% and < 2% Aromatics)	0.51	0.43	8
18	>460-580	Cyclo-Alkanes (≥ 90% and < 2% Aromatics)	0.63	0.54	8
19	>460-580	Alkanes (2 to < 8% Aromatics)	0.88	0.61	8
20	>460-580	Alkanes (8 to 22% Aromatics)	1.49	0.89	10
21	280-290	Aromatic Content (≥98%)	7.37	7.44	8
22	320-350	Aromatic Content (≥98%)	7.51	7.39	8
23	355-420	Aromatic Content (≥98%)	8.07	6.66	10
24	450-535	Aromatic Content (≥98%)	5.00	3.76	11

[a] Boiling points in degrees F. Average boiling point = (Initial boiling point + dry point) / 2

[b] Maximum Incremental Reactivity values in units of grams O<sub>3</sub> per gram VOC. "SAPRC-99" gives assignments of Kwok et al (2000) used current CARB regulations. "SAPRC-07" gives values derived recommended for the updated MIR scale. "Unc" gives the uncertainty code classification that is included in the reactivity tabulation in Table A-1. The uncertainty codes used here are as follows:

7. The estimated composition of this mixture is considered to be reasonably appropriate, and the major components do not have excessively high uncertainty. This code is also used for compounds whose mechanisms have not been evaluated but for which the methods used to estimate the mechanism have been found to be generally satisfactory.
8. The estimated composition of this mixture has more uncertainty, or includes components with more uncertain mechanisms. This code is also used for compounds whose estimated mechanisms have more uncertainty, but are based on reasonable assumptions.
- 10 The composition of this mixture has significant uncertainty or its major components have highly uncertain mechanisms. This code is also used for compounds whose mechanisms are highly uncertain.
- 11 The composition of this mixture has significant uncertainty and its major components also have extremely uncertain mechanisms. This code is also used for compounds whose mechanisms are questionable.

An alternative method for deriving hydrocarbon bin reactivities that avoids this problem is to estimate, for each bin, a representative composition in terms of individual types of compounds for which reactivities have been calculated. The reactivities in the MIR (or any other) reactivity scale can then be calculated from those of their constituents, and can be readily updated whenever the reactivity scale is changed. The general procedure for deriving a composition for each bin involves deriving carbon number distributions from boiling point data, and choosing compounds to be representative for each type of chemical category used in the bin definitions for each carbon number. Thus, given the carbon number and chemical category distributions for each bin, and assuming that the chemical category distributions are the same for each carbon number, one can then derive a representative composition for each bin.

As part of a previous CARB project, Carter and Malkina (2005) carried out an analysis of the available compositional data for representatives of various types of hydrocarbon solvents, and used the results to estimate compositions associated with each of the 24 CARB hydrocarbon bins. This was then used to calculate the reactivity values for each of these bins in the SAPRC-99 scale. This analysis is updated for this work based on new data for the heavier aromatics bins, and is updated to SAPRC-07 as discussed below.

## Methods

In order to derive compositions for each bin, it is necessary to (1) make specific assignments for each bin in terms of distributions of chemical types and boiling points, (2) derive carbon number distributions from boiling point distributions, and (3) assign specific compounds for each chemical type and carbon number. The bin definitions on Table 4 are not entirely specific concerning chemical composition assignments, so it is necessary to make assumptions in this regard. The specific chemical type assumptions and boiling point assumptions made by Carter and Malkina (2005) are indicated on Table 5. The type distribution assumptions are somewhat arbitrary but are consistent with the definitions on Table 4 and are based on assuming equal amounts of the various possible alkane types for each bin. The bin assignments do not specify types of aromatics, so a generic aromatic distribution is assigned for each carbon number as discussed below. The boiling point minima and maxima are based on those given in Table 4.

In order to derive carbon number distributions from boiling point ranges, Carter and Malkina (2005) summarized available boiling point information for relevant compounds and derived functions that best fit plots of carbon numbers vs. boiling points. The following relationships were derived for the three classes of compounds specified on Table 5:

$$nC \text{ (normal and cyclic alkanes)} = 3.95 + 2.81 (Bp/100) + 0.21 (Bp/100)^2 + 0.096 (Bp/100)^3$$

$$nC \text{ (branched alkanes)} = 3.95 + 2.81 [(Bp+13)/100] + 0.21 [(Bp+13)/100]^2 + 0.096 [(Bp+13)/100]^3$$

$$\begin{aligned} nC \text{ (aromatics)} &= 3.3 + 0.03372 Bp \text{ (for } Bp \leq 144.85^\circ\text{C)} \\ &= 0.4 + 0.05337 Bp \text{ (for } Bp > 144.85^\circ\text{C)} \end{aligned}$$

where  $nC$  is the carbon number and  $Bp$  is the boiling point in degrees C. The ability of these equations to fit the available boiling point data tabulated by Carter and Malkina (2005) are shown in Figure 3. In general, these relationships perform well for the normal alkanes but as expected there is more scatter in estimation of the carbon numbers for the other classes of compounds.

Since the above equations in general would predict non-integer carbon numbers for a given boiling point, it is necessary to derive a distribution of integer carbon numbers in order to relate these to actual compounds. For estimation purposes, we treat this as a mixture of compounds with the two carbon numbers surrounding the average, with relative weights derived to correspond to the average. Thus if

Table 5. Summary of chemical type distributions, boiling point ranges, and results of MIR calculations for each of the 24 CARB hydrocarbon bins.

Bin	Type distribution				Boiling Range (°F) [a]			SAPRC-99 MIR [a]			SAPRC-07 [b]	
	n-Alk.	Iso-Alk.	Cyc-Alk	Arom.	Avg	Min	Max	Calc.	CARB	Diff	Calc.	Diff
1	33%	33%	33%	-	143	80	205	1.62	2.08	28%	1.33	-18%
2	50%	50%	-	-	143	80	205	1.51	1.59	6%	1.23	-19%
3	-	-	100%	-	143	80	205	1.86	2.52	35%	1.53	-18%
4	32%	32%	32%	5%	143	80	205	1.66	2.24	35%	1.37	-17%
5	28%	28%	28%	15%	143	80	205	1.74	2.56	47%	1.47	-15%
6	33%	33%	33%	-	273	205	340	1.33	1.41	6%	1.08	-19%
7	50%	50%	-	-	273	205	340	1.17	1.17	0%	0.95	-19%
8	-	-	100%	-	273	205	340	1.66	1.65	0%	1.34	-19%
9	32%	32%	32%	5%	273	205	340	1.59	1.62	2%	1.35	-15%
10	28%	28%	28%	15%	273	205	340	2.11	2.03	-4%	1.88	-11%
11	33%	33%	33%	-	400	340	460	0.80	0.91	14%	0.63	-21%
12	50%	50%	-	-	400	340	460	0.73	0.81	11%	0.55	-24%
13	-	-	100%	-	400	340	460	0.93	1.01	8%	0.79	-16%
14	32%	32%	32%	5%	400	340	460	1.09	1.21	11%	0.91	-16%
15	28%	28%	28%	15%	400	340	460	1.67	1.82	9%	1.48	-11%
16	33%	33%	33%	-	520	460	580	0.57	0.57	0%	0.47	-18%
17	50%	50%	-	-	520	460	580	0.53	0.51	-4%	0.43	-19%
18	-	-	100%	-	520	460	580	0.64	0.63	-2%	0.54	-15%
19	32%	32%	32%	5%	520	460	580	0.74	0.88	18%	0.61	-18%
20	28%	28%	28%	15%	520	460	580	1.09	1.49	36%	0.89	-19%
21	-	-	-	100%	285	280	290	7.62	7.37	-3%	7.44	-2%
22	-	-	-	100%	335	320	350	7.31	7.51	3%	7.39	1%
23	-	-	-	100%	388	355	420	6.88	8.07	17%	6.66	-3%
24	-	-	-	100%	493	450	535	4.56	5.00	10%	3.76	-17%

[a] MIR values for SAPRC-99 in units of grams O<sub>3</sub> / gram solvent. "Calc" = calculated for the mixture assigned for this bin as discussed in this report. "CARB" = MIR assignment of Kwok et al (2000). "Diff" = Difference in the CARB assignment of Kwok et al (2000) relative to the calculated value. MIR data from Carter (2003).

[b] MIR values for SAPRC-07 in units of grams O<sub>3</sub> / gram solvent. "Calc" = calculated for the mixture assigned for this bin as discussed in this report. "Diff" = Difference between the SAPRC-07 value relative to the calculated SAPRC-99 value. (Data from Table A-1).



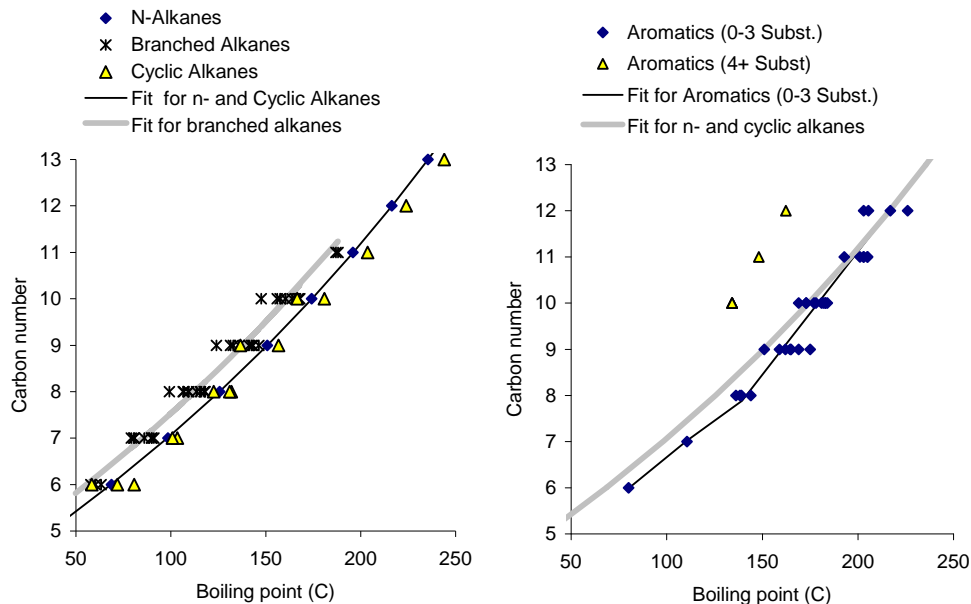


Figure 3. Plots of carbon numbers against boiling points for various alkanes and aromatic hydrocarbons (from Carter and Malkina, 2005).

$nC_{avg}$  is the carbon number derived by the above equations is, and if  $nC_1$  is the largest integer  $\leq nC_{avg}$ , and if  $nC_2 = nC_1 + 1$ , then the assumed carbon number distribution corresponding to  $nC_{avg}$  is given by:

$$\text{Mass fraction } (nC_1) = 1 - (nC_{avg} - nC_1)$$

$$\text{Mass fraction } (nC_2) = nC_{avg} - nC_1$$

Actual mixtures may in general have wider distributions of carbon numbers than predicted using this equation, but the effects of broader distributions of carbon numbers is taken into account by considering the boiling point ranges of the bins. For each bin, the carbon number distribution is derived from the boiling point range assignments as follows:

$$\begin{array}{l} \text{Mass fraction} \\ \text{in solvent} \\ \text{with carbon} \\ \text{number } n \end{array} = 0.5 \times \begin{array}{l} \text{Mass fraction with} \\ \text{carbon number } n \\ \text{calculated for } T_{avg} \end{array} + 0.25 \times \begin{array}{l} \text{Mass fraction with} \\ \text{carbon number } n \\ \text{calculated for} \\ (T_{avg} + T_{max})/2 \end{array} + 0.25 \times \begin{array}{l} \text{Mass fraction with} \\ \text{carbon number } n \\ \text{calculated for} \\ (T_{avg} + T_{min})/2 \end{array}$$

where  $T_{avg}$ ,  $T_{max}$ , and  $T_{min}$  are the average, minimum, and maximum for the boiling point range as given on Table 5, and the fractions with the given carbon number are calculated separately for normal, branched, and cyclic alkanes and for aromatics using the appropriate equation as indicated above.

For low boiling point aromatic solvents, it is assumed that the minimum aromatic carbon number is 6.5, which corresponds to a mixture of equal mass fractions of benzene and toluene. This tends to give predictions that are more consistent with the limited available compositional analysis of the solvents of this type. For alkanes, it is assumed that the minimum carbon number is 5, since this approach is not designed for gaseous or very low boiling point hydrocarbon mixtures.

For the alkane fractions, assignments of chemical compounds to each type and carbon number are fairly straightforward. For the normal alkanes, the assignment is clear since there is only one compound for each carbon number. The branched alkanes or cyclic alkanes with a given carbon number are represented by the generic SAPRC branched or cyclic alkane model species BR-C<sub>n</sub>, or CYC-C<sub>n</sub>, where n is the carbon number. The only exception is cycloalkanes with 5 carbons, which are represented by cyclopentane (CYCC5) explicitly. (Likewise, cycloalkanes with 6 carbons are assumed to be primarily cyclohexane, though the generic model species is used in these assignments to allow for use of other isomers in the future.) The specific compounds used to calculate the reactivities of these generic model species for the SAPRC-07 mechanism are shown in Table B-9 of the SAPRC-07 documentation report (Carter, 2009a). The assignments used for SAPRC-99 are the same or similar, and are given by Carter (2000). The choices of compounds are somewhat arbitrary for the larger carbon numbers, but are not inconsistent with the limited available analytical data.

Assignment of chemical compounds to the aromatic fractions is more uncertain because the bin definitions provide no specification of types of aromatics, and reactivities of aromatic isomers can vary significantly from compound to compound. The best approach is obviously to use a speciated analysis of the aromatics for reactivity estimation purposes. Because this analysis is usually not available, it is necessary to derive a “typical” aromatic composition for this purpose. The level of uncertainty in such estimates will depend on the degree of variability of reactivities of aromatic fractions of hydrocarbon solvents in general.

Table 6 lists the aromatic compounds identified by Carter and Malkina (2005) in 41 analyzed hydrocarbon solvents that had non-negligible aromatic content and speciated aromatic information, and gives the averages and standard deviations for the relative fractions of each within the same carbon number. The SAPRC-99 and SAPRC-07 MIR values for these compounds are also given on the table, indicating the variability of the reactivities of the compounds. Although the standard deviations of the averages on Table 6 indicate that there is relatively wide variability in the compositions for each carbon number, Carter and Malkina (2005) show that the variabilities of the MIRs of the aromatics with the given carbon numbers for the various solvents are relatively small. (This can also be seen in Figure 5, below, which shows relatively little variability in calculated MIRs for the aromatic hydrocarbon bins 21-23.) This suggests that reactivity estimates based on the average compositions shown on Table 6 may give reasonably good approximations to those derived from detailed speciated information.

Carter and Malkina (2005) did not have sufficient data to drive aromatic compositions for carbon numbers of 12 or greater, and estimated them by assuming that they have the same types of compounds as derived for C<sub>11</sub>. However, a composition analysis of the heavy aromatics, Bin 24, Aromatics-200 solvent conducted by Propper (2009) based on GC data made available at the Ignitable Liquids Reference Collection website (ILRC, 2009), indicates that the fraction of naphthalenes increases significantly with carbon number, approaching 100% at C<sub>14</sub> or greater. Based on this limited information, we assume that the fractions of naphthalenes (including tetralin and indan, which have similar reactivities as naphthalenes) increase with carbon number as shown on Table 7, which gives the composition assignments used for calculating the reactivities of these C<sub>12+</sub> aromatic fractions. The naphthalenes fraction is represented by equal parts of model species for unsubstituted and disubstituted naphthalenes (for which mechanisms have been derived based on available chamber data for naphthalene and 2,3-dimethylnaphthalene (Carter, 2009 and references therein) with the appropriate molecular weights. The alkylbenzene fractions are represented by assuming the same relative distributions of mono-, di-, and tri-substituted alkylbenzenes as C<sub>11</sub>, as also shown on Table 7. These composition assignments for the higher aromatics are somewhat arbitrary and highly uncertain, though probably not much more so than the estimated mechanisms and MIR values for the higher aromatic species themselves.

Table 6. List of C<sub>8</sub> - C<sub>11</sub> aromatic compounds identified in the hydrocarbon solvents used in this study for aromatic fraction analysis, and average contributions of the compounds to the total aromatics with the same carbon number.

Description	Model Species	nC	Contribution to carbon number [a]	MIR [b]	
				SAPRC-99	SAPRC-07
o-Xylene	O-XYLENE	8	41.8±31.7%	7.48	7.44
m-Xylene	M-XYLENE	8	34.5±19.1%	10.61	9.52
p-Xylene	P-XYLENE	8	13.0±7.2%	4.24	5.69
Ethyl Benzene	C2-BENZ	8	10.7±6.9%	2.79	2.93
1,2,4-Trimethyl Benzene	124-TMB	9	29.5±11.3%	7.18	8.64
1,2,3-Trimethyl Benzene	123-TMB	9	16.3±8.9%	11.25	11.66
m-Ethyl Toluene	M-ET-TOL	9	14.7±6.2%	9.37	7.21
1,3,5-Trimethyl Benzene	135-TMB	9	10.3±3.8%	11.22	11.44
p-Ethyl Toluene	P-ET-TOL	9	7.7±3.2%	3.75	4.32
o-Ethyl Toluene	O-ET-TOL	9	7.6±8.7%	6.61	5.43
n-Propyl Benzene	N-C3-BEN	9	5.5±3.4%	2.20	1.95
Indan	INDAN	9	5.0±5.7%	3.16	3.20
Isopropyl Benzene	I-C3-BEN	9	3.5±4.7%	2.32	2.43
C10 Trisubstituted Benzenes	C10-BEN3	10	35.4±7.5%	8.86	9.01
C10 Disubstituted Benzenes	C10-BEN2	10	23.4±11.3%	5.92	5.53
C10 Tetrasubstituted Benzenes	C10-BEN4	10	9.0±5.1%	8.86	9.01
Methyl Indans	ME-INDAN	10	7.3±5.9%	2.83	2.86
1,2,3,5 Tetramethyl Benzene	1235MBEN	10	6.9±5.0%	8.25	9.01
m-Diethyl Benzene	M-DE-BEN	10	4.6±2.4%	8.39	6.92
C10 Monosubstituted Benzenes	C10-BEN1	10	3.3±2.8%	1.97	2.27
p-Diethyl Benzene	P-DE-BEN	10	2.8±3.7%	3.36	4.31
n-Butyl Benzene	N-C4-BEN	10	2.7±3.5%	1.97	2.27
Naphthalene	NAPHTHAL	10	2.7±2.9%	3.26	3.24
o-Diethyl Benzene	O-DE-BEN	10	1.4±2.6%	5.92	5.34
Tetralin	TETRALIN	10	0.2±0.3%	2.83	2.86
s-Butyl Benzene	S-C4-BEN	10	0.2±0.5%	1.97	2.27
C11 Trisubstituted Benzenes	C11-BEN3	11	47.5±3.8%	8.02	7.91
C11 Tetrasubstituted Benzenes	C11-BEN4	11	23.9±1.2%	8.02	7.91
C11 Tetralin or Indane	C11-TET	11	9.6±2.6%	2.55	2.58
C11 Disubstituted Benzenes	C11-BEN2	11	7.3±1.2%	5.35	4.79
2-Methyl Naphthalene	2ME-NAPH	11	4.5±1.0%	4.61	2.96
C11 Pentasubstituted Benzenes	C11-BEN5	11	3.8±1.7%	8.02	7.91
C11 Monosubstituted Benzenes	C11-BEN1	11	2.5±0.5%	1.78	2.04
1-Methyl Naphthalene	1ME-NAPH	11	1.0±0.3%	4.61	2.96

[a] Averages and standard deviations for aromatics fractions for various solvents where speciated aromatic data are available (Carter and Malkina, 2005).

[b] MIR values in units of grams O<sub>3</sub> / gram compound.

Table 7. Composition assignments used to estimate reactivities of unspeciated C<sub>12</sub> - C<sub>16</sub> aromatic mixtures.

Carbon Number (n)	Naphthalenes Cn-NAPH	Monosubstituted benzenes Cn-BEN1	Disubstituted benzenes Cn-BEN2	Polysubstituted benzenes Cn-BEN3
11 [a]	15.1%	2.5%	7.3%	75.2%
12	30.0%	2.0%	6.0%	62.0%
13	50.0%	1.5%	4.3%	44.3%
14	75.0%	0.7%	2.1%	22.1%
15	90.0%	0.3%	0.9%	8.9%
16	100.0%			

[a] The model species used to represent C<sub>11</sub> aromatics are given in Table 6. The general types of model species are included here for comparison with C<sub>12+</sub>.

For the purpose of assigning compositions to the various aromatic-containing bins, the C<sub>6</sub> and C<sub>7</sub> aromatics are assigned benzene and toluene, respectively, the C<sub>8</sub> - C<sub>11</sub> aromatics are assigned the average compositions for the various carbon numbers as indicated on Table 6, and the C<sub>12+</sub> aromatics are assigned compositions based on assuming increasing naphthalene content as shown on Table 7. Some of these are given in terms of SAPRC detailed model species referring to mixtures of isomeric species assumed to have the same reactivity, and these in turn are assigned to individual compounds or lumped detailed model species with assigned mechanisms as indicated in Table B-9 of the SAPRC-07 documentation report (Carter, 2007). Note that in some cases the compounds assigned to these groups in SAPRC-99 are somewhat different, though the general approach is similar.

The methods discussed above to derive compositions and reactivities in the MIR and other scales for various hydrocarbon mixtures given type distributions and boiling point ranges has been implemented in a spreadsheet, HCcalc.xls, that is available for downloading from the SAPRC mechanism web site<sup>1</sup>. Comments in the spreadsheet indicate how to use the various macros to output the compositions or calculate reactivity values for various scales, and how to add or modify reactivity scales if needed. This spreadsheet was used to output the compositions given in Table B-1 for the various bins based on the type distributions and boiling point ranges in Table 5, and these compositions were used to calculate the MIR values for these various bins that are given in Table A-1 in this report.

The reactivity assignments made for the various bins can be evaluated by comparing the assigned or calculated bin reactivities with those calculated explicitly for various hydrocarbon mixtures that would fall into these bins, provided that sufficient analytical data are available for the mixtures. The analyzed mixtures for which we have sufficient analytical data for this purpose are summarized on Table 8. Most of these were used by Carter and Malkina (2005), though several mixtures they used have been deleted because of insufficient analytical data, and several have been added subsequently. The sources of the data are as follows, where the code letters are as indicated on Table 8:

- A. Data provided by the hydrocarbon panel of the American Chemistry Council (Jaques, 2002). The information provided included carbon number distribution and hydrocarbon type information for 77 types of solvents. This is a subset of the solvents used in the Kwok et al (2000) study. The type information was sufficient for reactivity analysis of the alkane fractions but not sufficient for the

<sup>1</sup> This file can be downloaded from [www.cert.ucr.edu/~carter/SAPRC/HCcalc.xls](http://www.cert.ucr.edu/~carter/SAPRC/HCcalc.xls).

Table 8. Summary of hydrocarbon solvents whose compositional information was used in this analysis of hydrocarbon solvent reactivity.

