

# **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). 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 (Carter, 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), 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, 2003) concerns the chemical mechanism used and the number and types of VOCs whose ozone impacts are calculated.

The previous MIR scales of Carter (2000, 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, of which 741 are represented using mechanisms explicitly derived for the compound, with the MIRs of the

remainder being estimated by assuming they have the same ozone impact per molecule as another chemically similar compound. In addition, ozone impacts for a total of 76 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, based on those provided by Carter (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 latest SAPRC-99 scale provided by Carter (2003a) are shown in Figure 1. The 1:1 and  $\pm 30\%$  lines are also shown. The average change (excluding the 10 outliers where the change was greater than 60%) in the MIR's was -13%, and the average absolute magnitude of the change (again excluding the outliers) was 15%. 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<sup>1</sup>.

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). The higher OH + NO<sub>2</sub> rate constant used in the updated mechanism may be one reason for this lower O<sub>3</sub> in the MIR scenarios. Sensitivity calculations or more analyses are needed to assess this in more detail.

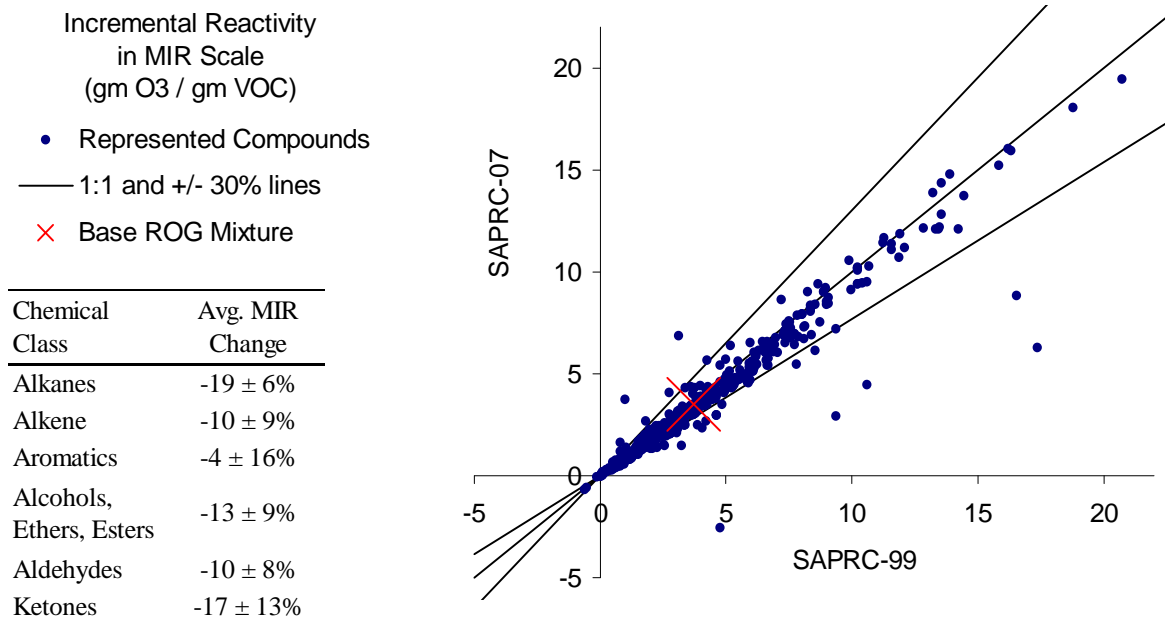


Figure 1. Plots of incremental reactivities in the MIR scale computed using the updated mechanism against those reported previously by Carter (2003a). Average MIR changes for different chemical classes are also shown.

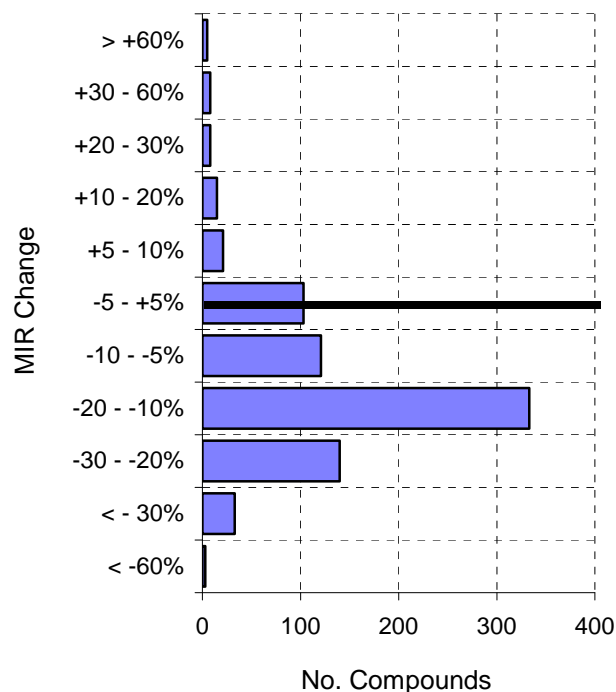
<sup>1</sup> The average for alcohols, ethers, and esters on Figure 1 excluded 3-methoxy-1-butanol, which had an incorrect rate constant in the SAPRC-99 mechanism.