ID	Description [a]	Src. [b]	Dist Range (F)	Avg C's	Type Summary (%)					MIR [c]
					N-Alk	Iso-Alk	Cy-Alk	Arom.	Naph	
CARB Bin 1										
1-A	Bin 1 solvent "A"	A	151-157	6.0	64	23	13	-	-	1.33
1-B	Bin 1 solvent "B"	A	148-185	6.2	32	49	19	-	-	1.22
1-C	Bin 1 solvent "C"	A	172-210	6.6	24	28	48	-	-	1.31
CARB Bin 2										
2-O	Bin 2 solvent "O"	A	148-201	6.3	25	68	6	1	-	1.24
2-D	Bin 2 solvent "D"	A	194-206	7.0	19	73	8	0	-	1.33
2-A	Bin 2 solvent "A"	A	150-159	6.0	50	49	1	-	-	1.19
2-B	Bin 2 solvent "B"	A	200-210	7.1	30	63	7	-	-	1.28
2-C	Bin 2 solvent "C"	A	142-170	6.1	29	62	9	-	-	1.22
2-E	Bin 2 solvent "E"	A	82-97	5.0	80	20	-	-	-	1.25
2-F	Bin 2 solvent "F"	A	95-140	5.2	73	26	1	-	-	1.25
2-G	Bin 2 solvent "G"	A	123-150	6.0	1	99	-	-	-	1.23
2-H	Bin 2 solvent "H"	A	151-157	6.0	83	8	9	-	-	1.16
2-I	Bin 2 solvent "I"	A	133-155	6.0	45	55	-	-	-	1.20
2-J	Bin 2 solvent "J"	A	190-210	7.0	7	91	2	-	-	1.36
2-K	Bin 2 solvent "K"	A	190-218	7.7	-	100	-	-	-	1.36
2-L	Bin 2 solvent "L"	A	140-145	6.0	4	95	1	-	-	1.23
2-M	Bin 2 solvent "M"	A	151-156	6.1	52	47	1	-	-	1.19
2-N	Bin 2 solvent "N"	A	151-156	6.0	48	45	7	-	-	1.19
CARB Bin 3										
3-B	Bin 3 solvent "B"	A	209-237	7.0	5	2	93	0	-	1.53
3-A	Bin 3 solvent "A"	A	174-180	6.2	-	13	87	-	-	1.21
CARB Bin 4										
4-A	Bin 4 solvent "A"	A	195-210	7.0	26	69	2	3	-	1.37
CP05	Lactol Spirits	B	185-220	7.3	8	29	56	7	-	1.56
CARB Bin 6										
6-G	Bin 6 solvent "G"	A	247-282	8.3	14	20	65	1	-	1.08
6-F	Bin 6 solvent "F"	A	209-230	7.3	20	16	64	0	-	1.26
6-A	Bin 6 solvent "A"	A	317-347	10.1	-	47	53	0	-	1.39
6-B	Bin 6 solvent "B"	A	312-356	9.8	17	25	58	-	-	0.92
6-C	Bin 6 solvent "C"	A	265-290	8.6	19	18	63	-	-	0.95
6-D	Bin 6 solvent "D"	A	241-292	8.2	18	27	55	-	-	1.18
6-E	Bin 6 solvent "E"	A	317-351	10.3	19	30	51	-	-	1.23
CP04	VM&P naphtha HT	B	240-285	8.3	19	34	47	-	-	0.84
CP14	VM&P Naphtha	B	244-287	8.3	20	32	47	1	-	1.13
CP23	VM&P Naphtha	B	260-288	8.5	9	25	66	1	-	1.20
CP24	VM&P Naphtha	B	244-287	8.4	9	24	66	1	-	1.25
CP29	aliphatic petroleum dist.	B	285-335	9.3	18	34	47	0	-	1.27
CP43	Mineral spirits	B	300-365	10.0	27	47	26	-	-	1.02
<u>VMP-NAPH</u>	<u>VMP Naphtha</u>	<u>C</u>	<u>240-304</u>	<u>8.7</u>	<u>13</u>	<u>44</u>	<u>42</u>	<u>0</u>	<u>=</u>	<u>0.82</u>

Table 8 (continued)

ID	Description [a]	Src. [b]	Dist Range (F)	Avg C's	Type Summary (%)					MIR [c]
					N-Alk	Iso-Alk	Cy-Alk	Arom.	Naph	
CARB Bin 7										
7-A	Bin 7 solvent "A"	A	201-210	7.1	35	62	3	-	-	0.95
7-B	Bin 7 solvent "B"	A	320-349	10.2	-	97	3	-	-	0.82
7-C	Bin 7 solvent "C"	A	250-320	9.2	-	100	-	-	-	1.01
7-D	Bin 7 solvent "D"	A	320-332	10.0	-	100	-	-	-	0.86
7-E	Bin 7 solvent "E"	A	204-218	8.0	-	100	-	-	-	1.35
CARB Bin 8										
8-A	Bin 8 solvent "A"	A	280-328	9.1	-	-	100	-	-	1.34
CARB Bin 9										
CP28	light naphtha solvent	B	195-225	7.5	23	40	35	2	-	1.30
9-A	Bin 9 solvent "A"	A	240-250	8.0	27	33	37	3	-	1.31
9-B	Bin 9 solvent "B"	A	158-270	6.7	28	41	28	3	-	1.26
CP12	Mineral Spirits	B	300-365	10.0	24	33	40	3	0	1.09
CP11	Mineral Spirits	B	300-365	9.9	20	30	47	3	0	1.07
CP30	VM&P naphtha	B	240-285	8.5	22	43	28	6	-	1.47
CARB Bin 10										
CP35	VM&P naphtha	B	247-282	8.4	17	29	45	10	-	1.75
CP01	VM&P naphtha	B	240-305	8.4	37	28	13	23	-	2.46
CARB Bin 11										
11-B	Bin 11 solvent "B"	A	374-405	11.5	22	21	57	0	-	0.63
11-I	Bin 11 solvent "I"	A	370-485	12.0	2	43	55	0	-	0.70
11-K	Bin 11 solvent "K"	A	395-445	11.8	2	43	55	0	-	0.71
11-L	Bin 11 solvent "L"	A	415-450	12.6	2	58	40	0	-	0.60
11-J	Bin 11 solvent "J"	A	380-410	10.9	2	28	70	0	-	0.82
11-A	Bin 11 solvent "A"	A	380-410	10.9	24	12	64	-	-	0.77
11-C	Bin 11 solvent "C"	A	315-390	9.9	18	24	58	-	-	0.94
11-D	Bin 11 solvent "D"	A	324-394	10.8	14	29	57	-	-	0.79
11-E	Bin 11 solvent "E"	A	370-408	11.9	20	29	51	-	-	0.65
11-F	Bin 11 solvent "F"	A	383-419	11.9	22	24	54	-	-	0.65
11-G	Bin 11 solvent "G"	A	408-453	12.7	22	32	46	-	-	0.59
11-H	Bin 11 solvent "H"	A	370-405	11.5	-	89	11	-	-	0.64
CP16	aliphatic petroleum dist.	B	351-415	11.3	31	42	27	-	-	0.67
CP18	aliphatic petroleum dist.	B	312-387	11.3	30	43	27	-	-	0.68
CP33	Mineral Spirits	B	324-402	10.4	24	42	34	1	-	0.84
<u>ASTM-1C</u>	<u>Low aromatic min. spirits</u>	<u>D</u>	<u>315-390</u>	<u>10.8</u>	<u>14</u>	<u>30</u>	<u>56</u>	<u>=</u>	<u>=</u>	<u>0.79</u>
CARB Bin 12										
12-A	Bin 12 solvent "A"	A	357-408	11.5	-	100	-	-	-	0.55
12-B	Bin 12 solvent "B"	A	388-459	12.2	-	100	-	-	-	0.62
12-C	Bin 12 solvent "C"	A	434-472	13.3	-	100	-	-	-	0.58
12-D	Bin 12 solvent "D"	A	355-400	11.8	-	100	-	-	-	0.52
12-E	Bin 12 solvent "E"	A	352-370	11.0	-	96	4	-	-	0.60
12-F	Bin 12 solvent "F"	A	354-385	11.5	-	97	3	-	-	0.68
12-G	Bin 12 solvent "G"	A	372-426	11.5	99	1	-	-	-	0.63
12-H	Bin 12 solvent "H"	A	432-469	13.2	99	1	-	-	-	0.53
<u>ASTM-3C1</u>	<u>Synthetic isoparaffinic</u>	<u>D</u>	<u>354-369</u>	<u>11.0</u>	<u>=</u>	<u>96</u>	<u>4</u>	<u>=</u>	<u>=</u>	<u>0.47</u>

Table 8 (continued)

ID	Description [a]	Src. [b]	Dist Range (F)	Avg C's	Type Summary (%)					MIR [c]
					N-Alk	Iso-Alk	Cy-Alk	Arom.	Naph	
CARB Bin 14										
CP03	Light HC solvent	B	379-405	11.6	4	54	40	2	2	0.91
14-C	Bin 14 solvent "C"	A	370-408	11.6	23	26	46	5	-	1.01
15-F	"Bin 15" solvent "F" [d]	A	320-396	10.4	19	30	46	5	-	1.22
15-D	"Bin 15" solvent "D" [d]	A	320-398	10.8	15	30	49	6	-	1.23
<u>ASTM-1B</u>	<u>Mineral Spirits 75</u>	<u>D,E</u>	<u>315-397</u>	<u>10.8</u>	<u>14</u>	<u>31</u>	<u>49</u>	<u>6</u>	<u>1</u>	1.11
14-A	Bin 14 solvent "A"	A	315-400	10.1	34	19	40	7	-	1.22
CARB Bin 15										
CP06	Mineral Spirits	B	324-402	10.2	10	33	47	10	1	1.48
CP20	Stoddard Solvent	B	312-387	10.1	10	31	49	10	1	1.52
CP25	Mineral Spirits	B	318-380	10.2	11	32	47	11	2	1.58
CP10	Mineral Spirits	B	307-389	10.1	9	31	49	11	1	1.60
CP26	Mineral Spirits	B	307-389	10.1	10	26	48	15	1	1.60
CP15	aliphatic petroleum dist.	B	351-415	10.1	13	27	44	15	1	1.79
CP02	300-66 solvent, M.S. 66	B	310-400	9.9	21	32	30	17	0	1.71
CP39	paraffinic petroleum dist.	B	315-397	9.9	21	29	32	18	1	2.03
<u>ASTM-1A</u>	<u>Regular mineral spirits</u>	<u>D,E</u>	<u>315-394</u>	<u>10.7</u>	<u>15</u>	<u>32</u>	<u>34</u>	<u>19</u>	<u>2</u>	2.01
CARB Bin 16										
16-A	Bin 16 solvent "A"	A	482-514	14.8	21	33	45	1	-	0.47
16-D	Bin 16 solvent "D"	A	460-525	14.4	2	63	35	0	-	0.55
16-E	Bin 16 solvent "E"	A	465-530	14.4	22	50	28	0	-	0.52
16-B	Bin 16 solvent "B"	A	540-593	17.1	18	21	61	-	-	0.50
16-C	Bin 16 solvent "C"	A	522-592	16.8	-	54	46	-	-	0.43
CARB Bin 17										
17-A	Bin 17 solvent "A"	A	451-536	14.0	-	100	-	-	-	0.49
17-B	Bin 17 solvent "B"	A	480-525	14.9	99	1	-	-	-	0.44
17-C	Bin 17 solvent "C"	A	489-541	14.5	97	2	2	-	-	0.45
CARB Bin 21										
CP19	Xylene	B	280-286	8.0	-	-	-	100	-	7.44
CP27	Xylene	B	280-286	8.0	-	-	-	100	-	7.31
CP34	Xylene	B	280-286	8.0	-	-	-	100	-	7.29
CP40	Xylene	B	280-286	8.0	-	-	-	100	-	7.37
CP41	Xylene	B	280-286	8.0	-	-	-	100	-	7.25
21-A	Xylene	G	279-289	8.0	-	-	-	100	-	7.17
CARB Bin 22										
CP07	Aromatic 100	B	320-348	9.1	-	-	-	100	1	7.15
CP13	Aromatic 100	B	320-348	9.1	0	0	0	100	1	7.72
CP21	Aromatic 100	B	320-348	9.1	-	0	-	100	2	7.64
CP31	Aromatic 100	B	320-348	9.0	-	-	-	100	1	7.51
CP36	Aromatic 100	B	320-348	9.1	-	-	-	100	2	7.58
CP42	Aromatic 100	B	320-348	9.1	-	-	-	100	2	7.56
22-A	Aromatic 100	F	316-352	9.0	-	-	-	100	-	7.78
<u>AROM-100</u>	<u>Aromatic 100</u>	<u>C</u>	<u>322-341</u>	<u>9.1</u>	<u>-</u>	<u>-</u>	<u>-</u>	<u>100</u>	<u>-</u>	7.79

Table 8 (continued)

ID	Description [a]	Src. [b]	Dist Range (F)	Avg C's	Type Summary (%)					MIR [c]
					N-Alk	Iso-Alk	Cy-Alk	Arom.	Naph	
CARB Bin 23										
CP08	Aromatic 150	B	343-407	10.0	-	-	-	100	17	6.66
CP17	Aromatic 150	B	343-407	10.1	-	-	0	100	12	7.33
CP22	Aromatic 150	B	343-407	10.0	-	-	-	100	14	7.80
CP32	Aromatic 150	B	343-407	10.0	-	0	-	100	19	7.31
CP37	Aromatic 150	B	343-407	10.1	-	-	-	100	17	7.48
23-A	Aromatic 150	F	363-423	10.9	-	-	-	100	10	7.30
23-B	Aromatic 150: NCFS 285	F	367-399	10.2	-	-	-	100	14	7.71
23-C	Aromatic 150: NCFS 75	F		10.7	-	-	-	100	11	7.36
CARB Bin 24										
24-A	Aromatic 200: ILRC 76	F	450-532	11.6	-	-	-	100	100	3.76

[a] Description that was provided with the solvent or from its MSDS sheet. Entries that are underlined are solvents that were studied in chamber experiments by Carter and Malkina (2005).

[b] Source codes for compositional information are as given in the text.

[c] Incremental reactivity in the SAPRC-07 MIR scale, in units of grams O<sub>3</sub> per gram solvent, calculated using the available compositional data or assigned to the solvent or the bin.

[d] The bin assignment indicated in the ACC designation was not consistent with the reported aromatic content. The bin assignment was modified to be consistent with Table 4

aromatics. For this reason, the solvents falling into the high aromatics bins (5, 10, 15 and 20-24) are removed from this dataset for this work, though they were included in the bin reactivity comparisons by Carter and Malkina (2005). This leaves 59 types of solvents useful for reactivity assessment for the purpose of this report.

- B. Data from the study of Censullo et al (2002), who conducted a detailed compositional analysis of 42 different hydrocarbon solvents, representing 19 of the 24 solvent bins. These data were not available at the time the Kwok et al (2000) work was carried out.
- C. Data provided by the American Chemistry Council (Jaques, 2003, 2004) and ExxonMobil Chemical (Medeiros, 2004) as needed for reactivity assessment for the six hydrocarbon solvents studied in the chamber experiments of Carter and Malkina (2005).
- D. Data provided as indicated above for "C", except that the boiling point ranges were taken from the MSDS sheet provided with the samples, and are considered to be approximate
- E. Data provided as indicated above for "C" except that detailed aromatic speciation data were provided separately by ExxonMobil Chemical (Medeiros, 2004).
- F. Data for 6 high aromatics were provided by Propper (2009) based on GC data at the ILRC (2009) website and additional analyses. These data were provided subsequent to the study of Carter and Malkina (2005).

The compositions for each of the solvents listed on Table 8 were used to derive MIR values for each in the SAPRC-99 or SAPRC-07 scale. These can then be compared with the bin reactivity assignments, as discussed in the following section.



## Results and Discussion

The compositions derived as discussed above for each of the hydrocarbon bins are given in Table B-1 at the end of this document. These are given in terms of SAPRC detailed model species for which MIR and other reactivity values have been derived (Carter, 2000, 2002, 2009). These were used to derive the MIR values given in Table A-1, Table 5, and Table 8. Table 5 also gives the SAPRC-99 bin MIR assignments of Kwok et al (2000), where they can be compared with the SAPRC-99 and SAPRC-07 values calculated for the bin compositions.

The changes in bin MIRs resulting from changing the methodology are shown on Table 5 and Figure 4, and Figure 5a. The comparison of the SAPRC-99 bin MIR's gives an indication of the effects of using the assigned composition approach of this work compared to the approach of Kwok et al (2000). The two methods agree to within  $\pm 15\%$  in all cases except for the lighter hydrocarbon bins containing cycloalkanes (Bins 1 and 3-5), and three of the four bins containing heavier aromatics (Bins 19, 20 and 23). Likely reasons for these differences are discussed below.

The discrepancies for the light hydrocarbon bins containing cycloalkanes may be due at least in part from the fact that the Kwok et al (2000) correlation between boiling points and carbon number predicts a MIR for cyclohexane that is  $\sim 60\%$  higher than the actual value. This is important for these bins because  $C_6$  is the largest carbon fraction assigned to these bins, and unspciated  $C_6$  cycloalkanes are assumed to be primarily cyclohexane. Because of chemical structural factors, the MIR calculated for cyclohexane is considerably lower than those calculated for the other light cycloalkanes that were used by Kwok et al (2000) to derive the boiling point vs. MIR correlation. In general, because of the lower number of isomers in the lighter solvents, MIR vs. boiling point estimation errors for individual compounds may be relatively more important for the lighter solvents than would be the case for the heavier solvents with larger numbers of possible isomers. On the other hand, compositional estimates, and the MIRs derived from them, are probably the least uncertain in the lighter solvents where the number of possible isomers is low. Therefore, for the lighter solvents at least, we believe that MIRs derived from compositional estimates are probably somewhat more reliable.

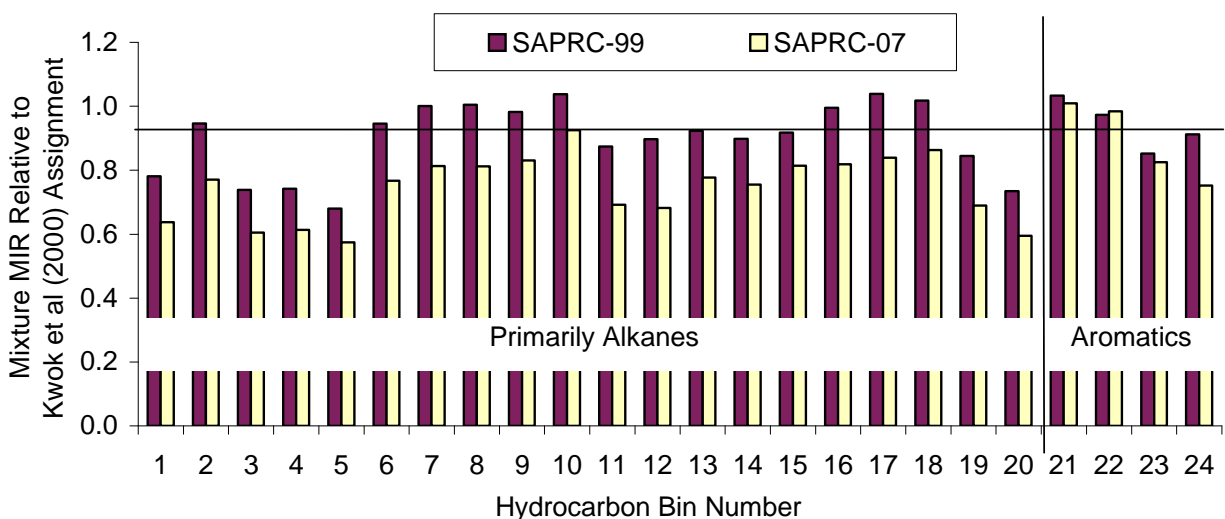


Figure 4. Changes in bin MIR values calculated using the mixture compositions in Table B-1 relative to the initial assignments of Kwok et al (2000). The SAPRC-99 data show the effects of changing the methodology only, and the SAPRC-07 data show the combined effects of changing the methodology and mechanism.

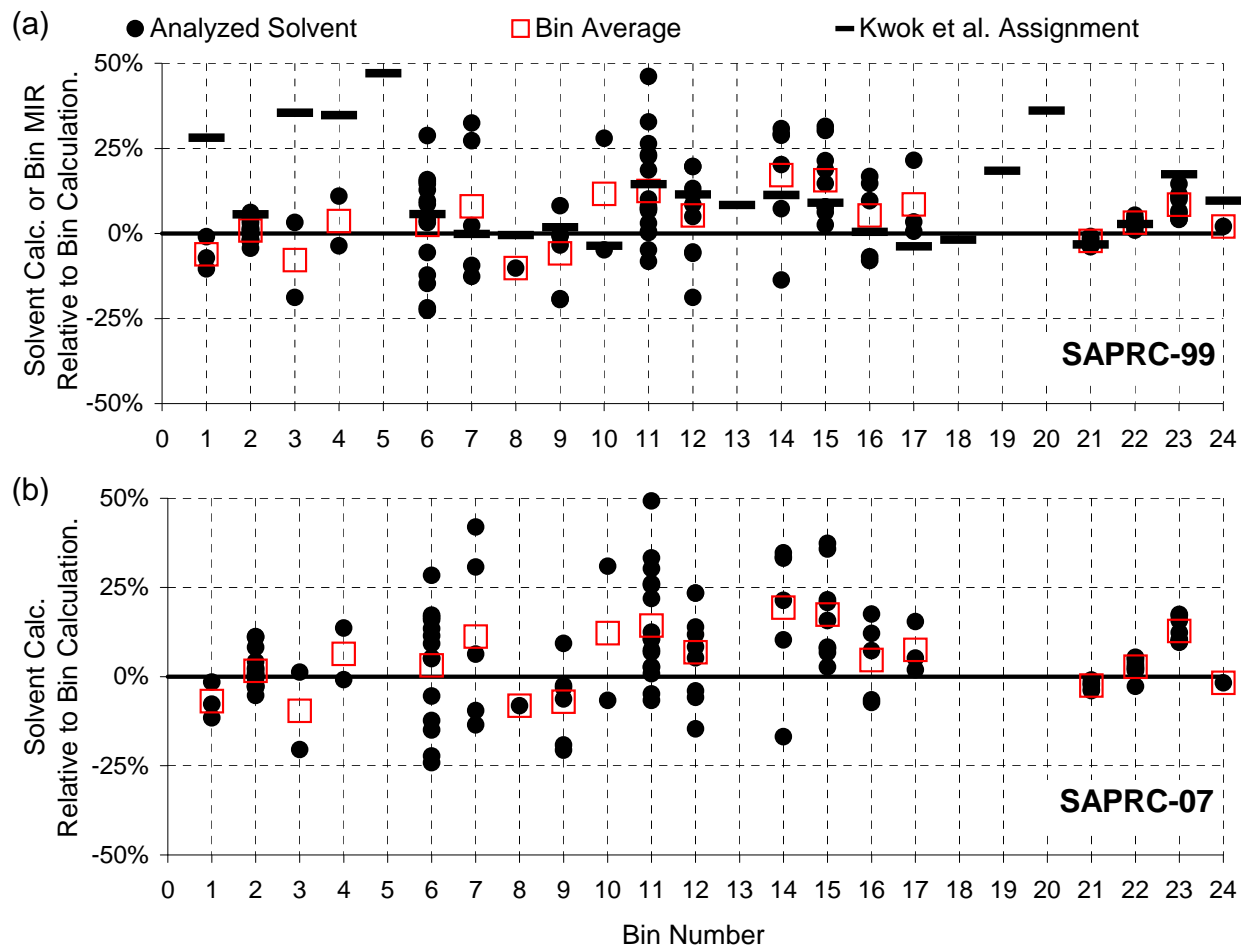


Figure 5. Plots of differences between assigned bin MIRs and explicitly calculated MIRs for the analyzed solvents. (a) Comparisons using SAPRC-99 MIRs, with bin assignments made by Kwok et al (2000) also shown. (b) Comparisons using SAPRC-07 MIRs.

The differences for the bins containing the heavier aromatics can be attributed, at least in part, to the relatively limited data available to derive reactivity estimates for such solvents, and the need to make assumptions about the distribution of compounds in the heavier aromatic fractions. We have no composition data for solvents in Bins 19 or 20, and the data we have for the solvents in Bins 23 and 24 were not, to our knowledge, used by Kwok et al (2000). Therefore we do not know the basis Kwok et al (2000) used to derive MIR estimates for solvents in these bins. It could have been based on solvents with inadequate detail in the aromatic speciation, as is the case for the solvents with source code "A" in Table 8). This would require Kwok et al (2000) making estimates concerning the aromatic type distributions for the purpose of deriving MIRs that might be different than what was derived in this work (as shown on Table 6 and Table 7). It is likely that they assumed much lower naphthalene fractions for the heaviest aromatics than we assume (see Table 7), since the Bin 24 solvent data we used as a basis for our estimates were probably not available to them. Since naphthalenes are less reactive than the alkylbenzenes, this would mean that they would estimate higher MIR values for these solvents than assumed in this work. It is surprising, however, that the discrepancy is not greater for Bin 24, which contains the highest amount of heavy aromatics for all the bins.

Comparisons of how well the SAPRC-99 MIR values calculated using the bin composition assignments compare with those calculated explicitly for the solvents listed on Table 8 are shown on Figure 5a. It can be seen that the composition calculation method performs significantly better for the four light hydrocarbon bins containing cycloalkanes than the Kwok et al (2000) assignments, and the performance is slightly better (though the differences may not be significant) for the heavy aromatic bins 23 and 24. In general, the composition calculation method predicts the MIRs for the solvents to within  $\pm 25\%$  in most cases, with the averages being within  $\pm 20\%$  in all cases. This is also the case for the Kwok et al (2000) method except for the four light hydrocarbon/cycloalkane bins. Note, however, that the good agreement for the aromatic bins shown in Figure 5b is not an independent test of the method, since the compositions of those solvents were used to derive the aromatic compositions used for the bin calculation.

The changes in bin MIRs resulting from changing the mechanism alone are shown on the last column of Table 5. It can be seen that the mechanism update causes decreases, by about 20% on the average, of the MIRs for the solvents that are primarily alkane mixtures. This is due to the  $\sim 20\%$  lower MIR values calculated for the heavier alkanes (see Table A-1). The MIR changes for the all-aromatic bins were generally less, and is consistent with the much more variable change in MIRs for the individual aromatic constituents, as shown on Table A-1. The greatest change for the all-aromatic bins is for Bin 24, and is attributable to the much lower MIRs calculated for the dialkylnaphthalenes, which are important constituents in the mixture derived for this bin.

The changes in MIR values resulting from both the change of methodology and the change of mechanism combined are shown in Figure 4 (the bars labeled "SAPRC-07") and in Table A-1. Since the mechanism change caused declines in MIRs for most of the bins, the reductions in MIRs in the bins where the methodology change had an effect were even greater. The relative changes ranged from essentially no change for the lighter aromatic bins 21 and 22, to almost 40% change for the light alkane bins with cycloalkanes. For most bins the MIR changes were on the order of 20-30%.

## Conclusions

The updated MIR assignments and uncertainty codes developed in this work are given in the last two columns of Table 4, and are included in the full MIR scale listing in Table A-1. The tables include the uncertainty codes associated with the reactivity assignments, based on those given on Table A-1 for the other compounds and mixtures. These reflect our subjective estimate of the overall level of uncertainty in the MIR assignments, which should be borne in mind when these reactivity values are used in regulatory applications. Footnotes to Table 4 indicate the meaning of these uncertainty assignments in the context of these bin mixtures. The heaviest aromatic bins have the highest uncertainties both for the compositions and the mechanisms, with the mechanisms for the higher molecular weight naphthalenes being particularly uncertain. Experimental work is recommended to reduce the significant uncertainties of these heavy aromatic bins.

The revised methodology for deriving hydrocarbon bin MIRs based on estimating compositions for each bin was found to perform at least as well in estimating reactivities of analyzed solvents as the methodology previously developed by the CARB, and is probably superior for bins containing light cycloalkanes and heavy aromatics. This methodology is concluded to be appropriate for deriving the bin reactivities in the new SAPRC-07 MIR scale, and has been used for this purpose. Although uncertainties remain, the recommended bin MIR values represent our best estimate given the available compositional and mechanistic information.

## REFERENCES

- Azzi, M., S. White and D. Angove (2008): "Review of the SAPRC-07 Chemical Mechanism," Report to the California Air Resources Board, November.
- CARB (2000): "Initial Statement of Reasons for the Proposed Amendments to the Regulation for Reducing Volatile Organic Compound Emissions from Aerosol Coating Products and Proposed Tables of Maximum Incremental Reactivity (MIR) Values, and Proposed Amendments to Method 310, 'Determination of Volatile Organic Compounds in Consumer Products'," California Air Resources Board, Sacramento, CA, May 5.
- CARB (2003): "Rulemaking on the Adoption Of Proposed Amendments to the Tables of Maximum Incremental Reactivity (MIR) Values," California Air Resources Board, December 3. Available at <http://www.arb.ca.gov/regact/mir2003/mir2003.htm>. Accessed August 14, 2009. Document giving MIR values is at <http://www.arb.ca.gov/regact/mir2003/fsor.doc>.
- Carter, W. P. L. (1990): "A Detailed Mechanism for the Gas-Phase Atmospheric Reactions of Organic Compounds," *Atmos. Environ.*, 24A, 481-518.
- Carter, W. P. L. (1994a): "Development of Ozone Reactivity Scales for Volatile Organic Compounds," *J. Air & Waste Manage. Assoc.*, 44, 881-899.
- Carter, W. P. L. (1994b): "Calculation of Reactivity Scales Using an Updated Carbon Bond IV Mechanism," Report Prepared for Systems Applications International Under Funding from the Auto/Oil Air Quality Improvement Research Program, April 12.
- Carter, W. P. L. (2000): "Documentation of the SAPRC-99 Chemical Mechanism for VOC Reactivity Assessment," Report to the California Air Resources Board, Contracts 92-329 and 95-308, May 8. Available at <http://cert.ucr.edu/~carter/absts.htm#sapr99> and <http://www.cert.ucr.edu/~carter/reactdat.htm>.
- Carter, W. P. L. (2003): "The SAPRC-99 Chemical Mechanism and Updated VOC Reactivity Scales, Updated and Corrected Data as of February 5, 2003," Available at <http://www.cert.ucr.edu/~carter/reactdat.htm>.
- Carter, W. P. L. (2008a): "Development of the SAPRC-07 Chemical Mechanism and Updated Ozone Reactivity Scales," Final report to the California Air Resources Board Contract No. 03-318. May 28.
- Carter, W. P. L. (2008b). "Reactivity Estimates for Selected Consumer Product Compounds," Final Report to the California Air Resources Board Contract 06-408, February 19. Available at <http://www.cert.ucr.edu/~carter/absts.htm#aminrep>.
- Carter, W. P. L. (2009a): "Development of the SAPRC-07 Chemical Mechanism and Updated Ozone Reactivity Scales," Final report to the California Air Resources Board Contract No. 03-318, as revised for Contracts 06-408 and 07-730. June 8. Available at [www.cert.ucr.edu/~carter/SAPRC](http://www.cert.ucr.edu/~carter/SAPRC).
- Carter, W. P. L. (2009b): "Peer Review of the SAPRC-07 Chemical Mechanism: Response to Reviewers' Comments," Prepared for California Air Resources Board Contract No. 07-730, March 19. Available at [www.cert.ucr.edu/~carter/SAPRC](http://www.cert.ucr.edu/~carter/SAPRC).

- Carter, W. P. L. and I. L. Malkina (2005): "Evaluation of Atmospheric Impacts of Selected Coatings VOC Emissions," Final report to the California Air Resources Board Contract No. 00-333, March 21. Available at <http://www.cert.ucr.edu/~carter/absts.htm#coatprt>.
- Censullo, A., C., D. R. Jones, and M. T. Wills (2002): "Investigation of Low Reactivity Solvents," Final Report for California Air Resources Board Contract 98-310, May 10.
- Derwent, R. G., M. E. Jenkin, and M. J. Pilling (2008): "Reactivity Scales and Comparative Tools for Chemical Mechanisms: SAPRC vs. MCM," Final Report to the California Air Resources Board.
- ILRC (2009): Ignitable Liquids Reference Collection, Developed by the ILRC Committee of the Technical Working Group for Fire and Explosives. Web site <http://ilrc.ucf.edu/>. Accessed June, 2009.
- Jaques, A (2004): "Sample Analysis for Products sent to Dr. W. Carter for CARB Architectural Coatings Research," revised compositional information provided by the Hydrocarbon Panel of the American Chemistry Council on March 8, 2004.
- Hanske, K. E. (2002): "Turpentine (Turpentine Oil, Wood Turpentine, Sulfate Turpentine, Sulfite Turpentine) [8006-64-2] Review of Toxicological Literature," Report to National Institute of Environmental Health Sciences, Research Triangle Park, NC, Contract N01-ES-65402, February.
- Harley, R. (2009): "SAPRC-07 Chemical Mechanism Peer Review Comments," Report to the California Air Resources Board, February 6.
- Kwok, E. S. C., C. Takemoto and A. Chew (2000): "Methods for Estimating Maximum Incremental Reactivity (MIR) of Hydrocarbon Solvents and their Classification," Appendix C to "Initial Statement of Reasons for the Proposed Amendments to the Regulation for Reducing Volatile Organic Compound Emissions from Aerosol Coating Products and Proposed Tables of Maximum Incremental Reactivity (MIR) Values, and Proposed Amendments to Method 310, 'Determination of Volatile Organic Compounds in Consumer Products'," California Air Resources Board, Sacramento, CA, May 5.
- Medeiros (2004): Arlean M. Medeiros, ExxonMobil Chemical Company, data provided to W. P. L. Carter by email, October 29.
- Propper, R (2009): Ralph Propper, Research Division, California Air Resources Board, Sacramento, California. Personal communication.
- Stockwell, W. R. (2009): "Peer Review of the SAPRC-07 Chemical Mechanism of Dr. William Carter," Draft report to the California Air Resources Board, March 9.

## APPENDIX A. TABLE OF MIR VALUES AND UNCERTAINTY CODES

Table A-1. Updated table of MIR values and uncertainty classifications. MIR values in the current CARB (2003) regulation are shown for comparison.

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
<u>Alkanes</u>										
1	methane	74-82-8	16.04	0.014	0.01	38%	1		0	6
2	ethane	74-84-0	30.07	0.26	0.31	-15%	1	3	0	1
3	propane	74-98-6	44.10	0.46	0.56	-18%	1	3	0	1
4	cyclopropane	75-19-4	42.08	0.082	0.10	-18%	1		0	6
5	n-butane	106-97-8	58.12	1.08	1.33	-19%	1	2	0	1
6	isobutane	75-28-5	58.12	1.17	1.35	-13%	1	3	0	2
7	cyclobutane	287-23-0	56.11	1.12	1.05	7%	1		0	6
8	n-pentane	109-66-0	72.15	1.23	1.54	-20%	1		0	6
9	branched C5 alkane(s)		72.15	1.36	1.68	-19%			0	8
10	neopentane	463-82-1	72.15	0.64	0.69	-7%	1		0	6
11	isopentane	78-78-4	72.15	1.36	1.68	-19%	1		0	6
12	cyclopentane	287-92-3	70.13	2.25	2.69	-16%	1		0	6
13	n-hexane	110-54-3	86.18	1.15	1.45	-20%	1	3	0	2
14	branched C6 alkane(s)		86.18	1.23	1.53	-19%			0	8
15	2,2-dimethyl butane	75-83-2	86.18	1.11	1.33	-16%	1		0	6
16	2,3-dimethyl butane	79-29-8	86.18	0.91	1.14	-20%	1		0	6
17	2-methyl pentane	107-83-5	86.18	1.41	1.80	-22%	1		0	6
18	3-methyl pentane	96-14-0	86.18	1.70	2.07	-18%	1		0	6
19	C6 cycloalkane(s)		84.16	1.16	1.46	-21%			0	8
20	cyclohexane	110-82-7	84.16	1.16	1.46	-21%	1	2	0	2
21	isopropyl cyclopropane	3638-35-5	84.16	1.15	1.52	-24%	1		0	6
22	methyl cyclopentane	96-37-7	84.16	2.06	2.42	-15%			0	7
23	unspeciated C6 alkane(s)		85.51	1.27	1.48	-14%			0	8
24	n-heptane	142-82-5	100.20	0.99	1.28	-23%	1		0	6
25	2,2,3-trimethyl butane	464-06-2	100.20	1.06	1.32	-20%	1		0	6
26	2,2-dimethyl pentane	590-35-2	100.20	1.05	1.22	-14%	1		0	6
27	2,3-dimethyl pentane	565-59-3	100.20	1.26	1.55	-19%			0	7
28	2,4-dimethyl pentane	108-08-7	100.20	1.46	1.65	-11%	1		0	6
29	2-methyl hexane	591-76-4	100.20	1.10	1.37	-19%			0	7
30	3,3-dimethyl pentane	562-49-2	100.20	1.13	1.32	-15%			0	7
31	3-methyl hexane	589-34-4	100.20	1.51	1.86	-19%			0	7
32	3-ethyl pentane	617-78-7	100.20	1.79					0	7
33	branched C7 alkane(s)		100.20	1.39	1.63	-15%			0	8
34	1,1-dimethyl cyclopentane	1638-26-2	98.19	1.01					0	7
35	1,2-dimethyl cyclopentane	2452-99-5	98.19	1.87					0	7
36	C7 cycloalkane(s)		98.19	1.58	1.99	-21%			0	7
37	1,3-dimethyl cyclopentane	2453-00-1	98.19	1.82	2.15	-15%			0	7
38	cycloheptane	291-64-5	98.19	1.83	2.26	-19%	1		0	6
39	ethyl cyclopentane	1640-89-7	98.19	1.89	2.27	-17%			0	7
40	methyl cyclohexane	108-87-2	98.19	1.58	1.99	-21%	1		0	6
41	unspeciated C7 alkane(s)		99.53	1.28	1.79	-29%			0	8
42	n-octane	111-65-9	114.23	0.82	1.11	-26%	1	1	0	2
43	branched C8 alkane(s)		114.23	1.35	1.57	-14%			0	8
44	2,2,3,3-tetramethyl butane	594-82-1	114.23	0.31	0.44	-30%	1		0	6

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
45	2,2,4-trimethyl pentane	540-84-1	114.23	1.20	1.44	-17%	1	3	0	2
46	2,2-dimethyl hexane	590-73-8	114.23	0.95	1.13	-16%	1		0	6
47	2,3,4-trimethyl pentane	565-75-3	114.23	0.96	1.23	-22%	1		0	6
48	2,3-dimethyl hexane	584-94-1	114.23	1.11	1.34	-17%			0	7
49	2,4-dimethyl hexane	589-43-5	114.23	1.62	1.80	-10%			0	7
50	2,5-dimethyl hexane	592-13-2	114.23	1.36	1.68	-19%			0	7
51	2-methyl heptane	592-27-8	114.23	0.99	1.20	-18%			0	7
52	3-methyl heptane	589-81-1	114.23	1.15	1.35	-15%			0	7
53	4-methyl heptane	589-53-7	114.23	1.16	1.48	-21%			0	7
54	2,3,3-trimethyl pentane	560-21-4	114.23	0.95					0	7
55	3,3-dimethyl hexane	563-16-6	114.23	1.16					0	7
56	2,2,3-trimethyl pentane	564-02-3	114.23	1.15					0	7
57	3,4-dimethyl hexane	583-48-2	114.23	1.41					0	7
58	3-ethyl 2-methyl pentane	609-26-7	114.23	1.25					0	7
59	C8 bicycloalkane(s)		110.20	1.41	1.75	-20%			0	8
60	1,1,2-trimethyl cyclopentane	4259-00-1	112.21	1.04					0	7
61	1,1,3-trimethyl cyclopentane	4516-69-2	112.21	0.94					0	7
62	1,1-dimethyl cyclohexane	590-66-9	112.21	1.13					0	7
63	1,2,3-trimethyl cyclopentane		112.21	1.52					0	7
64	1,2,4-trimethyl cyclopentane		112.21	1.43					0	7
65	1-methyl-3-ethyl cyclopentane		112.21	1.53					0	7
66	1,2-dimethyl cyclohexane	583-57-3	112.21	1.30					0	7
67	1,4-dimethyl cyclohexane	589-90-2	112.21	1.51					0	7
68	C8 cycloalkane(s)		112.21	1.37	1.75	-22%			0	8
69	1,3-dimethyl cyclohexane	591-21-9	112.21	1.41	1.72	-18%			0	7
70	cyclooctane	292-64-8	112.21	1.35	1.73	-22%	1		0	6
71	ethyl cyclohexane	1678-91-7	112.21	1.37	1.75	-22%			0	7
72	propyl cyclopentane	2040-96-2	112.21	1.57	1.91	-18%			0	7
73	unspciated C8 alkane(s)		113.56	1.19	1.64	-28%			0	8
74	n-nonane	111-84-2	128.26	0.71	0.95	-25%	1		0,+	6b
75	branched C9 alkane(s)		128.26	1.05	1.25	-16%			0	8b
76	2,2,5-trimethyl hexane	3522-94-9	128.26	1.06	1.33	-20%			0	7b
77	2,3,5-trimethyl hexane	1069-53-0	128.26	1.14	1.33	-14%	1		0	6b
78	2,4-dimethyl heptane	2213-23-2	128.26	1.29	1.48	-13%			0	7b
79	2-methyl octane	3221-61-2	128.26	0.75	0.96	-22%	1		0,+	6b
80	3,3-diethyl pentane	1067-20-5	128.26	1.14	1.35	-16%	1		0,+	6b
81	3,5-dimethyl heptane	926-82-9	128.26	1.45	1.63	-11%			0	7b
82	4-ethyl heptane	2216-32-2	128.26	1.13	1.44	-21%			0	7b
83	4-methyl octane	2216-34-4	128.26	0.87	1.08	-19%	1		0,+	6b
84	2,4,4-trimethyl hexane	16747-30-1	128.26	1.26					0	7b
85	3,3-dimethyl heptane	4032-86-4	128.26	1.05					0	7b
86	4,4-dimethyl heptane	1068-19-5	128.26	1.19					0	7b
87	2,2-dimethyl heptane	1071-26-7	128.26	0.93					0	7b
88	2,2,4-trimethyl hexane	16747-26-5	128.26	1.19					0	7b
89	2,6-dimethyl heptane	1072-05-5	128.26	0.96					0	7b
90	2,3-dimethyl heptane	3074-71-3	128.26	1.01					0	7b
91	2,5-dimethyl heptane	2216-30-0	128.26	1.25					0	7b
92	3-methyl octane	2216-33-3	128.26	0.91					0	7b
93	3,4-dimethyl heptane	922-28-1	128.26	1.15					0	7b
94	3-ethyl heptane	15869-80-4	128.26	1.01					0	7b
95	cis-hydrindane; bicyclo[4.3.0]nonane	496-10-6	124.22	1.20					0	7b

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]				
				New	Old	Chg	k a	Expt	Bias	Unc	
96	C9 bicycloalkane(s)		124.22	1.28	1.57	-18%				0	8b
97	1,2,3-trimethyl cyclohexane	1678-97-3	126.24	1.12						0	7b
98	1,3,5-trimethyl cyclohexane	1839-63-0	126.24	1.06						0	7b
99	1,1,3-trimethyl cyclohexane	3073-66-3	126.24	1.11	1.37	-19%	1			0	6b
100	1-ethyl-4-methyl cyclohexane	3728-56-1	126.24	1.33	1.62	-18%				0	7b
101	propyl cyclohexane	1678-92-8	126.24	1.19	1.47	-19%				0	7b
102	C9 cycloalkane(s)		126.24	1.26	1.55	-19%				0	8b
103	unspeciated C9 alkane(s)		127.59	0.99	2.13	-54%				0	8
104	n-decane	124-18-5	142.28	0.62	0.83	-26%	1			0,+	6b
105	branched C10 alkane(s)		142.28	0.86	1.09	-21%				0	8b
106	2,4,6-trimethyl heptane	2613-61-8	142.28	1.20						0	7b
107	2,4-dimethyl octane	4032-94-4	142.28	0.95	1.09	-13%				0	7b
108	2,6-dimethyl octane	2051-30-1	142.28	1.00	1.27	-21%	1	2		0,+	2b
109	2-methyl nonane	871-83-0	142.28	0.65	0.86	-24%	1	2		0,+	2b
110	3,4-diethyl hexane	19398-77-7	142.28	0.83	1.20	-31%	1	2		0,+	2b
111	3-methyl nonane	5911-04-6	142.28	0.68	0.89	-23%				0	7b
112	4-methyl nonane	17301-94-9	142.28	0.78	0.99	-21%				0	7b
113	4-propyl heptane	3178-29-8	142.28	0.94	1.24	-25%				0	7b
114	2,4,4-trimethyl heptane		142.28	1.23						0	7b
115	2,5,5-trimethyl heptane		142.28	1.17						0	7b
116	3,3-dimethyl octane	4110-44-5	142.28	1.01						0	7b
117	4,4-dimethyl octane	15869-95-1	142.28	1.06						0	7b
118	2,2-dimethyl octane	15869-87-1	142.28	0.77						0	7b
119	2,2,4-trimethyl heptane	14720-74-2	142.28	1.09						0	7b
120	2,2,5-trimethyl heptane		142.28	1.18						0	7b
121	2,3,6-trimethyl heptane	4032-93-3	142.28	0.82						0	7b
122	2,3-dimethyl octane	7146-60-3	142.28	0.79						0	7b
123	2,5-dimethyl octane		142.28	0.94						0	7b
124	2-methyl-3-ethyl heptane	14676-29-0	142.28	0.91						0	7b
125	4-ethyl octane	15869-86-0	142.28	0.71						0	7b
126	C10 bicycloalkane(s)		138.25	1.00	1.29	-22%				0	8b
127	isobutyl cyclohexane; (2-methylpropyl) cyclohexane	1678-98-4	140.27	0.90						0	8b
128	sec-butyl cyclohexane	7058-01-7	140.27	0.90						0	8b
129	C10 cycloalkane(s)		140.27	0.99	1.27	-22%				0	8b
130	1,3-diethyl cyclohexane	1678-99-5	140.27	1.16	1.34	-13%				0	7b
131	1,4-diethyl cyclohexane	1679-00-1	140.27	1.14	1.49	-24%				0	7b
132	1-methyl-3-isopropyl cyclohexane	16580-24-8	140.27	0.92	1.26	-27%				0	7b
133	butyl cyclohexane	1678-93-9	140.27	0.90	1.07	-15%	1			0	6b
134	unspeciated C10 alkane(s)		141.61	0.82	1.16	-29%				0	8
135	n-undecane	1120-21-4	156.31	0.55	0.74	-26%	1			0,+	6b
136	branched C11 alkane(s)		156.31	0.66	0.87	-24%				0	8b
137	2,3,4,6-tetramethyl heptane	61868-54-0	156.31	1.03	1.26	-19%				0	7b
138	2,6-dimethyl nonane	17302-28-2	156.31	0.72	0.95	-24%				0	7b
139	3,5-diethyl heptane	61869-02-1	156.31	1.02	1.21	-15%				0	7b
140	3-methyl decane	13151-34-3	156.31	0.58	0.77	-25%				0	7b
141	4-methyl decane	2847-72-5	156.31	0.61	0.80	-23%				0	7b
142	C11 bicycloalkane(s)		152.28	0.83	1.01	-18%				0	8b
143	C11 cycloalkane(s)		154.29	0.82	0.99	-17%				0	8b
144	1,3-diethyl-5-methyl cyclohexane	164259-42-1	154.29	0.96	1.11	-13%				0	7b



Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]				
				New	Old	Chg	k	a	Expt	Bias	Unc
145	1-ethyl-2-propyl cyclohexane	62238-33-9	154.29	0.73	0.95	-23%				0	7b
146	pentyl cyclohexane	4292-92-6	154.29	0.77	0.91	-16%				0	7b
147	unspeciated C11 alkane(s)		155.64	0.67	0.90	-26%				0	8
148	n-dodecane	112-40-3	170.33	0.50	0.66	-25%	1	2	0,+		3b
149	branched C12 alkane(s)		170.33	0.56	0.80	-29%				0	8b
150	2,3,5,7-tetramethyl octane	62199-32-0	170.33	0.84	1.06	-21%				0	7b
151	2,6-diethyl octane	62183-94-2	170.33	0.89	1.09	-18%				0	7b
152	3,6-dimethyl decane	17312-53-7	170.33	0.62	0.88	-29%				0	7b
153	3-methyl undecane	1002-43-3	170.33	0.53	0.70	-25%				0	7b
154	5-methyl undecane	1632-70-8	170.33	0.49	0.72	-32%				0	7b
155	C12 tricycloalkane(s)		164.29	0.74						0	8b
156	C12 bicycloalkane(s)		166.30	0.73	0.88	-17%				0	8b
157	C12 cycloalkane(s)		168.32	0.72	0.87	-17%				0	8b
158	1,3,5-triethyl cyclohexane	164259-43-2	168.32	0.94	1.06	-11%				0	7b
159	1-methyl-4-pentyl cyclohexane	75736-67-3	168.32	0.65	0.81	-19%				0	7b
160	hexyl cyclohexane	4292-75-5	168.32	0.57	0.75	-23%	1	2	0		2b
161	unspeciated C12 alkane(s)		169.66	0.61	0.81	-24%				0	8
162	n-tridecane	629-50-5	184.36	0.47	0.62	-24%	1		0,+		6b
163	branched C13 alkane(s)		184.36	0.54	0.73	-27%				0	8b
164	2,3,6-trimethyl 4-isopropyl heptane		184.36	0.85	1.24	-31%				0	7b
165	2,4,6,8-tetramethyl nonane	14638-54-1	184.36	0.69	0.94	-27%				0	7b
166	3,6-dimethyl undecane	17301-28-9	184.36	0.62	0.82	-24%				0	7b
167	3,7-diethyl nonane		184.36	0.81	1.08	-25%				0	7b
168	3-methyl dodecane	17312-57-1	184.36	0.49	0.64	-24%				0	7b
169	5-methyl dodecane	17453-93-9	184.36	0.41	0.64	-36%				0	7b
170	C13 tricycloalkane(s)		178.31	0.64						0	8b
171	C13 bicycloalkane(s)		180.33	0.64	0.79	-20%				0	8b
172	C13 cycloalkane(s)		182.35	0.63	0.78	-19%				0	8b
173	1,3-diethyl-5-propyl cyclohexane		182.35	0.89	0.96	-8%				0	7b
174	1-methyl-2-hexyl cyclohexane	92031-93-1	182.35	0.52	0.70	-26%				0	7b
175	heptyl cyclohexane	5617-41-4	182.35	0.49	0.66	-26%				0	7b
176	unspeciated C13 alkane(s)		183.69	0.56	0.73	-23%				0	8
177	n-tetradecane	629-59-4	198.39	0.46	0.58	-21%	1	2	0,+		3b
178	branched C14 alkane(s)		198.39	0.49	0.67	-27%				0	8b
179	2,4,5,6,8-pentamethyl nonane		198.39	0.87	1.11	-22%				0	7b
180	2-methyl 3,5-diisopropyl heptane		198.39	0.49	0.78	-37%				0	7b
181	3,7-dimethyl dodecane	82144-67-0	198.39	0.56	0.74	-24%				0	7b
182	3,8-diethyl decane	6224-52-8	198.39	0.53	0.68	-22%				0	7b
183	3-methyl tridecane	6418-41-3	198.39	0.45	0.57	-21%				0	7b
184	6-methyl tridecane	13287-21-3	198.39	0.40	0.62	-36%				0	7b
185	C14 tricycloalkane(s)		192.34	0.60						0	8b
186	C14 bicycloalkane(s)		194.36	0.59	0.71	-17%				0	8b
187	C14 cycloalkane(s)		196.37	0.59	0.71	-17%				0	8b
188	1,3-dipropyl-5-ethyl cyclohexane		196.37	0.84	0.94	-10%				0	7b
189	trans-1-methyl-4-heptyl cyclohexane	205324-73-8	196.37	0.47	0.58	-19%				0	7b
190	octyl cyclohexane	1795-15-9	196.37	0.45	0.60	-25%		2	0		7b
191	unspeciated C14 alkane(s)		197.72	0.52	0.67	-22%				0	8

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
192	n-pentadecane	629-62-9	212.41	0.44	0.53	-17%	1	4	0,+	3b
193	branched C15 alkane(s)		212.41	0.45	0.60	-26%			0	8b
194	2,6,8-trimethyl 4-isopropyl nonane		212.41	0.57	0.76	-25%			0	7b
195	3,7-dimethyl tridecane		212.41	0.50	0.64	-22%			0	7b
196	3,9-diethyl undecane	13286-72-1	212.41	0.46	0.62	-26%			0	7b
197	3-methyl tetradecane	18435-22-8	212.41	0.43	0.53	-19%			0	7b
198	6-methyl tetradecane	26730-16-5	212.41	0.37	0.57	-36%			0	7b
199	C15 tricycloalkane(s)		206.37	0.56					0	8b
200	C15 bicycloalkane(s)		208.38	0.56	0.69	-19%			0	8b
201	C15 cycloalkane(s)		210.40	0.55	0.68	-19%			0	8b
202	1,3,5-tripropyl cyclohexane		210.40	0.81	0.90	-10%			0	7b
203	1-methyl-2-octyl cyclohexane		210.40	0.45	0.60	-26%			0	7b
204	nonyl cyclohexane	2883-02-5	210.40	0.41	0.54	-24%			0	7b
205	1,3-diethyl-5-pentyl cyclohexane		210.40	0.61	0.99	-39%			0	7b
206	unspeciated C15 alkane(s)		211.74	0.49	0.61	-19%			0	8
207	n-hexadecane; n-C16	544-76-3	226.44	0.39	0.52	-24%	1	3	0,+	3b
208	branched C16 alkane(s)		226.44	0.42	0.54	-22%			0	8b
209	2,7-dimethyl 3,5-diisopropyl heptane		226.44	0.47	0.69	-33%			0	7b
210	3-methyl pentadecane	2882-96-4	226.44	0.41	0.50	-19%			0	7b
211	4,8-dimethyl tetradecane	175032-36-7	226.44	0.44	0.55	-21%			0	7b
212	7-methyl pentadecane	6165-40-8	226.44	0.40	0.51	-21%			0	7b
213	C16 tricycloalkane(s)		220.39	0.53					0	8b
214	C16 bicycloalkane(s)		222.41	0.52					0	8b
215	C16 cycloalkane(s)		224.43	0.49	0.61	-19%			0	8b
216	1,3-propyl-5-butyl cyclohexane		224.43	0.69	0.77	-10%			0	7b
217	1-methyl-4-nonyl cyclohexane	39762-40-8	224.43	0.41	0.55	-25%			0	7b
218	decyl cyclohexane	1795-16-0	224.43	0.38	0.50	-24%			0	7b
219	unspeciated C16 alkane(s)		225.77	0.45	0.55	-18%			0	8
220	n-heptadecane; n-C17	629-78-7	240.47	0.37	0.49	-25%			0,+	7b
221	branched C17 alkane(s)		240.47	0.40	0.51	-22%			0	8b
222	C17 tricycloalkane(s)		234.42	0.50					0	8b
223	C17 bicycloalkane(s)		236.44	0.49					0	8b
224	C17 cycloalkane(s)		238.45	0.46					0	8b
225	unspeciated C17 alkane(s)		239.80	0.43	0.52	-18%			0	8
226	n-octadecane; n-C18	593-45-3	254.49	0.35	0.44	-21%			0,+	7b
227	branched C18 alkane(s)		254.49	0.37	0.48	-22%			0	8b
228	C18 tricycloalkane(s)		248.45	0.47					0	8b
229	C18 bicycloalkane(s)		250.46	0.46					0	8b
230	C18 cycloalkane(s)		252.48	0.44					0	8b
231	unspeciated C18 alkane(s)		253.82	0.40	0.49	-18%			0	8
232	n-nonadecane; n-C19	629-92-5	268.52	0.33	0.44	-25%			0,+	7b
233	branched C19 alkane(s)		268.52	0.35					0	8b
234	C19 tricycloalkane(s)		262.47	0.44					0	8b
235	C19 bicycloalkane(s)		264.49	0.44					0	8b
236	C19 cycloalkane(s)		266.51	0.42					0	8b
237	n-eicosane; n-C20	112-95-8	282.55	0.31	0.42	-25%			0,+	7b
238	branched C20 alkane(s)		282.55	0.34					0	8b
239	C20 tricycloalkane(s)		276.50	0.42					0	8b
240	C20 bicycloalkane(s)		278.52	0.42					0	8b

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]				
				New	Old	Chg	k a	Expt	Bias	Unc	
241	C20 cycloalkane(s)		280.53	0.39						0	8b
242	n-henicosane; n-C21	629-94-7	296.57	0.30	0.40	-25%				0,+	7b
243	branched C21 alkane(s)		296.57	0.32						0	8b
244	C21 tricycloalkane(s)		290.53	0.40						0	8b
245	C21 bicycloalkane(s)		292.54	0.40						0	8b
246	C21 cycloalkane(s)		294.56	0.38						0	8b
247	n-docosane; n-C22	629-97-0	310.60	0.29	0.38	-25%				0,+	7b
248	branched C22 alkane(s)		310.60	0.31						0	8b
249	C22 tricycloalkane(s)		304.55	0.38						0	8b
250	C22 bicycloalkane(s)		306.57	0.38						0	8b
251	C22 cycloalkane(s)		308.58	0.36						0	8b
			<u>Alkenes</u>								
252	ethene	74-85-1	28.05	8.76	9.08	-4%	1	1	0		3d
253	propene	115-07-1	42.08	11.37	11.58	-2%	1	1	0		3d
254	1,2-propadiene; allene	463-49-0	40.06	8.11			1		0		11
255	1-butene	106-98-9	56.11	9.42	10.29	-8%	1	3	0		3d
256	C4 terminal alkenes		56.11	9.42	10.29	-8%			0		7
257	isobutene	115-11-7	56.11	6.14	6.35	-3%	1	3	0		3
258	cis-2-butene	590-18-1	56.11	13.89	13.22	5%	1		0		6
259	trans-2-butene	624-64-6	56.11	14.79	13.91	6%	1	1	0		3
260	C4 internal alkenes		56.11	14.34	13.57	6%			0		7
261	1,2-butadiene	590-19-2	54.09	9.03			1		0		11
262	1,3-butadiene	106-99-0	54.09	12.21	13.58	-10%	1		0		6
263	C4 alkenes		56.11	11.88	11.93	0%			0		8
264	1-pentene	109-67-1	70.13	6.97	7.79	-11%	1		0		6d
265	3-methyl-1-butene	563-45-1	70.13	6.76	6.99	-3%	1		0		6d
266	C5 terminal alkenes		70.13	6.97	7.79	-11%			0		7
267	2-methyl-1-butene	563-46-2	70.13	6.23	6.51	-4%	1		0		8
268	2-methyl-2-butene	513-35-9	70.13	13.72	14.45	-5%	1		0		6
269	cis-2-pentene	627-20-3	70.13	10.07	10.24	-2%	1		0		6
270	trans-2-pentene	646-04-8	70.13	10.25	10.23	0%	1		0		6
271	2-pentenenes		70.13	10.16	10.23	-1%			0		7
272	C5 internal alkenes		70.13	10.16	10.23	-1%			0		7
273	cyclopentene	142-29-0	68.12	6.55	7.38	-11%	1		0		8
274	trans-1,3-pentadiene	2004-70-8	68.12	12.10					0		8
275	cis-1,3-pentadiene	1574-41-0	68.12	12.10					0		8
276	1,4-pentadiene	591-93-5	68.12	8.92			1		0		8
277	1,2-pentadiene	591-95-7	68.12	7.59			1		0		11
278	3-methyl-1,2-butadiene	598-25-4	68.12	9.95			1		0		11
279	Isoprene; 2-methyl-1,3-butadiene	78-79-5	68.12	10.28	10.69	-4%	1	2	0		1
280	cyclopentadiene	542-92-7	66.10	6.75	7.61	-11%			0		8
281	C5 alkenes		70.13	8.57	9.01	-5%			0		8
282	1-hexene	592-41-6	84.16	5.28	6.17	-14%	1	4	0		4d
283	3,3-dimethyl-1-butene	558-37-2	84.16	5.61	6.06	-7%	1		0		8d
284	3-methyl-1-pentene	760-20-3	84.16	5.93	6.22	-5%			0		8
285	4-methyl-1-pentene	691-37-2	84.16	5.48	6.26	-12%			0		8
286	C6 terminal alkenes		84.16	5.28	6.17	-14%			0		8
287	2,3-dimethyl-1-butene	563-78-0	84.16	4.61	4.77	-3%			0		8
288	2-ethyl-1-butene	760-21-4	84.16	4.93	5.04	-2%			0		8
289	2-methyl-1-pentene	763-29-1	84.16	5.12	5.18	-1%	1		0		8
290	2,3-dimethyl-2-butene	563-79-1	84.16	12.13	13.32	-9%	1		0		8

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
291	2-methyl-2-pentene	625-27-4	84.16	10.70	12.28	-13%	1		0	8
292	cis 4-methyl-2-pentene		84.16	7.88					0	8
293	cis-2-hexene	7688-21-3	84.16	8.06	8.44	-4%			0	8
294	cis-3-hexene	7642-09-3	84.16	7.33	8.22	-11%			0	8
295	cis-3-methyl-2-pentene	922-62-3	84.16	12.15	12.84	-5%			0	8
296	trans-3-methyl-2-pentene	616-12-6	84.16	12.81					0	8
297	trans-4-methyl-2-pentene	674-76-0	84.16	7.88			1		0	8
298	trans-2-hexene	4050-45-7	84.16	8.37	8.44	-1%			0	8
299	trans-3-hexene	13269-52-8	84.16	7.30	8.16	-11%			0	8
300	2-hexenes	592-43-8	84.16	8.21	8.44	-3%			0	8
301	C6 internal alkenes		84.16	8.21	8.44	-3%			0	8
302	3-methyl cyclopentene	1120-62-3	82.14	4.92					0	8
303	1-methyl cyclopentene	693-89-0	82.14	12.11	13.95	-13%			0	8
304	cyclohexene	110-83-8	82.14	4.81	5.45	-12%	1	4	0	4
305	trans,trans-2,4-hexadiene	5194-51-4	82.14	8.57					0	8
306	trans-1,3-hexadiene	20237-34-7	82.14	10.03					0	8
307	trans-1,4-hexadiene	7319-00-8	82.14	8.36			1		0	8
308	C6 cyclic olefins or di-olefins		82.14	8.41	8.65	-3%			0	8
309	C6 alkenes		84.16	6.75	6.88	-2%			0	8
310	trans-4-methyl-2-hexene		98.19	6.96	7.88	-12%			0	8
311	trans-3-methyl-2-hexene		98.19	9.80	14.17	-31%			0	8
312	2,3-dimethyl-2-hexene		112.21	8.28	10.41	-20%			0	8
313	1-heptene	592-76-7	98.19	4.25	4.20	1%	1		0	8d
314	3,4-dimethyl-1-pentene	7385-78-6	98.19	4.66					0	8
315	3-methyl-1-hexene	3404-61-3	98.19	4.24					0	8
316	2,4-dimethyl-1-pentene	2213-32-3	98.19	5.81					0	8
317	2,3-dimethyl-1-pentene	3404-72-6	98.19	4.97					0	8
318	3,3-dimethyl-1-pentene	3404-73-7	98.19	4.71					0	8
319	2-methyl-1-hexene	6094-02-6	98.19	4.92					0	8
320	2,3,3-trimethyl-1-butene	594-56-9	98.19	4.33	4.62	-6%			0	8
321	C7 terminal alkenes		98.19	4.25	4.20	1%			0	8
322	4,4-dimethyl-cis-2-pentene	762-63-0	98.19	6.45					0	8
323	2,4-dimethyl-2-pentene	625-65-0	98.19	9.03					0	8
324	2-methyl-2-hexene	2738-19-4	98.19	9.22					0	8
325	3-ethyl-2-pentene	816-79-5	98.19	9.49					0	8
326	3-methyl-trans-3-hexene	3899-36-3	98.19	9.44					0	8
327	cis-2-heptene	6443-92-1	98.19	6.94					0	8
328	2-methyl-trans-3-hexene	692-24-0	98.19	6.03					0	8
329	3-methyl-cis-3-hexene	4914-89-0	98.19	9.44					0	8
330	3,4-dimethyl-cis-2-pentene	4914-91-4	98.19	8.91					0	8
331	2,3-dimethyl-2-pentene	10574-37-5	98.19	9.45			1		0	8
332	cis-3-heptene	7642-10-6	98.19	6.10	6.96	-12%			0	8
333	trans-4,4-dimethyl-2-pentene	690-08-4	98.19	6.45	6.99	-8%	1		0	8
334	trans-2-heptene	14686-13-6	98.19	6.92	7.33	-6%	1		0	8
335	trans-3-heptene	14686-14-7	98.19	6.09	6.96	-13%			0	8
336	cis-3-methyl-2-hexene	10574-36-4	98.19	9.80	13.38	-27%			0	8
337	2-heptenes		98.19	6.09	6.96	-12%			0	8
338	C7 internal alkenes		98.19	6.09	6.96	-13%			0	8
339	1-methyl cyclohexene	591-49-1	96.17	6.41	7.81	-18%	1		0	8
340	4-methyl cyclohexene	591-47-9	96.17	4.02	4.48	-10%			0	8
341	C7 cyclic olefins or di-olefins		96.17	7.07	7.49	-6%			0	8
342	C7 alkenes		98.19	5.17	5.76	-10%			0	8

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
343	1-octene	111-66-0	112.21	3.12	3.45	-10%			0	8
344	C8 terminal alkenes		112.21	3.12	3.45	-10%			0	8
345	2,4,4-trimethyl-1-pentene	107-39-1	112.21	3.24					0	8
346	3-methyl-2-isopropyl-1-butene	111823-35-9	112.21	3.17	3.29	-4%			0	8
347	trans-2-octene	13389-42-9	112.21	5.81					0	8
348	2-methyl-2-heptene	627-97-4	112.21	8.10					0	8
349	cis-4-octene	7642-15-1	112.21	4.55	5.94	-23%			0	8
350	trans-2,2-dimethyl 3-hexene	690-93-7	112.21	4.81	5.97	-19%			0	8
351	trans-2,5-dimethyl 3-hexene	692-70-6	112.21	4.63	5.44	-15%			0	8
352	trans-3-octene	14919-01-8	112.21	5.14	6.13	-16%			0	8
353	trans-4-octene	14850-23-8	112.21	4.63	5.90	-22%	1		0	8
354	3-octenes		112.21	5.14	6.13	-16%			0	8
355	C8 internal alkenes		112.21	4.63	5.90	-22%			0	8
356	2,4,4-trimethyl-2-pentene	107-40-4	112.21	6.13	8.52	-28%			0	8
357	1,2-dimethyl cyclohexene	1674-10-8	110.20	5.43	6.77	-20%			0	8
358	C8 cyclic olefins or di-olefins		110.20	4.71	6.01	-22%			0	8
359	C8 alkenes		112.21	3.88	4.68	-17%			0	8
360	1-nonene	124-11-8	126.24	2.48	2.76	-10%			0	8
361	C9 terminal alkenes		126.24	2.48	2.76	-10%			0	8
362	4,4-dimethyl-1-pentene	762-62-9	126.24	3.00					0	8
363	4-nonene	2198-23-4	126.24	4.37					0	8
364	3-nonenes		126.24	4.37	5.31	-18%			0	8
365	C9 internal alkenes		126.24	4.37	5.31	-18%			0	8
366	trans-4-nonene	10405-85-3	126.24	4.37	5.23	-16%			0	8
367	C9 cyclic olefins or di-olefins		124.22	4.44	5.40	-18%			0	8
368	C9 alkenes		126.24	3.43	4.03	-15%			0	8
369	1-decene	872-05-9	140.27	2.07	2.28	-9%			0	8
370	C10 terminal alkenes		140.27	2.07	2.28	-9%			0	8
371	3,4-diethyl-2-hexene	59643-70-8	140.27	3.25	3.95	-18%			0	8
372	cis-5-decene	7433-78-5	140.27	3.52	4.89	-28%			0	8
373	trans-4-decene	19398-89-1	140.27	3.72	4.50	-17%			0	8
374	C10 3-alkenes		140.27	3.72	4.50	-17%			0	8
375	C10 internal alkenes		140.27	3.72	4.50	-17%			0	8
376	C10 cyclic olefins or di-olefins		138.25	3.78	4.56	-17%			0	8
377	3-carene	13466-78-9	136.23	3.13	3.21	-3%	1	3	0	4
378	$\alpha$ -pinene	80-56-8	136.23	4.38	4.29	2%	1	2	0	4
379	$\beta$ -pinene	127-91-3	136.23	3.38	3.28	3%	1	2	0	4
380	d-limonene	5989-27-5	136.23	4.40	3.99	10%	1	2	0	4
381	sabinene	3387-41-5	136.23	4.01	3.67	9%	1	3	0	4
382	Terpinolene	586-62-9	136.23	6.16					0	8
383	Camphene	79-92-5	136.23	4.38					0	8
384	terpene (monoterpenes)		136.23	3.91	3.79	3%			0	8
385	C10 alkenes		140.27	3.17	3.39	-6%			0	8
386	1-undecene	821-95-4	154.29	1.78	1.95	-9%			0	8
387	C11 terminal alkenes		154.29	1.78	1.95	-9%			0	8
388	trans-5-undecene	764-97-6	154.29	3.46	4.23	-18%			0	8
389	C11 3-alkenes		154.29	3.46	4.23	-18%			0	8
390	C11 internal alkenes		154.29	3.46	4.23	-18%			0	8
391	C11 cyclic olefins or di-olefins		152.28	3.50	4.29	-18%			0	8
392	C11 alkenes		154.29	2.62	3.09	-15%			0	8
393	C12 terminal alkenes		168.32	1.56	1.72	-9%			0	8
394	1-dodecene	112-41-4	168.32	1.56	1.72	-9%			0	8

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
395	C12 2-alkenes		168.32	3.02	3.75	-20%			0	8
396	C12 3-alkenes		168.32	3.02	3.75	-20%			0	8
397	C12 internal alkenes		168.32	3.02	3.75	-20%			0	8
398	trans-5-dodecene	7206-16-8	168.32	3.02	3.74	-19%			0	8
399	C12 cyclic olefins or di-olefins		166.30	3.05	3.79	-19%			0	8
400	C12 alkenes		168.32	2.29	2.73	-16%			0	8
401	1-tridecene	2437-56-1	182.35	1.41	1.55	-9%			0	8
402	C13 terminal alkenes		182.35	1.41	1.55	-9%			0	8
403	trans-5-tridecene	23051-84-5	182.35	2.49	3.38	-26%			0	8
404	C13 3-alkenes		182.35	2.49	3.38	-26%			0	8
405	C13 internal alkenes		182.35	2.49	3.38	-26%			0	8
406	C13 cyclic olefins or di-olefins		180.33	2.51	3.42	-26%			0	8
407	C13 alkenes		182.35	1.95	2.46	-21%			0	8
408	1-tetradecene	1120-36-1	196.37	1.27	1.41	-10%			0	8
409	C14 terminal alkenes		196.37	1.27	1.41	-10%			0	8
410	trans-5-tetradecene	41446-66-6	196.37	2.26	3.08	-27%			0	8
411	C14 3-alkenes		196.37	2.26	3.08	-27%			0	8
412	C14 internal alkenes		196.37	2.26	3.08	-27%			0	8
413	C14 cyclic olefins or di-olefins		194.36	2.29	3.11	-26%			0	8
414	C14 alkenes		196.37	1.77	2.28	-22%			0	8
415	1-pentadecene	13360-61-7	210.40	1.19	1.27	-6%			0	8
416	C15 terminal alkenes		210.40	1.19	1.27	-6%			0	8
417	trans-5-pentadecene	74392-33-9	210.40	2.08	2.82	-26%			0	8
418	C15 3-alkenes		210.40	2.08	2.82	-26%			0	8
419	C15 internal alkenes		210.40	2.08	2.82	-26%			0	8
420	C15 cyclic olefins or di-olefins		208.38	2.10	2.85	-26%			0	8
421	C15 alkenes		210.40	1.63	2.06	-21%			0	8
<u>Aromatic Hydrocarbons</u>										
422	benzene	71-43-2	78.11	0.69	0.81	-15%	1	2	0?	4
423	toluene	108-88-3	92.14	3.88	3.97	-2%	1	2	0	4
424	ethyl benzene	100-41-4	106.17	2.93	2.79	5%	1	3	0	4
425	m-xylene	108-38-3	106.17	9.52	10.61	-10%	1	1	0	4
426	o-xylene	95-47-6	106.17	7.44	7.49	-1%	1	2	0	4
427	p-xylene	106-42-3	106.17	5.69	4.25	34%	1	3	0	4
428	C8 disubstituted benzenes	1330-20-7	106.17	7.57	7.48	1%			0	8
429	isomers of ethylbenzene		106.17	6.39	5.16	24%			0	8
430	styrene	100-42-5	104.15	1.65	1.95	-16%	1	2	0	2
431	Unspeciated C8 Aromatics		106.17	7.42					0	8
432	C9 monosubstituted benzenes		120.19	1.95	2.20	-12%			0	8
433	n-propyl benzene	103-65-1	120.19	1.95	2.20	-12%	1		0	8
434	isopropyl benzene; cumene	98-82-8	120.19	2.43	2.32	5%	1		0	8
435	C9 disubstituted benzenes		120.19	5.65	6.61	-15%			0	8
436	m-ethyl toluene	620-14-4	120.19	7.21	9.37	-23%	1		0	8
437	o-ethyl toluene	611-14-3	120.19	5.43	6.61	-18%	1		0	8
438	p-ethyl toluene	622-96-8	120.19	4.32	3.75	15%	1		0	8
439	C9 trisubstituted benzenes	25551-13-7	120.19	10.58	9.90	7%			0	8
440	1,2,3-trimethyl benzene	526-73-8	120.19	11.66	11.26	4%	1	2	0	4
441	1,2,4-trimethyl benzene	95-63-6	120.19	8.64	7.18	20%	1	2	0	4
442	1,3,5-trimethyl benzene	108-67-8	120.19	11.44	11.22	2%	1	2	0	4
443	isomers of propyl benzene		120.19	6.06	6.12	-1%			0	8
444	indene	95-13-6	116.16	1.48	3.21	-54%			0	10
445	indane	496-11-7	118.18	3.20	3.17	1%			0	10

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]				
				New	Old	Chg	k	a	Expt	Bias	Unc
446	allylbenzene	300-57-2	118.18	1.45						0	8
447	$\alpha$ -methyl styrene	98-83-9	118.18	1.45	1.72	-16%				0	8
448	C9 styrenes		118.18	1.45	1.72	-16%				0	8
449	$\beta$ -methyl styrene	637-50-3	118.18	0.95			1			0	8
450	Unspeciated C9 Aromatics		120.09	7.92						0	8
451	C10 monosubstituted benzenes		134.22	2.27	1.97	15%				0	8
452	n-butyl benzene	104-51-8	134.22	2.27	1.97	15%				0	8
453	sec-butyl benzene	135-98-8	134.22	2.27	1.97	15%				0	8
454	tert-butyl benzene	98-06-6	134.22	1.89			1			0	8
455	o-cymene; 1-methyl-2-(1-methylethyl) benzene	527-84-4	134.22	5.34						0	8
456	1-methyl-2-n-propyl benzene	1074-17-5	134.22	5.34						0	8
457	m-cymene; 1-methyl-3-(1-methylethyl) benzene	535-77-3	134.22	6.92						0	8
458	1-methyl-3-n-propyl benzene	1074-43-7	134.22	6.92						0	8
459	1-methyl-4-n-propyl benzene	1074-55-1	134.22	4.31						0	8
460	C10 disubstituted benzenes		134.22	5.53	5.92	-7%				0	8
461	m-C10 disubstituted benzenes		134.22	6.92						0	8
462	o-C10 disubstituted benzenes		134.22	5.34						0	8
463	p-C10 disubstituted benzenes		134.22	4.31						0	8
464	m-diethyl benzene	141-93-5	134.22	6.92	8.39	-18%				0	8
465	o-diethyl benzene	135-01-3	134.22	5.34	5.92	-10%				0	8
466	1-methyl-4-isopropyl benzene; p-cymene	99-87-6	134.22	4.32			1			0	8
467	p-diethyl benzene	105-05-5	134.22	4.31	3.36	28%				0	8
468	1,2,3-C10 trisubstituted benzenes		134.22	9.89						0	8
469	1,2,4-C10 trisubstituted benzenes		134.22	7.35						0	8
470	1,3,5-C10 trisubstituted benzenes		134.22	9.80						0	8
471	1,2,3,4-tetramethyl benzene	488-23-3	134.22	9.01						0	8
472	1,2,4,5-tetramethyl benzene	95-93-2	134.22	9.01						0	8
473	1,2-dimethyl-3-ethyl benzene	933-98-2	134.22	9.89						0	8
474	1,2-dimethyl-4-ethyl benzene	934-80-5	134.22	7.35						0	8
475	1,3-dimethyl-2-ethyl benzene	2870-04-4	134.22	9.89						0	8
476	1,3-dimethyl-4-ethyl benzene	874-41-9	134.22	7.35						0	8
477	1,3-dimethyl-5-ethyl benzene	934-74-7	134.22	9.80						0	8
478	1,4-dimethyl-2-ethyl benzene	1758-88-9	134.22	7.35						0	8
479	1,2,3,5-tetramethyl benzene	527-53-7	134.22	9.01	8.25	9%				0	8
480	C10 trisubstituted benzenes		134.22	9.01	8.86	2%				0	8
481	C10 tetrasubstituted benzenes		134.22	9.01	8.86	2%				0	8
482	butylbenzenes		134.22	5.60	5.48	2%				0	8
483	methyl indanes		132.20	2.86	2.83	1%				0	10
484	tetralin; 1,2,3,4-tetrahydronaphthalene	119-64-2	132.20	2.86	2.83	1%	1	4	+	5	
485	naphthalene	91-20-3	128.17	3.24	3.26	-1%	1	4	+	5	
486	C10 styrenes		132.20	1.30	1.53	-15%				0	8
487	Unspeciated C10 Aromatics		133.91	7.03	5.48	28%				0	8
488	n-pentyl benzene	538-68-1	148.24	2.04						0	8
489	C11 monosubstituted benzenes		148.24	2.04	1.78	14%				0	8
490	m-C11 disubstituted benzenes		148.24	5.98						0	8

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
491	o-C11 disubstituted benzenes		148.24	4.60					0	8
492	p-C11 disubstituted benzenes		148.24	3.77					0	8
493	1-butyl-2-methyl benzene		148.24	4.60					0	8
494	1-ethyl-2-n-propyl benzene		148.24	4.60					0	8
495	o-tert-butyl toluene; 1-(1,1-dimethylethyl)-2-methyl benzene	1074-92-6	148.24	4.60					0	8
496	1-methyl-3-n-butyl benzene	1595-04-6	148.24	5.98					0	8
497	p-isobutyl toluene; 1-methyl-4-(2-methylpropyl) benzene	5161-04-6	148.24	3.77					0	8
498	C11 disubstituted benzenes		148.24	4.79	5.35	-11%			0	8
499	1,2,3-C11 trisubstituted benzenes		148.24	8.64					0	8
500	1,2,4-C11 trisubstituted benzenes		148.24	6.44					0	8
501	1,3,5-C11 trisubstituted benzenes		148.24	8.65					0	8
502	pentamethyl benzene	700-12-9	148.24	7.91					0	8
503	1-methyl-3,5-diethyl benzene	2050-24-0	148.24	8.65					0	8
504	C11 trisubstituted benzenes		148.24	7.91	8.03	-1%			0	8
505	C11 tetrasubstituted benzenes		148.24	7.91	8.03	-1%			0	8
506	C11 pentasubstituted benzenes		148.24	7.91	8.03	-1%			0	8
507	pentyl benzenes		148.24	4.75	4.96	-4%			0	8
508	C11 tetralins or indanes		146.23	2.58	2.56	1%			+	10
509	methyl naphthalenes	1321-94-4	142.20	2.96	4.61	-36%			+	10
510	1-methyl naphthalene	90-12-0	142.20	2.96	4.61	-36%			+	10
511	2-methyl naphthalene	91-57-6	142.20	2.96	4.61	-36%			+	10
512	Unspecified C11 Aromatics		147.72	6.82	4.96	38%			0	8
513	C12 monosubstituted benzenes		162.27	1.83	1.63	12%			0	8
514	m-C12 disubstituted benzenes		162.27	5.35					0	8
515	o-C12 disubstituted benzenes		162.27	4.11					0	8
516	p-C12 disubstituted benzenes		162.27	3.38					0	8
517	1,3-di-n-propyl benzene		162.27	4.11					0	8
518	1,4 di-isopropyl benzene		162.27	3.38					0	8
519	3-isopropyl cumene; 1,3-di-isopropyl benzene	99-62-7	162.27	5.35					0	8
520	C12 disubstituted benzenes		162.27	4.28	4.90	-13%			0	8
521	1,2,3-C12 trisubstituted benzenes		162.27	7.74					0	8
522	1,2,4-C12 trisubstituted benzenes		162.27	5.78					0	8
523	1,3,5-C12 trisubstituted benzenes		162.27	7.79					0	8
524	1-(1,1-dimethylethyl)-3,5-dimethylbenzene	98-19-1	162.27	7.79					0	8
525	C12 trisubstituted benzenes		162.27	7.10	7.33	-3%			0	8
526	C12 tetrasubstituted benzenes		162.27	7.10	7.33	-3%			0	8
527	C12 pentasubstituted benzenes		162.27	7.10	7.33	-3%			0	8
528	C12 hexasubstituted benzenes		162.27	7.10	7.33	-3%			0	8
529	hexyl benzenes		162.27	4.26	4.53	-6%			0	8
530	C12 tetralins or indanes		160.26	2.36	2.33	1%			0	10
531	1-ethyl naphthalene	1127-76-0	156.22	2.69					+	10



Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]				
				New	Old	Chg	k	a	Expt	Bias	Unc
532	C12 naphthalenes		156.22	3.76						+	10
533	C12 monosubstituted naphthalene		156.22	2.69	4.20	-36%				+	10
534	C12 disubstituted naphthalenes		156.22	4.84	5.54	-13%				+	10
535	2,3-dimethyl naphthalene	581-40-8	156.22	4.84	5.54	-13%	1	4		+	5
536	dimethyl naphthalenes		156.22	4.84	5.54	-13%				+	10
537	Unspeciated C12 Aromatics		159.90	6.02	4.53	33%				0	8
538	C13 monosubstituted benzenes		176.30	1.67	1.50	11%				0	8
539	m-C13 disubstituted benzenes		176.30	4.80						0	8
540	o-C13 disubstituted benzenes		176.30	3.67						0	8
541	p-C13 disubstituted benzenes		176.30	3.03						0	8
542	C13 disubstituted benzenes		176.30	3.84	4.50	-15%				0	8
543	1,2,3-C13 trisubstituted benzenes		176.30	6.94						0	8
544	1,2,4-C13 trisubstituted benzenes		176.30	5.20						0	8
545	1,3,5-C13 trisubstituted benzenes		176.30	7.04						0	8
546	C13 trisubstituted benzenes		176.30	6.39	6.75	-5%				0	8
547	C13 tetralins or indanes		174.28	2.17						0	10
548	C13 naphthalenes		170.25	3.45						0	10
549	C13 monosubstituted naphthalene		170.25	2.47	3.86	-36%				0	10
550	C13 disubstituted naphthalenes		170.25	4.44	5.08	-13%				0	10
551	C13 trisubstituted naphthalenes		170.25	4.44	5.08	-13%				0	10
552	Unspeciated C13 Aromatics		175.85	4.88						0	8
553	C14 monosubstituted benzenes		190.32	1.53						0	8
554	m-C14 disubstituted benzenes		190.32	4.32						0	8
555	o-C14 disubstituted benzenes		190.32	3.30						0	8
556	p-C14 disubstituted benzenes		190.32	2.75						0	8
557	C14 disubstituted benzenes		190.32	3.46						0	8
558	1,2,3-C14 trisubstituted benzenes		190.32	6.31						0	8
559	1,2,4-C14 trisubstituted benzenes		190.32	4.75						0	8
560	1,3,5-C14 trisubstituted benzenes		190.32	6.44						0	8
561	C14 trisubstituted benzenes		190.32	5.84						0	8
562	C14 tetralins or indanes		188.31	2.01						0	10
563	C14 naphthalenes		184.28	3.19						0	10
564	Unspeciated C14 Aromatics		189.87	3.93						0	8
565	C15 monosubstituted benzenes		204.35	1.42						0	8
566	C15 disubstituted benzenes		204.35	3.15						0	8
567	m-C15 disubstituted benzenes		204.35	3.93						0	8
568	o-C15 disubstituted benzenes		204.35	3.00						0	8
569	p-C15 disubstituted benzenes		204.35	2.51						0	8
570	C15 trisubstituted benzenes		204.35	5.35						0	8
571	1,2,3-C15 trisubstituted benzenes		204.35	5.77						0	8
572	1,2,4-C15 trisubstituted benzenes		204.35	4.35						0	8

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
573	1,3,5-C15 trisubstituted benzenes		204.35	5.92					0	8
574	C15 tetralins or indanes		202.34	1.87					0	10
575	C15 naphthalenes		198.30	2.97					0	10
576	Unspeciated C15 Aromatics		203.90	3.35					0	8
577	C16 monosubstituted benzenes		218.38	1.32					0	8
578	m-C16 disubstituted benzenes		218.38	3.60					0	8
579	o-C16 disubstituted benzenes		218.38	2.74					0	8
580	p-C16 disubstituted benzenes		218.38	2.30					0	8
581	C16 disubstituted benzenes		218.38	2.88					0	8
582	1,2,3-C16 trisubstituted benzenes		218.38	5.31					0	8
583	1,2,4-C16 trisubstituted benzenes		218.38	4.01					0	8
584	1,3,5-C16 trisubstituted benzenes		218.38	5.47					0	8
585	C16 trisubstituted benzenes		218.38	4.93					0	8
586	C16 tetralins or indanes		216.36	1.75					0	10
587	C16 naphthalenes		212.33	2.77					0	10
588	Unspeciated C16 Aromatics		217.93	2.96					0	8
589	C17 monosubstituted benzenes		232.40	1.24					0	8
590	C17 disubstituted benzenes		232.40	2.71					0	8
591	C17 trisubstituted benzenes		232.40	4.63					0	8
592	C17 tetralins or indanes		230.39	1.64					0	10
593	C17 naphthalenes		226.36	2.60					0	10
594	C18 monosubstituted benzenes		246.43	1.17					0	8
595	C18 disubstituted benzenes		246.43	2.55					0	8
596	C18 trisubstituted benzenes		246.43	4.37					0	8
597	C18 tetralins or indanes		244.41	1.55					0	10
598	C18 naphthalenes		240.38	2.45					0	10
599	C19 monosubstituted benzenes		260.46	1.11					0	8
600	C19 disubstituted benzenes		260.46	2.42					0	8
601	C19 trisubstituted benzenes		260.46	4.13					0	8
602	C19 tetralins or indanes		258.44	1.46					0	10
603	C19 naphthalenes		254.41	2.31					0	10
604	C20 monosubstituted benzenes		274.48	1.05					0	8
605	C20 disubstituted benzenes		274.48	2.29					0	8
606	C20 trisubstituted benzenes		274.48	3.92					0	8
607	C20 tetralins or indanes		272.47	1.39					0	10
608	C20 naphthalenes		268.44	2.19					0	10
609	C21 monosubstituted benzenes		288.51	1.00					0	8
610	C21 disubstituted benzenes		288.51	2.18					0	8
611	C21 trisubstituted benzenes		288.51	3.73					0	8
612	C21 tetralins or indanes		286.49	1.32					0	10
613	C21 naphthalenes		282.46	2.08					0	10
614	C22 monosubstituted benzenes		302.54	0.96					0	8
615	C22 disubstituted benzenes		302.54	2.08					0	8
616	C22 trisubstituted benzenes		302.54	3.56					0	8
617	C22 tetralins or indanes		300.52	1.26					0	10
618	C22 naphthalenes		296.49	1.98					0	10

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
<u>Oxygenated Organics</u>										
619	carbon monoxide	630-08-0	28.01	0.053	0.06	-12%	1	2	0	1
620	formaldehyde	50-00-0	30.03	9.24	8.97	3%	1	1	0	1b
621	methanol	67-56-1	32.04	0.65	0.71	-8%	1	3	0	2
622	formic acid	64-18-6	46.03	0.062	0.08	-22%	1		0	6
623	ethylene oxide	75-21-8	44.05	0.037	0.04	-8%	1		0	6
624	acetaldehyde	75-07-0	44.05	6.34	6.84	-7%	1	2	0	1
625	ethanol	64-17-5	46.07	1.45	1.69	-14%	1	3	0	2
626	dimethyl ether	115-10-6	46.07	0.76	0.93	-18%	1	3	0	2
627	glyoxal	107-22-2	58.04	12.13	14.22	-15%	1		0	6
628	methyl formate	107-31-3	60.05	0.054	0.06	-11%	1		0	6
629	acetic acid	64-19-7	60.05	0.66	0.50	32%	1		0	6
630	glycolaldehyde	141-46-8	60.05	4.96					0	7
631	ethylene glycol	107-21-1	62.07	3.01	3.36	-10%	1	2	0	2
632	glycolic acid	79-14-1	76.05	2.32	2.67	-13%			0	8
633	peroxyacetic acid	79-21-0	76.05	0.52	12.62	-96%			0	8
634	acrolein	107-02-8	56.06	7.24	7.60	-5%	1	3	0	2
635	trimethylene oxide	503-30-0	58.08	4.32	5.22	-17%	1		0	6
636	propylene oxide	75-56-9	58.08	0.28	0.32	-13%	1		0	6
637	propionaldehyde	123-38-6	58.08	6.83	7.89	-13%	1		0	6
638	acetone	67-64-1	58.08	0.35	0.43	-19%	1	1	0	2
639	isopropyl alcohol	67-63-0	60.10	0.59	0.71	-17%	1	2	0	2
640	n-propyl alcohol	71-23-8	60.10	2.38	2.74	-13%	1		0	6
641	acrylic acid	79-10-7	72.06	11.10	11.66	-5%			0	8
642	methyl glyoxal	78-98-8	72.06	16.02	16.21	-1%	1		0	6
643	1,3-dioxolane	646-06-0	74.08	4.73	5.47	-14%			0	7
644	ethyl formate	109-94-4	74.08	0.45	0.52	-13%	1		0	6
645	methyl acetate	79-20-9	74.08	0.067	0.07	-4%	1	2	0	2
646	propionic acid	79-09-4	74.08	1.17	0.79	49%			0	7
647	hydroxy acetone	116-09-6	74.08	3.15	3.08	2%	1		0	8
648	propylene glycol	57-55-6	76.09	2.48	2.75	-10%	1	2	0	2
649	dimethoxy methane	109-87-5	76.09	0.89	1.04	-14%	1		0	6
650	2-methoxy ethanol	109-86-4	76.09	2.83	2.98	-5%	1		0	6
651	dimethyl carbonate	616-38-6	90.08	0.055	0.06	-8%	1	2	0	2
652	dihydroxy acetone	96-26-4	90.08	3.89	4.02	-3%			0	8
653	glycerol	56-81-5	92.09	3.05	3.27	-7%			0	7
654	furan	110-00-9	68.07	8.86	16.54	-46%	1	3	-	4
655	crotonaldehyde	4170-30-3	70.09	9.14	10.07	-9%	1		0	8
656	methacrolein	78-85-3	70.09	5.84	6.23	-6%	1	2	0	2
657	cyclobutanone	1191-95-3	70.09	0.59	0.68	-14%	1		0	8
658	methylvinyl ketone	78-94-4	70.09	9.39	8.73	8%	1	3	0	2
659	tetrahydrofuran	109-99-9	72.11	4.10	4.95	-17%	1		0	6
660	1,2-epoxy butane	106-88-7	72.11	0.86	1.02	-16%	1		0	6
661	2-methyl propanal	78-84-2	72.11	5.05	5.87	-14%	1		0	7
662	butanal	123-72-8	72.11	5.75	6.74	-15%	1		0	7
663	C4 aldehydes		72.11	5.75	6.74	-15%			0	7
664	methyl ethyl ketone	78-93-3	72.11	1.43	1.49	-4%	1	2	0	2
665	isobutyl alcohol	78-83-1	74.12	2.41	2.24	8%	1		0	6
666	n-butyl alcohol	71-36-3	74.12	2.76	3.34	-17%	1		0	6
667	sec-butyl alcohol	78-92-2	74.12	1.30	1.60	-19%	1		0	6
668	tert-butyl alcohol	75-65-0	74.12	0.39	0.45	-14%	1	2	+	2
669	diethyl ether	60-29-7	74.12	3.61	4.01	-10%	1	2	0	2

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
670	gamma-butyrolactone	96-48-0	86.09	0.90	1.15	-22%			0	7
671	methacrylic acid	79-41-4	86.09	18.04	18.78	-4%			0	8
672	methyl acrylate	96-33-3	86.09	11.21	12.24	-8%			0	8
673	vinyl acetate	108-05-4	86.09	3.11	3.26	-5%			0	8
674	hydroxyl-methacrolein	40364-84-9	86.09	6.04	6.61	-9%			0	8
675	biacetyl	431-03-8	86.09	19.43	20.73	-6%	1		0	6
676	1,4-dioxane	123-91-1	88.11	2.48	2.71	-8%			0	7
677	ethyl acetate	141-78-6	88.11	0.59	0.64	-7%	1	2	0	3
678	methyl propionate	554-12-1	88.11	0.63	0.71	-11%	1		0	6
679	n-propyl formate	110-74-7	88.11	0.73	0.93	-21%	1		0	6
680	isopropyl formate	625-55-8	88.11	0.35	0.42	-18%			0	7
681	isobutyric acid	79-31-2	88.11	1.15	1.22	-6%			0	7
682	butanoic acid	107-92-6	88.11	1.75	1.78	-2%			0	7
683	methoxy-acetone	5878-19-3	88.11	1.94	2.14	-9%	1		0	8
684	1,3-butanediol	107-88-0	90.12	3.21			1		0	6
685	1,2-butanediol	584-03-2	90.12	2.43	2.21	10%	1		0	6
686	1,4-butanediol	110-63-4	90.12	2.61	3.22	-19%			0	7
687	2,3-butanediol		90.12	4.23			1		0	6
688	1-methoxy-2-propanol	107-98-2	90.12	2.33	2.62	-11%	1	2	0	2
689	2-ethoxy-ethanol	110-80-5	90.12	3.57	3.78	-5%	1	3	0	2
690	2-methoxy-1-propanol	1589-47-5	90.12	2.92	3.01	-3%			0	7
691	3-methoxy-1-propanol	1320-67-8	90.12	3.71	4.01	-7%			0	7
692	propylene carbonate	108-32-7	102.09	0.27	0.25	6%	1	2	+	2
693	methyl lactate	547-64-8	104.10	2.59	2.75	-6%	1		0	6
694	diethylene glycol	111-46-6	106.12	3.23	3.55	-9%			0	7
695	malic acid	6915-15-7	134.09	6.77	7.51	-10%			0	8
696	2-methyl furan	534-22-5	82.10	8.02			1	3	0	4
697	3-methyl furan	930-27-8	82.10	6.64			1	3	0	4
698	cyclopentanone	120-92-3	84.12	1.08	1.43	-24%	1		0	8
699	C5 cyclic ketones		84.12	1.08	1.43	-24%			0	8
700	cyclopentanol	96-41-3	86.13	1.65	1.96	-16%	1		0	6
701	$\alpha$ -methyl tetrahydrofuran	96-47-9	86.13	3.78	4.62	-18%	1		0	6
702	tetrahydropyran	142-68-7	86.13	3.05	3.81	-20%	1		0	6
703	2-methyl-3-butene-2-ol	115-18-4	86.13	4.73	5.12	-8%	1		0	8
704	2,2-dimethylpropanal; pivaldehyde	630-19-3	86.13	4.71	5.40	-13%	1		0	8
705	3-methylbutanal; isovaleraldehyde	590-86-3	86.13	4.79	5.52	-13%	1		0	8
706	pentanal; valeraldehyde	110-62-3	86.13	4.89	5.76	-15%	1		0	8
707	C5 aldehydes		86.13	4.89	5.76	-15%			0	8
708	2-pentanone	107-87-9	86.13	2.70	3.07	-12%	1	2	0	2
709	3-pentanone	96-22-0	86.13	1.18	1.45	-19%	1		0	6
710	C5 ketones		86.13	2.70	3.07	-12%			0	7
711	methyl isopropyl ketone	563-80-4	86.13	1.58	1.64	-3%	1		0	6
712	2-pentanol	6032-29-7	88.15	1.54	1.74	-12%	1		0	6
713	3-pentanol	584-02-1	88.15	1.56	1.73	-10%	1		0	6
714	pentyl alcohol	71-41-0	88.15	2.71	3.35	-19%	1		0	6
715	isoamyl alcohol; 3-methyl-1- butanol	123-51-3	88.15	3.04	2.73	11%	1		0	6
716	2-methyl-1-butanol	137-32-6	88.15	2.30	2.60	-12%			0	7
717	ethyl isopropyl ether	625-54-7	88.15	3.61	3.86	-7%			0	7
718	methyl n-butyl ether	628-28-4	88.15	2.99	3.66	-18%	1		0	6

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
719	methyl t-butyl ether	1634-04-4	88.15	0.70	0.78	-11%	1	3	0	2
720	ethyl acrylate	140-88-5	100.12	7.55	8.78	-14%			0	8
721	methyl methacrylate	80-62-6	100.12	15.22	15.84	-4%			0	8
722	glutaraldehyde	111-30-8	100.12	4.14	4.79	-14%			0	8
723	lumped C5+ unsaturated carbonyl species		100.12	6.18					0	8
724	2,4-pentanedione	123-54-6	100.12	0.98	1.02	-4%			0	8
725	tetrahydro-2-furanmethanol; tetrahydrofurfuryl alcohol	97-99-4	102.13	3.19	3.54	-10%			0	7
726	ethyl propionate	105-37-3	102.13	0.73	0.79	-8%	1		0	6
727	isopropyl acetate	108-21-4	102.13	1.03	1.12	-8%	1	2	0	2
728	methyl butyrate	623-42-7	102.13	1.04	1.18	-12%	1		0	6
729	methyl isobutyrate	547-63-7	102.13	0.58	0.70	-17%	1	2	0	2
730	n-butyl formate	592-84-7	102.13	0.77	0.95	-18%	1		0	6
731	propyl acetate	109-60-4	102.13	0.73	0.87	-16%	1		0	6
732	3-methyl butanoic acid	503-74-2	102.13	4.11	4.26	-4%			0	7
733	2,2-dimethoxy-propane	77-76-9	104.15	0.46	0.52	-12%			0	7
734	1-ethoxy-2-propanol	1569-02-4	104.15	2.96	3.25	-9%			0	7
735	2-propoxy-ethanol	2807-30-9	104.15	3.17	3.52	-10%			0	7
736	3-ethoxy-1-propanol	111-35-3	104.15	3.94	4.24	-7%	1		0	6
737	3-methoxy-1-butanol	2517-43-3	104.15	3.75	0.97	287%	1		0	6
738	2-methoxyethyl acetate	110-49-6	118.13	1.08	1.18	-8%			0	7
739	ethyl lactate	97-64-3	118.13	2.39	2.71	-12%	1		0	6
740	methyl isopropyl carbonate	51729-83-0	118.13	0.59	0.69	-14%	1	2	0	2
741	2-(2-methoxyethoxy) ethanol	111-77-3	120.15	2.54	2.90	-13%			0	7
742	pentaerythritol	115-77-5	136.15	2.09	2.42	-14%			0	7
743	phenol	108-95-2	94.11	2.69	1.82	48%			0	8
744	2-ethyl furan	3208-16-0	96.13	6.85					0	8
745	2,5-dimethyl furan	625-86-5	96.13	7.60			1	3	0	4
746	cyclohexanone	108-94-1	98.14	1.26	1.61	-22%	1	2	0	2
747	C6 cyclic ketones		98.14	1.26	1.61	-22%			0	7
748	mesityl oxide; 2-methyl-2- penten-4-one	141-79-7	98.14	6.31	17.37	-64%			0	8
749	cyclohexanol	108-93-0	100.16	1.84	2.25	-18%	1		0	6
750	hexanal	66-25-1	100.16	4.18	4.98	-16%	1		0	8
751	C6 aldehydes		100.16	4.18	4.98	-16%			0	8
752	4-methyl-2-pentanone	108-10-1	100.16	3.74	4.31	-13%	1	2	0	3
753	methyl n-butyl ketone	591-78-6	100.16	3.00	3.55	-15%	1		0	8
754	methyl tert-butyl ketone	75-97-8	100.16	0.62	0.78	-21%	1		0	8
755	C6 ketones		100.16	3.00	3.55	-15%			0	8
756	1-hexanol	111-27-3	102.17	2.56	2.74	-7%	1		0	6
757	2-hexanol	626-93-7	102.17	1.97	2.46	-20%	1		0	6
758	4-methyl-2-pentanol; methyl isobutyl carbinol	108-11-2	102.17	2.52	2.89	-13%			0	7
759	di-n-propyl ether	111-43-3	102.17	2.93	3.24	-9%	1		0	6
760	ethyl n-butyl ether	628-81-9	102.17	3.33	3.86	-14%	1		0	6
761	ethyl tert-butyl ether	637-92-3	102.17	1.93	2.11	-9%	1		0	6
762	methyl tert-amyl ether; TAME	994-05-8	102.17	1.61	2.14	-25%	1		0	6
763	diisopropyl ether	108-20-3	102.17	3.39	3.56	-5%			0	7
764	ethyl methacrylate	97-63-2	114.14	12.15					0	8
765	ethyl butyrate	105-54-4	116.16	1.11	1.25	-11%	1		0	6
766	isobutyl acetate	110-19-0	116.16	0.58	0.67	-13%			0	7

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
767	methyl pivalate	598-98-1	116.16	0.33	0.39	-15%	1	2	0	2
768	n-butyl acetate	123-86-4	116.16	0.78	0.89	-12%	1	2	0,+	2
769	n-propyl propionate	106-36-5	116.16	0.79	0.93	-15%	1		0	6
770	sec-butyl acetate	105-46-4	116.16	1.25	1.43	-13%	1		0	6
771	tert-butyl acetate	540-88-5	116.16	0.172	0.20	-14%	1	3	0	2
772	diacetone alcohol	123-42-2	116.16	0.57	0.68	-17%			0	8
773	methyl pentanoate; methyl valerate	624-24-8	116.16	1.00					0	7
774	1,2-dihydroxyhexane	6920-22-5	118.17	2.45	2.75	-11%			0	7
775	2-methyl-2,4-pentanediol	107-41-5	118.17	1.39	1.04	34%	1		0	6
776	ethylene glycol diethyl ether; 1,2-diethoxyethane	629-14-1	118.17	2.81	2.84	-1%			0	7
777	acetal (1,1-diethoxyethane)	105-57-7	118.17	3.43	3.68	-7%			0	7
778	1-propoxy-2-propanol; propylene glycol n-propyl ether	1569-01-3	118.17	2.56	2.86	-11%			0	7
779	2-butoxy-ethanol	111-76-2	118.17	2.78	2.90	-4%	1	2	0	2
780	3 methoxy-3 methyl-butanol	56539-66-3	118.17	1.46	1.74	-16%			0	7
781	n-propoxy-propanol	30136-13-1	118.17	3.62	3.84	-6%			0	7
782	hydroxypropyl acrylate	2918-23-2	130.14	4.74	5.56	-15%			0	8
783	1-methoxy-2-propyl acetate	108-65-6	132.16	1.62	1.71	-5%	1	2	0,+	2
784	2-ethoxyethyl acetate	111-15-9	132.16	1.75	1.90	-8%			0	7
785	2-methoxy-1-propyl acetate	70657-70-4	132.16	1.06	1.12	-6%			0	7
786	methoxypropanol acetate	84540-57-8	132.16	1.76	1.97	-10%			0	7
787	2-(2-ethoxyethoxy) ethanol	111-90-0	134.17	3.11	3.19	-2%	1	3	0	2
788	dipropylene glycol isomer (1-[2-hydroxypropyl]-2-propanol)	110-98-5	134.17	2.20	2.48	-11%			0	7
789	dimethyl succinate	106-65-0	146.14	0.21	0.23	-8%	1	2	0	2
790	ethylene glycol diacetate	111-55-7	146.14	0.62	0.72	-13%			0	7
791	adipic acid; hexanedioic acid	124-04-9	146.14	2.94	3.37	-13%			0	8
792	triethylene glycol	112-27-6	150.17	3.11	3.41	-9%			0	7
793	benzaldehyde	100-52-7	106.12	-0.67	0.00	0%	1	3	0	2
794	C7 alkyl phenols	1319-77-3	108.14	2.34	2.34	0%			0	5
795	m-cresol	108-39-4	108.14	2.34	2.34	0%		4	-,0	5
796	p-cresol	106-44-5	108.14	2.34	2.34	0%		4	0?	5
797	o-cresol	95-48-7	108.14	2.34	2.34	0%	1	4	?	5
798	benzyl alcohol	100-51-6	108.14	4.98			1	2	0	4
799	methoxybenzene; anisole	100-66-3	108.14	6.49			1		0	8
800	C7 cyclic ketones		112.17	1.10	1.41	-22%			0	8
801	heptanal	111-71-7	114.19	3.54	4.23	-16%	1		0	8
802	C7 aldehydes		114.19	3.54	4.23	-16%			0	8
803	2-methyl-hexanal	925-54-2	114.19	3.40	3.97	-14%			0	8
804	2-heptanone	110-43-0	114.19	2.24	2.80	-20%	1	3	?	4
805	2-methyl-3-hexanone	7379-12-6	114.19	1.45	1.79	-19%			0	8
806	di-isopropyl ketone	565-80-0	114.19	1.23	1.63	-24%	1		0	8
807	C7 ketones		114.19	2.24	2.80	-20%			0	8
808	5-methyl-2-hexanone	110-12-3	114.19	2.28	2.10	9%	1		0	8
809	3-methyl-2-hexanone	2550-21-2	114.19	2.43	2.81	-14%			0	8
810	1-heptanol	111-70-6	116.20	1.75	2.21	-21%	1		0	6
811	dimethylpentanol; 2,3-dimethyl-1-pentanol	10143-23-4	116.20	2.13	2.51	-15%			0	7
812	4,4-diethyl-3-oxahexane	919-94-8	116.20	1.86	2.03	-8%			0	7
813	n-butyl acrylate	141-32-2	128.17	4.87	5.52	-12%			0	8

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
814	isobutyl acrylate	106-63-8	128.17	4.57	5.05	-10%			0	8
815	butyl propionate	590-01-2	130.18	0.79	0.89	-11%			0	7
816	amyl acetate; n-pentyl acetate	628-63-7	130.18	0.78	0.96	-19%			0	7
817	n-propyl butyrate	105-66-8	130.18	0.99	1.17	-15%	1		0	6
818	isoamyl acetate; 3-methyl-butyl acetate	123-92-2	130.18	1.02	1.18	-13%			0	7
819	2-methyl-1-butyl acetate	624-41-9	130.18	1.01	1.17	-13%			0	7
820	methyl hexanoate	106-70-7	130.18	0.96					0	7
821	1-tert-butoxy-2-propanol	57018-52-7	132.20	1.53	1.71	-10%			0	7
822	2-tert-butoxy-1-propanol	94023-15-1	132.20	1.75	1.81	-3%			0	7
823	n-butoxy-2-propanol; propylene glycol n-butyl ether	5131-66-8	132.20	2.59	2.70	-4%			0	7
824	ethyl 3-ethoxy propionate	763-69-9	146.18	3.46	3.61	-4%			0	7
825	diisopropyl carbonate	6482-34-4	146.18	0.94	1.04	-10%			0	7
826	2-(2-propoxyethoxy) ethanol	6881-94-3	148.20	2.71	3.00	-10%			0	7
827	dipropylene glycol methyl ether: 1-methoxy-2-(2-hydroxypropoxy)-propane		148.20	1.87	2.21	-15%			0	7
828	dipropylene glycol methyl ether: 2-(2-methoxypropoxy)-1-propanol	13588-28-8	148.20	2.46	2.70	-9%			0	7
829	1,2-propylene glycol diacetate	623-84-7	160.17	0.58	0.94	-39%			0	7
830	dimethyl glutarate	1119-40-0	160.17	0.39	0.51	-23%	1	2	0	2
831	2-[2-(2-methoxyethoxy) ethoxy] ethanol	112-35-6	164.20	2.44	2.62	-7%			0	7
832	tolualdehyde		120.15	-0.59	0.00	0%			0	7
833	4-vinyl phenol	2628-17-3	120.15	1.43					0	11
834	2,4-dimethyl phenol	105-67-9	122.16	2.07					0	8
835	2,5-dimethyl phenol		122.16	2.07					0	8
836	3,4-dimethyl phenol	95-65-8	122.16	2.07					0	8
837	2,3-dimethyl phenol	526-75-0	122.16	2.07					0	8
838	2,6-dimethyl phenol	576-26-1	122.16	2.07					0	8
839	C8 alkyl phenols		122.16	2.07	2.07	0%			0	8
840	$\beta$ -phenethyl alcohol; 2-phenyl ethyl alcohol	98-85-1	122.16	4.41					-	11
841	C8 cyclic ketones		126.20	0.98	1.25	-22%			0	8
842	2-butyl tetrahydrofuran	1004-29-1	128.21	2.00	2.53	-21%			0	7
843	octanal	124-13-0	128.21	3.03	3.65	-17%			0	8
844	C8 aldehydes		128.21	3.03	3.65	-17%			0	8
845	2-octanone	111-13-7	128.21	1.31	1.66	-21%	1		0	8
846	C8 ketones		128.21	1.31	1.66	-21%			0	8
847	1-octanol	111-87-5	130.23	1.35	2.01	-33%	1	2	+	2
848	2-ethyl-1-hexanol	104-76-7	130.23	1.90	2.20	-14%			0	7
849	2-octanol	4128-31-8	130.23	1.86	2.16	-14%	1	2	+	2
850	3-octanol	20296-29-1	130.23	2.16	2.57	-16%	1	2	+	2
851	4-octanol	589-62-8	130.23	2.10	3.07	-32%	1		0	6
852	5-methyl-1-heptanol	7212-53-5	130.23	1.70	1.95	-13%			0	7
853	di-isobutyl ether	628-55-7	130.23	1.12	1.29	-13%	1		0	6
854	di-n-butyl ether	142-96-1	130.23	2.70	3.17	-15%	1		0	6
855	2-phenoxyethanol; ethylene glycol phenyl ether	122-99-6	138.16	4.35	3.61	21%			0	8
856	butyl methacrylate	97-88-1	142.20	8.47	9.09	-7%			0	8

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
857	isobutyl methacrylate	97-86-9	142.20	8.39	8.99	-7%			0	8
858	hexyl acetates		144.21	0.74					0	7
859	2,3-dimethylbutyl acetate		144.21	0.70	0.84	-17%			0	7
860	2-methylpentyl acetate		144.21	0.91	1.11	-18%			0	7
861	3-methylpentyl acetate		144.21	1.00	1.31	-24%			0	7
862	4-methylpentyl acetate		144.21	0.76	0.92	-17%			0	7
863	isobutyl isobutyrate	97-85-8	144.21	0.55	0.61	-9%			0	7
864	n-butyl butyrate	109-21-7	144.21	1.02	1.12	-9%	1		0	6
865	n-hexyl acetate	142-92-7	144.21	0.63	0.87	-27%			0	7
866	methyl amyl acetate; 4-methyl-2-pentanol acetate	108-84-9	144.21	1.28	1.46	-13%			0	7
867	n-pentyl propionate	624-54-4	144.21	0.66	0.79	-17%			0	7
868	2-ethyl hexanoic acid	149-57-5	144.21	3.19	3.49	-9%			0	7
869	methyl heptanoate	106-73-0	144.21	0.76					0	7
870	2-ethyl-1,3-hexanediol	94-96-2	146.23	1.95	2.62	-26%			0	7
871	2-n-hexyloxyethanol	112-25-4	146.23	1.98	2.45	-19%			0	7
872	2,2,4-trimethyl-1,3-pentanediol	144-19-4	146.23	1.46	1.74	-16%			0	7
873	phthalic anhydride	85-44-9	148.12	2.50					0	8
874	methylparaben; 4-hydroxybenzoic acid, methyl ester	99-76-3	152.15	1.66					0	11
875	2-butoxyethyl acetate	112-07-2	160.21	1.53	1.67	-8%			0	7
876	2-methoxy-1-(2-methoxy-1-methylethoxy)-propane; dipropylene glycol dimethyl ether	89399-28-0	162.23	1.91	2.09	-9%			0	7
877	2-(2-butoxyethoxy)-ethanol	112-34-5	162.23	2.26	2.87	-21%		2	0	7
878	dipropylene glycol ethyl ether	15764-24-6	162.23	2.60	2.75	-6%			0	7
879	dimethyl adipate	627-93-0	174.19	1.72	1.95	-12%	1		0	6
880	2-(2-ethoxyethoxy) ethyl acetate	112-15-2	176.21	1.39	1.50	-7%			0	7
881	2-[2-(2-ethoxyethoxy) ethoxy] ethanol	112-50-5	178.23	2.33	2.66	-12%			0	7
882	tetraethylene glycol	112-60-7	194.23	2.38	2.84	-16%			0	7
883	cinnamic aldehyde	104-55-2	132.16	4.68					0	10
884	Cinnamic alcohol	104-54-1	134.18	0.84					-1	10
885	2,3,5-trimethyl phenol	697-82-5	136.19	1.86					0	8
886	2,3,6-trimethyl phenol	2416-94-6	136.19	1.86					0	8
887	C9 alkyl phenols		136.19	1.86	1.86	0%			0	8
888	isophorone; 3,5,5-trimethyl-2-cyclohexenone	78-59-1	138.21	4.48	10.58	-58%			0	8
889	C9 cyclic ketones		140.22	0.88	1.13	-22%			0	8
890	2-propyl cyclohexanone	94-65-5	140.22	1.43	1.71	-16%			0	8
891	4-propyl cyclohexanone	40649-36-3	140.22	1.74	2.08	-16%			0	8
892	1-nonene-4-one	61168-10-3	140.22	3.03	3.39	-11%			0	8
893	trimethyl cyclohexanol	1321-60-4	142.24	1.75	2.17	-19%			0	7
894	2-nonanone	821-55-6	142.24	1.00	1.30	-23%	1		0	8
895	di-isobutyl ketone; 2,6-dimethyl-4-heptanone	108-83-8	142.24	2.56	2.94	-13%	1		0	8
896	C9 ketones		142.24	1.00	1.30	-23%			0	8
897	dimethyl heptanol; 2,6-dimethyl-2-heptanol	13254-34-7	144.25	0.88	1.07	-18%			0	7
898	2,6-dimethyl-4-heptanol	108-82-7	144.25	1.98	2.37	-17%			0	7



Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
899	1-phenoxy-2-propanol	770-35-4	152.19	1.54	1.73	-11%			0	8
900	2,4-dimethylpentyl acetate		158.24	0.85	0.98	-13%			0	7
901	2-methylhexyl acetate		158.24	0.64	0.89	-29%			0	7
902	3-ethylpentyl acetate		158.24	1.03	1.24	-17%			0	7
903	3-methylhexyl acetate		158.24	0.83	1.01	-18%			0	7
904	4-methylhexyl acetate		158.24	0.76	0.91	-16%			0	7
905	5-methylhexyl acetate		158.24	0.54	0.79	-32%			0	7
906	isoamyl isobutyrate	2050-01-3	158.24	0.76	0.89	-14%			0	7
907	n-heptyl acetate	112-06-1	158.24	0.59	0.73	-19%			0	7
908	methyl octanoate	111-11-5	158.24	0.64					0	7
909	1-(butoxyethoxy)-2-propanol	124-16-3	176.25	1.82	2.08	-13%			0	7
910	dipropylene glycol n-propyl ether isomer #1		176.25	1.89	2.13	-11%			0	7
911	dipropylene glycol methyl ether acetate isomer #1		190.24	1.30	1.41	-8%			0	7
912	dipropylene glycol methyl ether acetate isomer #2		190.24	1.43	1.58	-9%			0	7
913	dipropylene glycol methyl ether acetate isomers	88917-22-0	190.24	1.37	1.49	-8%			0	7
914	2-[2-(2-propoxyethoxy) ethoxy] ethanol	23305-64-8	192.25	2.05	2.46	-17%			0	7
915	tripropylene glycol	24800-44-0	192.25	2.07					0	7
916	2,5,8,11-tetraoxatridecan-13-ol	23783-42-8	208.25	1.86	2.15	-14%			0	7
917	glyceryl triacetate	102-76-1	218.20	0.51	0.57	-11%			0	7
918	anethol; p-propenyl-anisole	104-46-1	148.20	0.76					0	11
919	C10 alkyl phenols		150.22	1.68	1.68	0%			0	8
920	camphor	76-22-2	152.23	0.45					0	8
921	$\alpha$ -terpineol	98-55-5	154.25	4.50	5.16	-13%			0	8
922	citronellol; 3,7-dimethyl-6-octen-1-ol	106-22-9	154.25	5.63					0	8
923	hydroxycitronella	107-75-5	154.25	2.50					0	8
924	C10 cyclic ketones		154.25	0.80	1.02	-21%			0	8
925	menthol	89-78-1	156.27	1.35	1.70	-21%			0	7
926	linalool	78-70-6	156.27	5.28					0	8
927	2-decanone	693-54-9	156.27	0.82	1.06	-22%	1		0	8
928	C10 ketones		156.27	0.82	1.06	-22%			0	8
929	8-methyl-1-nonanol; isodecyl alcohol	25339-17-7	158.28	0.99	1.23	-20%			0	7
930	1-decanol	112-30-1	158.28	1.00	1.22	-18%			0	7
931	3,7-dimethyl-1-octanol	106-21-8	158.28	1.13	1.42	-21%			0	7
932	di-n-pentyl ether	693-65-2	158.28	2.02	2.64	-24%	1		0	6
933	1,2-diacetyl benzene	704-00-7	162.19	2.17			1		0	8
934	2,4-dimethylhexyl acetate		172.26	0.70	0.93	-24%			0	7
935	2-ethyl-hexyl acetate	103-09-3	172.26	0.60	0.79	-24%			0	7
936	3,4-dimethyl-hexyl acetate		172.26	0.81	1.16	-30%			0	7
937	3,5-dimethyl-hexyl acetate		172.26	0.92	1.09	-16%			0	7
938	3-ethyl-hexyl acetate		172.26	0.84	1.03	-18%			0	7
939	3-methyl-heptyl acetate		172.26	0.61	0.76	-19%			0	7
940	4,5-dimethyl-hexyl acetate		172.26	0.63	0.86	-27%			0	7
941	4-methyl-heptyl acetate		172.26	0.60	0.72	-17%			0	7
942	5-methyl-heptyl acetate		172.26	0.55	0.73	-25%			0	7
943	n-octyl acetate	112-14-1	172.26	0.52	0.64	-19%			0	7

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]				
				New	Old	Chg	k	a	Expt	Bias	Unc
944	geraniol	106-24-1	172.26	4.97						0	8
945	methyl nonanoate	1731-84-6	172.26	0.54						0	7
946	2-(2-ethylhexyloxy) ethanol	1559-35-9	174.28	1.45	1.71	-15%				0	7
947	propylparaben	94-13-3	180.20	1.40						0	11
948	2-(2-hexyloxyethoxy) ethanol	112-59-4	190.28	1.73	2.03	-15%				0	7
949	glycol ether DPnB; dipropylene glycol n-butyl ether; 1-(2-butoxy-1-methylethoxy)-2-propanol)	29911-28-2	190.28	1.73	1.96	-12%				0	7
950	2-(2-butoxyethoxy) ethyl acetate	124-17-4	204.26	1.30	1.38	-6%				0	7
951	2-[2-(2-butoxyethoxy) ethoxy] ethanol	143-22-6	206.28	1.85	2.24	-17%				0	7
952	tripropylene glycol monomethyl ether	25498-49-1	206.28	1.81	1.90	-5%				0	7
953	C11 alkyl phenols		164.24	1.54	1.54	0%				0	8
954	2-ethyl-hexyl acrylate	103-11-7	184.28	2.43	2.42	1%				0	8
955	2,3,5-trimethyl-hexyl acetate		186.29	0.79	0.86	-8%				0	7
956	2,3-dimethyl-heptyl acetate		186.29	0.65	0.84	-22%				0	7
957	2,4-dimethyl-heptyl acetate		186.29	0.62	0.88	-29%				0	7
958	2,5-dimethyl-heptyl acetate		186.29	0.72	0.86	-16%				0	7
959	2-methyloctyl acetate		186.29	0.47	0.63	-26%				0	7
960	3,5-dimethyl-heptyl acetate		186.29	0.74	1.01	-26%				0	7
961	3,6-dimethyl-heptyl acetate		186.29	0.71	0.87	-18%				0	7
962	3-ethyl-heptyl acetate		186.29	0.57	0.71	-19%				0	7
963	4,5-dimethyl-heptyl acetate		186.29	0.63	0.96	-35%				0	7
964	4,6-dimethyl-heptyl acetate		186.29	0.72	0.83	-13%				0	7
965	4-methyloctyl acetate		186.29	0.56	0.68	-18%				0	7
966	5-methyloctyl acetate		186.29	0.50	0.67	-25%				0	7
967	n-nonyl acetate	143-13-5	186.29	0.47	0.58	-19%				0	7
968	methyl decanoate	110-42-9	186.29	0.48						0	7
969	C12 alkyl phenols		178.27	1.42	1.42	0%				0	8
970	2,6,8-trimethyl-4-nonanone; isobutyl heptyl ketone	123-18-2	184.32	1.57	1.86	-16%				0	8
971	trimethylnonanolthreoerythro; 2,6,8-trimethyl-4-nonanol	123-17-1	186.33	1.24	1.55	-20%				0	7
972	3,6-dimethyl-octyl acetate		200.32	0.72	0.88	-18%				0	7
973	3-isopropyl-heptyl acetate		200.32	0.49	0.71	-31%				0	7
974	4,6-dimethyl-octyl acetate		200.32	0.70	0.85	-18%				0	7
975	methyl undecanoate	1731-86-8	200.32	0.45						0	7
976	1-hydroxy-2,2,4-trimethylpentyl-3-isobutyrate	18491-15-1	216.32	0.84	0.92	-8%				0	7
977	3-hydroxy-2,2,4-trimethylpentyl-1-isobutyrate	77-68-9	216.32	0.72	0.88	-18%				0	7
978	2,2,4-trimethyl-1,3-pentanediol monoisobutyrate and isomers (texanol®)	25265-77-4	216.32	0.76	0.89	-15%	1	2		0	2
979	substituted C7 ester (C12)		216.32	0.76	0.92	-17%				0	7
980	substituted C9 ester (C12)		216.32	0.76	0.89	-15%				0	7
981	diethylene glycol mono-(2-ethylhexyl) ether	1559-36-0	218.33	1.46						0	7
982	diethyl phthalate	84-66-2	222.24	1.56						0	8
983	dimethyl sebacate	106-79-6	230.30	0.40	0.48	-18%				0	7

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
984	diisopropyl adipate	6938-94-9	230.30	1.22	1.42	-14%			0	7
985	3,6,9,12-tetraoxa-hexadecan-1-ol	1559-34-8	250.33	1.62	1.90	-15%			0	7
986	triethyl citrate	77-93-0	276.28	0.66					0	8
987	3,5,7-trimethyl-octyl acetate		214.34	0.60	0.83	-28%			0	7
988	3-ethyl-6-methyl-octyl acetate		214.34	0.57	0.80	-29%			0	7
989	4,7-dimethyl-nonyl acetate		214.34	0.45	0.64	-30%			0	7
990	methyl dodecanoate; methyl laurate	111-82-0	214.34	0.42	0.53	-20%			0	7
991	tripropylene glycol n-butyl ether	55934-93-5	248.36	1.55					0	7
992	amyl cinnamal	122-40-7	202.29	3.06					0	10
993	isobornyl methacrylate	7534-94-3	222.32	5.37	8.64	-38%			+	10
994	2,3,5,7-tetramethyl-octyl acetate		228.37	0.57	0.74	-24%			0	7
995	3,5,7-trimethyl-nonyl acetate		228.37	0.56	0.76	-26%			0	7
996	3,6,8-trimethyl-nonyl acetate		228.37	0.53	0.72	-27%			0	7
997	methyl tridecanoate	1731-88-0	228.37	0.40					0	7
998	hexyl cinnamal	101-86-0	216.32	2.86					0	10
999	2,6-di-tert-butyl-p-cresol	128-37-0	220.35	1.15					0	10
1000	2-ethyl-hexyl benzoate	5444-75-7	234.33	0.93					0	10
1001	2,4,6,8-tetramethyl-nonyl acetate		242.40	0.46	0.63	-28%			0	7
1002	3-ethyl-6,7-dimethyl-nonyl acetate		242.40	0.55	0.76	-27%			0	7
1003	4,7,9-trimethyl-decyl acetate		242.40	0.37	0.55	-32%			0	7
1004	methyl myristate; methyl tetradecanoate	124-10-7	242.40	0.39	0.47	-18%			0	7
1005	methyl cis-9-pentadecenoate		254.41	1.73					0	8
1006	methyl cis-9-hexadecenoate; methyl palmitoleate	1120-25-8	268.43	1.64					0	8
1007	methyl pentadecanoate	7132-64-1	256.42	0.42					0	7
1008	2,3,5,6,8-pentamethyl-nonyl acetate		256.42	0.59	0.74	-20%			0	7
1009	3,5,7,9-tetramethyl-decyl acetate		256.42	0.43	0.58	-26%			0	7
1010	5-ethyl-3,6,8-trimethyl-nonyl acetate		256.42	0.71	0.77	-8%			0	7
1011	dibutyl phthalate	84-74-2	278.34	1.20					0	8
1012	2,2,4-trimethyl-1,3-pentanediol diisobutyrate	6846-50-0	286.41	0.34					0	7
1013	methyl hexadecanoate; methyl palmitate	112-39-0	270.45	0.40					0	7
1014	Methyl cis-9-heptadecenoate		282.46	1.56					0	8
1015	methyl heptadecanoate; methyl margarate	1731-92-6	284.48	0.38					0	7
1016	methyl linolenate; methyl cis,cis,cis-9,12,15-octadecatrienoate	301-00-8	292.46	2.23					0	8
1017	methyl linoelate; methyl cis,cis-9,12-octadecadienoate	112-63-0	294.47	1.77					0	8
1018	methyl cis-9-octadecenoate; methyl oleate	112-62-9	296.49	1.48					0	8
1019	methyl octadecanoate; methyl stearate	112-61-8	298.50	0.36					0	7

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
<u>Other Organic Compounds</u>										
1020	methylamine	74-89-5	31.06	7.29			1		+	13a,n
1021	methyl chloride	74-87-3	50.49	0.036	0.03	22%	1		0	10
1022	methyl nitrite	624-91-9	61.04	10.50			1		0	6
1023	nitromethane	75-52-5	61.04	0.065	7.86	-99%	1		0	8
1024	carbon disulfide	75-15-0	76.14	0.23			1	2	0	2
1025	dichloromethane	75-09-2	84.93	0.039	0.07	-45%	1		0	10
1026	methyl bromide	74-83-9	94.94	0.018	0.02	-11%	1		0	10
1027	chloroform	67-66-3	119.38	0.020	0.03	-33%	1		0	10
1028	methyl iodide	74-88-4	141.94	-0.53					0	3
1029	carbon tetrachloride	56-23-5	153.82	0	0.00	0%			0	1
1030	chloropicrin; trichloro-nitro-methane	76-06-2	164.38	1.80			1	2	0	1
1031	methylene bromide	74-95-3	173.83	0	0.00	0%			0	1
1032	acetylene	74-86-2	26.04	0.93	1.25	-25%	1	2	-	3
1033	dimethyl amine	124-40-3	45.08	2.95	9.37	-69%	1		+	13a,n
1034	ethyl amine	75-04-7	45.08	5.48	7.80	-30%	1		+	13a,n
1035	ethanolamine	141-43-5	61.08	6.53	5.97	9%		3a	+	12a,n
1036	vinyl chloride	75-01-4	62.50	2.70	2.92	-8%	1		0	10
1037	ethyl chloride	75-00-3	64.51	0.27	0.25	8%	1		0	10
1038	1,1-difluoroethane; HFC-152a	75-37-6	66.05	0.016	0.00		1		+	6
1039	methyl isothiocyanate	556-61-6	73.12	0.31			1	2	0	2
1040	nitroethane	79-24-3	75.07	0.060	12.79	-100%	1		0	7
1041	dimethyl sulfoxide; DMSO	67-68-5	78.13	6.46	6.90	-6%	1	2	-2,0	4
1042	chloroacetaldehyde	107-20-0	78.50	12.00			1		0	7
1043	1,1-dichloroethene	75-35-4	96.94	1.69					0	10
1044	trans-1,2-dichloroethene	156-60-5	96.94	1.65	0.81	103%	1		0	10
1045	cis-1,2-dichloroethene		96.94	1.65					0	10
1046	1,1-dichloroethane	75-34-3	98.96	0.065	0.10	-35%	1		0	10
1047	1,2-dichloroethane	107-06-2	98.96	0.21	0.10	107%	1		0	10
1048	1,1,1,2-tetrafluoroethane; HFC-134a	811-97-2	102.03	.0007	0.00		1		0	6
1049	ethyl bromide	74-96-4	108.97	0.121	0.11	10%	1		0	20
1050	trichloroethylene	79-01-6	131.39	0.61	0.60	1%	1	2x	+2	20
1051	1,1,1-trichloroethane	71-55-6	133.40	0.005	0.00		1		0	10
1052	1,1,2-trichloroethane	79-00-5	133.40	0.082	0.06	37%	1		0	10
1053	perchloroethylene	127-18-4	165.83	0.029	0.04	-28%	1		0	10
1054	1,2-dibromoethane	106-93-4	187.86	0.098	0.05	96%	1		0	20
1055	methyl acetylene	74-99-7	40.06	6.57	6.45	2%	1		-	7
1056	acrylonitrile	107-13-1	53.06	2.16			1		0	10
1057	trimethyl amine	75-50-3	59.11	6.03	7.06	-15%	1		+	13a,n
1058	isopropyl amine	75-31-0	59.11	6.93				4a	+	12a,n
1059	N-methyl acetamide**	79-16-3	73.09	19.63	19.70	0%			+	*UL*
1060	1-amino-2-propanol	78-96-6	75.11	5.17	13.42	-61%			+	13a,n
1061	3-chloropropene		76.52	11.98					0	10
1062	1-nitropropane	108-03-2	89.09	0.20	16.16	-99%			0	8
1063	2-nitropropane	79-46-9	89.09	0.104	16.16	-99%	1		0	6
1064	chloroacetone	78-95-5	92.52	9.22			1	3	0	5
1065	trans-1,3-dichloropropene	10061-02-6	110.97	4.92			1	2m	0	3
1066	cis-1,3-dichloropropene	10061-01-5	110.97	3.61			1	2m	0	3
1067	1,3-dichloropropene mixture		110.97	4.19			1	2	0	2
1068	1,2-dichloropropane	78-87-5	112.99	0.28					0	10

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
1069	trans-1,3,3,3-tetrafluoropropene	1645-83-6	114.04	0.091			1	2	0	1
1070	2,3,3,3-tetrafluoropropene	754-12-1	114.04	0.27			1	2	0	1
1071	n-propyl bromide	106-94-5	122.99	0.40	0.35	16%	1	2x	-,+2	20n
1072	1,1,1,3,3-pentafluoropropane	460-73-1	134.05	.0007			1		0	6
1073	3,3-dichloro-1,1,1,2,2-pentafluoropropane; HCFC-225ca	422-56-0	202.94	0.003			1		0	6
1074	1,3-dichloro-1,1,2,2,3-pentafluoropropane; HCFC-225cb	507-55-1	202.94	.0010			1		0	6
1075	1,3-butadiyne	460-12-8	50.06	5.53					0	11
1076	1-buten-3-yne; vinyl acetylene	689-97-4	52.07	10.15					0	11
1077	2-butyne	503-17-3	54.09	15.95	16.33	-2%	1		0	10
1078	ethyl acetylene	107-00-6	54.09	5.95	6.20	-4%	1		-	7
1079	tert-butyl amine	75-64-9	73.14	-3.15			1	4a	-	12a
1080	morpholine	110-91-8	87.12	1.85	15.43	-88%			+	13a,n
1081	ethyl methyl ketone oxime; methyl ethyl ketoxime	96-29-7	87.12	1.52	22.04	-93%			0	10
1082	dimethylaminoethanol	108-01-0	89.14	5.41	4.76	14%	1		+	13a,n
1083	2-amino-1-butanol	96-20-8	89.14	4.78					+	13a,n
1084	2-amino-2-methyl-1-propanol	124-68-5	89.14	-2.57	15.08	-100%		3a	-	12a
1085	1-chlorobutane	109-69-3	92.57	1.04					0	10
1086	diethylenetriamine**	111-40-0	103.17	15.10	13.03	16%			+	*UL*
1087	diethanol-amine	111-42-2	105.14	2.36	4.05	-42%			+	13a,n
1088	2-(chloro-methyl)-3-chloro-propene	1871-57-4	125.00	6.85	1.13	506%	1	4	-	20
1089	n-butyl bromide	109-65-9	137.02	0.78	0.60	30%	1	2x	-,+2	20n
1090	1,1,1,3,3-pentafluorobutane; HFC-365mfc	406-58-6	148.07	.0006			1		0	6
1091	n-methyl-2-pyrrolidone	872-50-4	99.13	2.28	2.56	-11%	1	2	0	2
1092	2-amino-2-ethyl-1,3-propanediol	115-70-8	119.16	-0.93					-	13a
1093	hydroxyethylethylene urea**	3699-54-5	130.15	10.91	14.75	-26%			+	*UL*
1094	methyl-nonafluoro-butyl ether	163702-07-6	234.06	0.052					0	8
1095	methyl-nonafluoro-isobutyl ether	163702-08-7	234.06	0.052					0	8
1096	methoxy-perfluoro-n-butane	163702-07-6	250.06	.0005			1		0	6
1097	methoxy-perfluoro-isobutene	163702-08-7	250.06	.0005			1		0	6
1098	1,1,1,2,2,3,4,5,5,5-decafluoropentane; HFC-43-10mee	138495-42-8	252.05	.0002			1		0	6
1099	triethyl amine	121-44-8	101.19	3.66	16.60	-78%			+	13a,n
1100	triethylene diamine	280-57-9	112.17	3.31					+	13a,n
1101	monochlorobenzene	108-90-7	112.56	0.31	0.36	-15%	1		0	8
1102	nitrobenzene	98-95-3	123.11	0.054	0.07	-23%	1		0	8
1103	p-dichlorobenzene	106-46-7	147.00	0.171	0.20	-15%			0	10
1104	o-dichlorobenzene	95-50-1	147.00	0.171					0	8
1105	triethanolamine	102-71-6	149.19	4.08	2.76	48%			+	13a,n
1106	hexamethyl-disiloxane	107-46-0	162.38	-0.027			1	3	0	5
1107	hydroxymethyl-disiloxane		164.35	-0.131			1	3	0	5
1108	hexafluoro-benzene	392-56-3	186.05	0.045			1		0	8
1109	ethoxy-perfluoro-n-butane	163702-05-4	264.09	0.008			1		0	6
1110	ethoxy-perfluoro-isobutane	163702-06-5	264.09	0.009			1		0	6

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]				
				New	Old	Chg	k a	Expt	Bias	Unc	
1111	ethyl nonafluorobutyl ether	163702-05-4	264.09	0.192						+	8
1112	ethyl nonafluoroisobutyl ether	163702-06-5	264.09	0.192						+	8
1113	perfluoro-n-hexane	355-42-0	338.04	0						0	1
1114	2-chlorotoluene	95-49-8	126.58	2.82						1	8
1115	m-nitrotoluene	99-08-1	137.14	0.48			1			0	8
1116	benzotrifluoride	98-08-8	146.11	0.28	0.26	9%	1			0	8
1117	p-trifluoromethyl-chloro- benzene	98-56-6	180.55	0.121	0.11	10%	1			0	8
1118	p-toluene isocyanate	622-58-2	133.15	1.03	0.93	11%	1	2		0	5
1119	3-(chloromethyl)-heptane	123-04-6	148.67	0.88						0	10
1120	cyclosiloxane D4; octamethylcyclotetrasiloxane	556-67-2	296.62	-0.056			1	3		0	5
1121	cumene hydroperoxide; 1- methyl-1- phenylethylhydroperoxide**	80-15-9	152.19	8.83	12.61	-30%				+	*UL*
1122	2,4-toluene diisocyanate	584-84-9	174.16	-0.072			1	2		0	5
1123	2,6-toluene diisocyanate	91-08-7	174.16	-0.072				4		0	5
1124	toluene diisocyanate (mixed isomers)	26471-62-5	174.16	-0.072	0.00	0%				0	5
1125	Molinate; S-ethyl hexahydro- 1H-azepine-1-carbothioate	2212-67-1	187.30	1.43						0	7
1126	EPTC; S-ethyl dipropyl- thiocarbamate	759-94-4	189.32	1.58			1	2		0	2
1127	triisopropanolamine	122-20-3	191.27	2.60						+	13a,n
1128	dexpanthenol; pantothenylol**	81-13-0	205.25	5.98	9.35	-36%				+	*UL*
1129	pebulate; S-propyl butylethylthiocarbamate	1114-71-2	203.34	1.58						0	7
1130	cyclosiloxane D5; decamethylcyclopentasiloxane	541-02-6	370.77	-0.068			1	4		0	5
1131	thiobencarb; S-[4-chlorobenzyl] N,N-diethylthiolcarbamate	28249-77-6	257.78	0.65						0	8
1132	methylene diphenylene diisocyanate	101-68-8	250.25	0.87	0.79	10%				0	8
1133	lauryl pyrrolidone	2687-96-9	253.42	0.89						0	11
<u>CARB Hydrocarbon Bins</u>											
1134	CARB Hydrocarbon Bin 1		14.25	1.33	2.08	-36%				0	7c
1135	CARB Hydrocarbon Bin 2		14.37	1.23	1.59	-23%				0	7c
1136	CARB Hydrocarbon Bin 3		14.03	1.53	2.52	-39%				0	7c
1137	CARB Hydrocarbon Bin 4		14.19	1.37	2.24	-39%				0	7c
1138	CARB Hydrocarbon Bin 5		14.06	1.47	2.56	-43%				0	7c
1139	CARB Hydrocarbon Bin 6		14.18	1.08	1.41	-23%				0	7c
1140	CARB Hydrocarbon Bin 7		14.26	0.95	1.17	-19%				0	7c
1141	CARB Hydrocarbon Bin 8		14.03	1.34	1.65	-19%				0	7c
1142	CARB Hydrocarbon Bin 9		14.13	1.35	1.62	-17%				0	7c
1143	CARB Hydrocarbon Bin 10		14.04	1.88	2.03	-8%				0	7c
1144	CARB Hydrocarbon Bin 11		14.14	0.63	0.91	-31%				0	8c
1145	CARB Hydrocarbon Bin 12		14.20	0.55	0.81	-32%				0	8c
1146	CARB Hydrocarbon Bin 13		14.03	0.79	1.01	-22%				0	8c
1147	CARB Hydrocarbon Bin 14		14.10	0.91	1.21	-24%				0	8c
1148	CARB Hydrocarbon Bin 15		14.02	1.48	1.82	-19%				0	8c
1149	CARB Hydrocarbon Bin 16		14.11	0.47	0.57	-18%				0	8c
1150	CARB Hydrocarbon Bin 17		14.16	0.43	0.51	-16%				0	8c

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
1151	CARB Hydrocarbon Bin 18		14.03	0.54	0.63	-14%			0	8c
1152	CARB Hydrocarbon Bin 19		14.09	0.61	0.88	-31%			0	8c
1153	CARB Hydrocarbon Bin 20		14.03	0.89	1.49	-41%			0	10c
1154	CARB Hydrocarbon Bin 21		13.27	7.44	7.37	1%			0	8c
1155	CARB Hydrocarbon Bin 22		13.36	7.39	7.51	-2%			0	8c
1156	CARB Hydrocarbon Bin 23		13.41	6.66	8.07	-17%			0	10c
1157	CARB Hydrocarbon Bin 24		13.47	3.76	5.00	-25%			0	11c
<u>Other Complex Mixtures</u>										
1158	Base ROG Mixture			3.50	3.71	-6%			0	7
1159	final LEV – RFA			3.44					0	7
1160	TLEV Exhaust -- RFA			3.89					0	7
1161	TLEV exhaust – phase 2			3.85					0	7
1162	Final LEV -- Phase 2			3.34					0	7
1163	TLEV Exhaust -- LPG			1.99					0	7
1164	TLEV Exhaust -- CNG			0.70					0	7
1165	TLEV Exhaust -- E-85			2.46					0	7
1166	TLEV Exhaust -- M-85			1.53					0	7
1167	composite mineral spirit (naphthas or lactol spirits) (ARB Profile ID 802)			1.75					0	7
1168	Safety-Kleen Mineral Spirits "A" (Type I-B, 91% Alkanes)			1.11				2	0,+	7
1169	Safety-Kleen Mineral Spirits "B" (Type II-C)			0.65				2	0,+	7
1170	Safety-Kleen Mineral Spirits "C" (Type II-C)			0.65				2	0,+	7
1171	Exxon Exxol® D95 Fluid			0.55				2	0	7
1172	Safety-Kleen Mineral Spirits "D" (Type II-C)			0.65				2	0,+	7
1173	Exxon Isopar® M Fluid			0.54				2	0	7
1174	thinning solvent/mineral spirits (Cal Poly SLO 1996)			1.79					0	7
1175	Aromatic 100®			7.38				2	0	7
1176	Kerosene			1.46				2	0	7
1177	Regular mineral spirits			1.73				2	0	7
1178	Reduced Aromatics Mineral Spirits			1.08				2	0	7
1179	Dearomatized Alkanes, mixed, predominately C10-C12			0.80				2	0	7
1180	VMP Naphtha			1.12				2	0	7
1181	Synthetic isoparaffinic alkane mixture, predominately C10- C12			0.68				2	0	7
1182	Oxo-Tridecyl Acetate			0.54	0.67	-20%			0	7
1183	Oxo-Dodecyl Acetate			0.58	0.72	-20%			0	7
1184	Oxo-Decyl Acetate			0.66	0.83	-20%		2	0	7
1185	Oxo-Nonyl Acetate			0.69	0.85	-19%			0	7
1186	Oxo-Octyl Acetate			0.78	0.96	-19%			0	7
1187	Oxo-Heptyl Acetate			0.80	0.97	-17%			0	7
1188	Oxo-Hexyl Acetate			0.84	1.03	-18%			0	7
1189	turpentine	8006-64-2		4.12				note [e]	0	7

Table A-1 (continued)

No. [a]	Description [b]	CAS	MWt	MIR [c]			Codes [d]			
				New	Old	Chg	k a	Expt	Bias	Unc
1190	soy methyl esters; alkyl C16-C18 methyl esters			1.52			note [f]	0	8	

## Notes:

[a] VOCs in this table are organized into various sections, and ordered in those sections as described below. Individual compounds or simple mixtures of isomers assumed to have the same reactivity are categorized as alkanes, alkenes, aromatic hydrocarbons, oxygenates (compounds with C, H, and O's only), and other organics. Compounds or isomeric mixtures are then sorted by carbon number, and then as follows depending on the category: Alkanes by normal, branched, or cyclic alkanes; alkenes by external, internal, cyclic, and di- and polyunsaturated alkenes; aromatic hydrocarbons by mono-, di-, and polysubstituted benzenes, indans and tetralins and naphthalenes; oxygenated and other organics by molecular weight. Complex mixtures are ordered by bin number or time the mixture was added to the MIR list, as applicable.

[b] A "\*\*\*" after the name means that no MIR estimate was developed for this compound and the the upper limit MIR (ULMIR) was used for this compound.

[c] Calculated ozone impact in the maximum incremental reactivity (MIR) scale in units of grams O<sub>3</sub> per gram VOC. Column labels: "New" = current updated values calculated using the SAPRC-07 mechanism as documented by Carter (2009). "Old" = MIR values used in the CARB (2003) regulation. Those with a "\*" are not represented in the SAPRC-99 mechanism and the CARB assigned them Upper Limit MIRs for regulatory purposes. For the CARB hydrocarbon bins, the "Old" values are those of Kwok et al (2000).

[d] The various types of codes related to uncertainties are as follows. These are from Carter (2009).

“k a” ... Codes indicating availability of measurement data for the reaction rate constants

- 1 The OH radical rate constant has been measured. If the compound is consumed primarily by photolysis, this code means that absorption cross section and quantum yield are available. Not applicable for mixtures or compounds represented by another compound using the "lumped molecule" method.
- blank Either the OH radical rate constant or (if primarily photoreactive) the photolysis rate parameters had to be estimated, or this compound is represented by another compound using the "lumped molecule" method. Not applicable for mixtures.

“Expt” ... Environmental Chamber Data Availability Codes (if blank, no suitable evaluation data are available). See Carter (2009) for results of evaluations of the mechanisms against chamber data.

- 1 Extensive evaluation data for a variety of conditions.
- 2 Sufficient data available. At least 2 and often 3 types of evaluation experiments to test data under different conditions.
- 3 Limited evaluation data; usually representing one set of conditions, or some inconsistencies in evaluation results.
- 3a Evaluation data exist for 2 or more sets of conditions, but uncertainties exist concerning amount of compound available to react in the gas phase. See Carter (2008).
- 4 Data from only a single experiment is available, results from different experiments gave inconsistent results, or problems exist with the data.
- 4a Data from only a single experiment is available, and uncertainties exist concerning the amount of compound available for reaction in the gas phase. See Carter (2008).
- m This compound was studied in a mixture with the other isomer. Since the reactivities of the two isomers are different, the uncertainty classification has been increased over that of the mixture that was studied.
- x No attempt was made to improve the mechanism performance to fit the available data.

“Bias” ... Probable reactivity prediction bias codes (if blank, this compound has not been rated)

Chamber data available

No chamber data available



Table A-1 (continued)

0	No apparent bias	Direction of bias is unknown
+	Some indication of positive bias	Positive bias considered to be more likely than not
-	Some indication of negative bias	Negative bias is considered to be more likely than not
±2	Bias found to be relatively large	Bias may be relatively large
x,x	If two codes given, first indicates observed or probable bias for predictions of rates of NO oxidation and O <sub>3</sub> formation, which is important in affecting MIR reactivity, and the second indicates observed or probable bias for low NO <sub>x</sub> conditions. E.g. “0,+” if chamber data available indicates that the model simulated rates of NO oxidation and O <sub>3</sub> formation but overpredicted final O <sub>3</sub> yields in NO <sub>x</sub> -limited experiments.	
?	There is some inconsistency in the data concerning this bias indication (or lack thereof), or the bias is unknown but may be large.	
a	The reactivity predictions and representation in the mechanism is based on the assumption that this compound is completely available for reaction in the gas phase. This is likely not to be the case for this compound. Thus the reactivity estimate may be high for compounds that have positive O <sub>3</sub> impacts and low for compounds that are calculated to be inhibitors.	

“Unc” ... Uncertainty codes (if blank, this compound or mixture has not been rated)

The following codes are used when experimental data are available to evaluate the reactivity predictions of the mechanism and the mechanism was (or would have been) adjusted to fit the data as appropriate to improve the fits.

- 1 The mechanism appears to be reasonably well established or at least its predictions appear to be reasonably well evaluated. This does not rule out possible changes in reactivity values if the base mechanism, scenario conditions, or reactivity metrics are changed. Also used for compounds known or expected to be inert or to have upper limit reactivities much less than methane.
- 2 The mechanism has been evaluated at least to some extent, rate constant data are available for its major reactions, and is not considered to have large uncertainties. If a likely bias is indicated it is probably not large.
- 3 The mechanism has been evaluated at least to some extent and rate constant data are available for its major reactions, but the mechanism has some uncertainties or apparent inconsistencies with available laboratory data, or there are some uncertainties in the evaluation data. If a likely bias is indicated it is probably not large.
- 4 The mechanism has been evaluated at least to some extent and rate constant data are available for its major reactions, but the mechanism has some uncertainties, apparent inconsistencies with available laboratory data exist that may be significant, or the available evaluation database is limited or has problems. If a likely bias of ±1 is indicated it is probably not large.
- 5 A highly parameterized mechanism has been adjusted to simulate chamber data. The appropriateness of the parameterization, and its ability to extrapolate to ambient conditions, is uncertain.

The following codes are used for compounds for which no experimental data exist to evaluate reactivity predictions of the mechanism, or where such data, if any, were not taken into account when developing the mechanism.

- 6 The mechanism has not been evaluated but at least the important reaction rate(s) have been measured and the methods used to estimate the mechanism have been found to generally perform reasonably well for compounds where evaluation data are available, or the mechanisms are not expected to be highly complex. If a likely bias is indicated it is based on evaluation results for similar compounds.

Table A-1 (continued)

- 7 The mechanism has not been evaluated and the reaction rates had to be estimated, but the methods used to estimate the rate constant(s) and mechanism have been found to generally perform reasonably well for compounds where evaluation data are available. If a likely bias is indicated it is based on evaluation results for similar compounds. This code is also used for mixture or lumped molecule or mixture representations that are considered to be reasonably appropriate.
- 8 The estimated mechanism and/or relevant rate constant(s) or photolysis rates have some uncertainties, but mechanisms based on similar assumptions have been found to perform satisfactorily for related compounds, or the mechanisms are not expected to be highly complex. The applicability of these assumptions to this compound, or the extrapolation of mechanisms for smaller compounds to one of this size, has some uncertainty. This code is also used for mixture or lumped molecule representations whose appropriateness has some uncertainty.

The uncertainty codes below mean that use of the reactivity values in regulatory applications needs to take uncertainty into account

- 10 The estimated mechanism is sufficiently uncertain that it needs to be evaluated. This code is also used for mixture or lumped molecule representations whose appropriateness is considered to be highly uncertain. However, the representation employed is the current best estimate, and the direction of the bias is unknown.
- 11 The estimated mechanism is extremely uncertain and needs to be evaluated. This code is also used for mixture or lumped molecule representations whose appropriateness is questionable, but no better alternative exists, and the bias of using the representation is unknown. However, the representation employed is the current best estimate, and the direction of the bias is unknown.
- 12 An estimated mechanism for the gas-phase reactions for this compound has been developed and has been evaluated at least qualitatively against available chamber data, but its estimated atmospheric ozone impact is highly uncertain because the amount of emitted compound available for reaction in the gas-phase is unknown. One important issue is that this compound may be removed by gas-phase reaction with HNO<sub>3</sub>, whose presence depends on ambient conditions and may not be appropriately represented in the scenarios used for reactivity assessment. For such compounds two reactivity values are given, and “upper limit magnitude” reactivity value based on assuming that all the emitted VOC is available for gas-phase reaction and that reaction with HNO<sub>3</sub> is negligible (as may be applicable if the HNO<sub>3</sub> formed in gas-phase reactions is removed from the gas phase by other means) and one also assuming that all the emitted VOC is available for gas-phase reaction except that the reaction with gas-phase HNO<sub>3</sub> is fast and there is no other sink for HNO<sub>3</sub> formed in the gas-phase reactions.
- 13 Same as code 12 except that no chamber data are available to test the estimated gas-phase mechanism.
- 20 The representation or estimated mechanism used is considered to be biased, and the direction of the likely bias is indicated by the bias code. Best estimate mechanisms have not been developed.
- UL No mechanism or MIR estimate has been derived for this compound. Upper limit MIR estimates are given.

Additional codes used where applicable

- s Portions of the mechanism are unknown or highly uncertain and simplified or parameterized representation has been adjusted at least in part to fit available data for this or related compounds. This is used primarily for alkylbenzenes.
- d Portions of this mechanism appear to be inconsistent with available laboratory data. This is used primarily for the 1-alkenes, where radical yields in O<sub>3</sub> reactions have to be reduced to simulate chamber data.

Table A-1 (continued)

- u The mechanism is unknown and a parameterized mechanism adjusted to fit the data for this or related compounds is employed.
  - m This uncertainty code is only applicable for mixtures whose composition has been analyzed using state-of-the-science methods. Rating of effects of compositional uncertainties is beyond the scope of the project (but see discussion in Carter and Malkina (2005) for hydrocarbon mixtures).
  - b The reactivity predictions may be more sensitive than usual to changes in the base mechanism or scenario conditions.
  - n Chamber data for this or related compounds suggest that the mechanism may overpredict ozone under conditions where  $\text{NO}_x$  is limited. This should affect MIR values but will lead to too high reactivities in lower  $\text{NO}_x$  scenarios.
  - a This compound may react with  $\text{HNO}_3$  to form a non-volatile salt, which may reduce the availability for this compound to react in the gas phase. The importance of this process under atmospheric conditions is uncertain because (a) the salt may revolatilize to the gas-phase species and the equilibrium constant is unknown, (b) the sources and other sinks for  $\text{HNO}_3$  may vary significantly from scenario to scenario and have not been established for the reactivity assessment scenarios, and (c) if ammonia or other amines are present they may compete for the  $\text{HNO}_3$  and reduce the importance of this process for this amine, and the importance of these processes have not been established for the reactivity scenarios. In order to derive an upper limit ozone impact estimate, the reactivities of these compounds have been calculated assuming that removal by reaction with  $\text{HNO}_3$  is uncertain. If this process is important, the magnitude of the actual ozone impact may be an order of magnitude or more low. Therefore, the tabulated reactivity values are upper limits for positively reactive compounds, and lower limits for ozone inhibitors.
  - c CARB hydrocarbon bins are defined as described by Kwok et al (2000), and the SAPRC-99 bin MIRs derived by Kwok et al (2000) for use in CARB regulations are given in the "old" column. The data in the "new" column were calculated based on estimated compositions in each bin, as discussed in the "Hydrocarbon Bin MIR Calculation" section of this report. See the "Hydrocarbon Bin MIR Calculation" section of this report for a discussion of the bin MIR calculation methodologies and for tables showing effects of changing only the methodology or the mechanism.
  - + This may appropriately be considered to be an upper limit estimate in the ozone impact of this compound.
  - This may appropriately be considered to be an upper limit estimate in the amount of ozone inhibition caused by this compound. The upper limit reactivity is zero.
- [e] Turpentine composition used is 66% a-pinene, 24% b-pinene, 5% d-limonene, 3% camphene, 1% 3-carene, and 1% terpinolene, based on recommendation of CARB staff (Dongmin Luo, CARB Research Division, personal communication, August 19, 2009. This is consistent with the range of data reported by Hanske (2002).
- [f] Soy methyl ester composition used is: methyl palmitate: 10%; methyl linolenate: 5%; methyl oleate: 25%; methyl linoelate: 55%; and methyl stearate: 5%. This is based on recommendation of CARB staff (Carla Takemoto, Stationary Source Division, personal communication, August 26, 2009.

**APPENDIX B. MIXTURE COMPOSITIONS USED TO CALCULATE  
HYDROCARBON BIN REACTIVITIES**

Table B-1. Compositions of mixtures assigned to the CARB hydrocarbon bins. From Table B-10 of Carter (2009).

Wt %	Constituent	Wt %	Constituent
Bin 1		Bin 5	
10.1%	n-pentane	8.6%	n-pentane
20.3%	n-hexane	17.3%	n-hexane
2.9%	n-heptane	2.5%	n-heptane
2.9%	branched C5 alkanes	2.5%	branched C5 alkanes
20.6%	branched C6 alkanes	17.5%	branched C6 alkanes
9.8%	branched C7 alkanes	8.4%	branched C7 alkanes
10.1%	cyclopentane	8.6%	cyclopentane
20.3%	C6 cycloalkanes	17.3%	C6 cycloalkanes
2.9%	C7 cycloalkanes	2.5%	C7 cycloalkanes
Bin 2		7.4%	benzene
15.1%	n-pentane	7.6%	toluene
30.5%	n-hexane	Bin 6	
4.4%	n-heptane	3.2%	n-heptane
4.4%	branched C5 alkanes	16.7%	n-octane
30.8%	branched C6 alkanes	12.8%	n-nonane
14.8%	branched C7 alkanes	0.7%	n-decane
Bin 3		10.3%	branched C8 alkanes
30.2%	cyclopentane	17.7%	branched C9 alkanes
61.0%	C6 cycloalkanes	5.3%	branched C10 alkanes
8.8%	C7 cycloalkanes	3.2%	C7 cycloalkanes
Bin 4		16.7%	C8 cycloalkanes
9.6%	n-pentane	12.8%	C9 cycloalkanes
19.3%	n-hexane	0.7%	C10 cycloalkanes
2.8%	n-heptane	Bin 7	
2.8%	branched C5 alkanes	4.8%	n-heptane
19.5%	branched C6 alkanes	25.0%	n-octane
9.4%	branched C7 alkanes	19.2%	n-nonane
9.6%	cyclopentane	1.1%	n-decane
19.3%	C6 cycloalkanes	15.5%	branched C8 alkanes
2.8%	C7 cycloalkanes	26.6%	branched C9 alkanes
2.5%	benzene	7.9%	branched C10 alkanes
2.5%	toluene	Bin 8	
		9.5%	C7 cycloalkanes
		50.0%	C8 cycloalkanes
		38.4%	C9 cycloalkanes
		2.1%	C10 cycloalkanes

Table B-1 (continued)

Wt %	Constituent	Wt %	Constituent
Bin 9		Bin 10	
3.01%	n-heptane	2.69%	n-heptane
15.83%	n-octane	14.16%	n-octane
12.16%	n-nonane	10.88%	n-nonane
0.67%	n-decane	0.60%	n-decane
9.81%	branched C8 alkanes	8.77%	branched C8 alkanes
16.85%	branched C9 alkanes	15.07%	branched C9 alkanes
5.02%	branched C10 alkanes	4.49%	branched C10 alkanes
3.01%	C7 cycloalkanes	2.69%	C7 cycloalkanes
15.83%	C8 cycloalkanes	14.16%	C8 cycloalkanes
12.16%	C9 cycloalkanes	10.88%	C9 cycloalkanes
0.67%	C10 cycloalkanes	0.60%	C10 cycloalkanes
1.56%	toluene	4.68%	toluene
0.28%	ethyl benzene	0.83%	ethyl benzene
0.05%	n-propyl benzene	0.14%	n-propyl benzene
0.03%	isopropyl benzene (cumene)	0.09%	isopropyl benzene (cumene)
0.89%	m-xylene	2.67%	m-xylene
1.08%	o-xylene	3.24%	o-xylene
0.34%	p-xylene	1.01%	p-xylene
0.13%	m-ethyl toluene	0.38%	m-ethyl toluene
0.07%	o-ethyl toluene	0.20%	o-ethyl toluene
0.07%	p-ethyl toluene	0.20%	p-ethyl toluene
0.14%	1,2,3-trimethyl benzene	0.42%	1,2,3-trimethyl benzene
0.25%	1,2,4-trimethyl benzene	0.76%	1,2,4-trimethyl benzene
0.09%	1,3,5-trimethyl benzene	0.26%	1,3,5-trimethyl benzene
0.04%	indan	0.13%	indan
Bin 11		Bin 13	
3.1%	n-decane	9.2%	C10 cycloalkanes
15.2%	n-undecane	45.7%	C11 cycloalkanes
12.8%	n-dodecane	38.5%	C12 cycloalkanes
2.2%	n-tridecane	6.5%	C13 cycloalkanes
6.3%	branched C11 alkanes		
18.3%	branched C12 alkanes		
8.7%	branched C13 alkanes		
3.1%	C10 cycloalkanes		
15.2%	C11 cycloalkanes		
12.8%	C12 cycloalkanes		
2.2%	C13 cycloalkanes		
Bin 12			
4.6%	n-decane		
22.8%	n-undecane		
19.3%	n-dodecane		
3.3%	n-tridecane		
9.4%	branched C11 alkanes		
27.5%	branched C12 alkanes		
13.1%	branched C13 alkanes		

Table B-1 (continued)

Wt %	Constituent	Wt %	Constituent
	Bin 14		Bin 15
2.93%	n-decane	2.62%	n-decane
14.47%	n-undecane	12.94%	n-undecane
12.20%	n-dodecane	10.92%	n-dodecane
2.07%	n-tridecane	1.85%	n-tridecane
5.97%	branched C11 alkanes	5.35%	branched C11 alkanes
17.40%	branched C12 alkanes	15.56%	branched C12 alkanes
8.30%	branched C13 alkanes	7.42%	branched C13 alkanes
2.93%	C10 cycloalkanes	2.62%	C10 cycloalkanes
14.47%	C11 cycloalkanes	12.94%	C11 cycloalkanes
12.20%	C12 cycloalkanes	10.92%	C12 cycloalkanes
2.07%	C13 cycloalkanes	1.85%	C13 cycloalkanes
0.24%	C10 trisubstituted benzenes	0.71%	C10 trisubstituted benzenes
0.16%	C10 disubstituted benzenes	0.47%	C10 disubstituted benzenes
0.06%	C10 tetrasubstituted benzenes	0.18%	C10 tetrasubstituted benzenes
0.05%	methyl indans	0.15%	methyl indans
0.05%	1,2,3,5 tetramethyl benzene	0.14%	1,2,3,5 tetramethyl benzene
0.03%	m-diethyl benzene	0.09%	m-diethyl benzene
0.02%	C10 monosubstituted benzenes	0.07%	C10 monosubstituted benzenes
0.02%	p-diethyl benzene	0.06%	p-diethyl benzene
0.02%	n-butyl benzene	0.05%	n-butyl benzene
0.02%	naphthalene	0.05%	naphthalene
0.01%	o-diethyl benzene	0.03%	o-diethyl benzene
1.04%	C11 trisubstituted benzenes	3.13%	C11 trisubstituted benzenes
0.52%	C11 tetrasubstituted benzenes	1.57%	C11 tetrasubstituted benzenes
0.21%	C11 tetralin or indan	0.63%	C11 tetralin or indan
0.16%	C11 disubstituted benzenes	0.48%	C11 disubstituted benzenes
0.10%	2-methyl naphthalene	0.29%	2-methyl naphthalene
0.08%	C11 pentasubstituted benzenes	0.25%	C11 pentasubstituted benzenes
0.05%	C11 monosubstituted benzenes	0.16%	C11 monosubstituted benzenes
0.02%	1-methyl naphthalene	0.07%	1-methyl naphthalene
0.04%	C12 monosubstituted benzenes	0.11%	C12 monosubstituted benzenes
0.11%	C12 disubstituted benzenes	0.33%	C12 disubstituted benzenes
1.13%	C12 trisubstituted benzenes	3.40%	C12 trisubstituted benzenes
0.55%	C12 naphthalenes	1.65%	C12 naphthalenes
0.01%	C13 disubstituted benzenes	0.01%	C13 monosubstituted benzenes
0.13%	C13 trisubstituted benzenes	0.04%	C13 disubstituted benzenes
0.15%	C13 naphthalenes	0.40%	C13 trisubstituted benzenes
		0.46%	C13 naphthalenes

Table B-1 (continued)

Wt %	Constituent	Wt %	Constituent
Bin 16		Bin 19	
7.6%	n-tetradecane	7.27%	n-tetradecane
16.6%	n-pentadecane	15.81%	n-pentadecane
8.1%	n-C16	7.69%	n-C16
0.9%	n-C17	0.89%	n-C17
1.3%	branched C14 alkanes	1.20%	branched C14 alkanes
9.6%	branched C15 alkanes	9.09%	branched C15 alkanes
14.4%	branched C16 alkanes	13.72%	branched C16 alkanes
8.1%	branched C17 alkanes	7.65%	branched C17 alkanes
7.6%	C14 cycloalkanes	7.27%	C14 cycloalkanes
16.6%	C15 cycloalkanes	15.81%	C15 cycloalkanes
8.1%	C16 cycloalkanes	7.69%	C16 cycloalkanes
Bin 17		0.89%	C17 cycloalkanes
11.5%	n-tetradecane	0.01%	C14 monosubstituted benzenes
25.0%	n-pentadecane	0.03%	C14 disubstituted benzenes
12.1%	n-C16	0.32%	C14 trisubstituted benzenes
1.4%	n-C17	1.08%	C14 naphthalenes
1.9%	branched C14 alkanes	0.01%	C15 monosubstituted benzenes
14.4%	branched C15 alkanes	0.02%	C15 disubstituted benzenes
21.7%	branched C16 alkanes	0.23%	C15 trisubstituted benzenes
12.1%	branched C17 alkanes	2.30%	C15 naphthalenes
Bin 18		1.00%	C16 naphthalenes
23.6%	C14 cycloalkanes		
51.4%	C15 cycloalkanes		
25.0%	C16 cycloalkanes		

Table B-1 (continued)

Wt %	Constituent	Wt %	Constituent
	Bin 20		Bin 22
6.50%	n-tetradecane	3.14%	n-propyl benzene
14.15%	n-pentadecane	2.00%	isopropyl benzene (cumene)
6.88%	n-C16	1.42%	C10 monosubstituted benzenes
0.80%	n-C17	1.17%	n-butyl benzene
1.08%	branched C14 alkanes	0.08%	s-butyl benzene
8.13%	branched C15 alkanes	8.40%	m-ethyl toluene
12.28%	branched C16 alkanes	4.37%	o-ethyl toluene
6.84%	branched C17 alkanes	4.40%	p-ethyl toluene
6.50%	C14 cycloalkanes	10.01%	C10 disubstituted benzenes
14.15%	C15 cycloalkanes	1.95%	m-diethyl benzene
6.88%	C16 cycloalkanes	0.58%	o-diethyl benzene
0.80%	C17 cycloalkanes	1.19%	p-diethyl benzene
0.03%	C14 monosubstituted benzenes	0.00%	isomers of propylbenzene
0.09%	C14 disubstituted benzenes	9.32%	1,2,3-trimethyl benzene
0.96%	C14 trisubstituted benzenes	16.87%	1,2,4-trimethyl benzene
3.24%	C14 naphthalenes	5.90%	1,3,5-trimethyl benzene
0.02%	C15 monosubstituted benzenes	2.95%	1,2,3,5 tetramethyl benzene
0.07%	C15 disubstituted benzenes	0.02%	isomers of butylbenzene
0.68%	C15 trisubstituted benzenes	15.12%	C10 trisubstituted benzenes
6.90%	C15 naphthalenes	3.85%	C10 tetrasubstituted benzenes
3.01%	C16 naphthalenes	2.87%	indan
	Bin 21	1.15%	naphthalene
0.44%	toluene	3.14%	methyl indans
10.28%	ethyl benzene	0.10%	tetralin
0.18%	n-propyl benzene		
0.12%	isopropyl benzene (cumene)		
33.15%	m-xylene		
40.24%	o-xylene		
12.53%	p-xylene		
0.49%	m-ethyl toluene		
0.26%	o-ethyl toluene		
0.26%	p-ethyl toluene		
0.55%	1,2,3-trimethyl benzene		
0.99%	1,2,4-trimethyl benzene		
0.35%	1,3,5-trimethyl benzene		
0.17%	indan		



Table B-1 (concluded)

Wt %	Constituent	Wt %	Constituent
	Bin 23		Bin 24
4.69%	C10 trisubstituted benzenes	0.19%	C13 monosubstituted benzenes
3.11%	C10 disubstituted benzenes	0.57%	C13 disubstituted benzenes
1.20%	C10 tetrasubstituted benzenes	5.90%	C13 trisubstituted benzenes
0.97%	methyl indans	6.66%	C13 naphthalenes
0.92%	1,2,3,5 tetramethyl benzene	0.46%	C14 monosubstituted benzenes
0.60%	m-diethyl benzene	1.36%	C14 disubstituted benzenes
0.44%	C10 monosubstituted benzenes	14.09%	C14 trisubstituted benzenes
0.37%	p-diethyl benzene	47.73%	C14 naphthalenes
0.36%	n-butyl benzene	0.07%	C15 monosubstituted benzenes
0.36%	naphthalene	0.20%	C15 disubstituted benzenes
0.18%	o-diethyl benzene	2.04%	C15 trisubstituted benzenes
0.03%	tetralin	20.73%	C15 naphthalenes
0.02%	s-butyl benzene		
0.01%	isomers of butylbenzene		
35.67%	C11 trisubstituted benzenes		
17.94%	C11 tetrasubstituted benzenes		
7.22%	C11 tetralin or indan		
5.45%	C11 disubstituted benzenes		
3.36%	2-methyl naphthalene		
2.84%	C11 pentasubstituted benzenes		
1.86%	C11 monosubstituted benzenes		
0.77%	1-methyl naphthalene		
0.24%	C12 monosubstituted benzenes		
0.70%	C12 disubstituted benzenes		
7.21%	C12 trisubstituted benzenes		
3.49%	C12 naphthalenes		