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%	3	0.4%
< -30%	33	4%
-30 - -20%	140	18%
-20 - -10%	333	42%
-10 - -5%	121	15%
-5 - +5%	103	13%
+5 - 10%	21	3%
+10 - 20%	15	2%
+20 - 30%	8	1%
+30 - 60%	8	1%
> +60%	5	0.6%
Abs Chg < 30%	741	94%
New MIRs	347	31%

[a] Based on SAPRC-99 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.



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 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 chloroaldehyde products predicted to be formed. It is interesting to note that except for the compound with the erroneous mechanism that was corrected, all the changes are less than about 150%. 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.

## 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 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 Reason
	Old	New	Change	
3-Methoxy-1-butanol	0.97	3.75	287%	1
2-Amino-2-methyl-1-propanol	4.75	-2.57	-154%	2
2-(Chloromethyl)-3-chloropropene	3.13	6.85	119%	3
1,2-Dibromoethane	0.046	0.098	111%	4
1,2-Dichloroethane	0.098	0.21	111%	3
trans-1,2-Dichloroethene	0.81	1.65	103%	3
Dimethyl amine	9.37	2.95	-69%	2
Mesityl oxide (2-methyl-2-penten-4-one)	17.37	6.31	-64%	5
3,5,5-trimethyl-2-cyclohexenone	10.58	4.48	-58%	5
Indene	3.21	1.48	-54%	
Propionic acid	0.79	1.17	48%	
Triethanolamine	2.75	4.08	48%	2
Phenol	1.82	2.69	48%	6
Furan	16.54	8.86	-46%	7
2,4-Toluene diisocyanate	-0.133	-0.072	-46%	
CARB Hydrocarbon Bin 5	2.56	1.47	-43%	8
1,1,2-Trichloroethane	0.058	0.082	42%	2
Diethanol amine	4.05	2.36	-42%	2
Dichloromethane	0.066	0.039	-41%	
Chloroform	0.034	0.020	-41%	
CARB Hydrocarbon Bin 20	1.49	0.89	-41%	8
1,2-Propylene glycol diacetate	0.94	0.58	-39%	
CARB Hydrocarbon Bin 3	2.52	1.53	-39%	8
CARB Hydrocarbon Bin 4	2.24	1.37	-39%	8
Unspeciated C11 aromatics	4.96	6.84	38%	9
2-Methyl 3,5-diisopropyl heptane	0.78	0.49	-37%	
Methyl naphthalenes	4.61	2.96	-36%	
CARB Hydrocarbon Bin 1	2.08	1.33	-36%	8
1,1-Dichloroethane	0.101	0.065	-35%	
2-Methyl-2,4-pentanediol	1.03	1.39	35%	
4,5-Dimethylheptyl acetate	0.96	0.63	-34%	
p-Xylene	4.24	5.69	34%	
6-Methyl tetradecane	0.55	0.37	-33%	
5-Methyl dodecane	0.62	0.41	-33%	
6-Methyl tridecane	0.59	0.40	-33%	
2,7-Dimethyl 3,5-diisopropyl heptane	0.69	0.47	-33%	
Acetic acid	0.50	0.66	32%	
1-Octanol	1.99	1.35	-32%	
5-Methylhexyl acetate	0.79	0.54	-32%	
3-Isopropylheptyl acetate	0.71	0.49	-32%	
4,7,9-Trimethyldecyl acetate	0.55	0.37	-32%	
CARB Hydrocarbon Bin 12	0.81	0.55	-32%	8
2,3,6-Trimethyl 4-isopropyl heptane	1.24	0.85	-31%	
4-Octanol	3.04	2.10	-31%	
2,2,3,3-Tetramethyl butane	0.44	0.31	-31%	



Table 2 (continued)

Compound	MIR (gm O <sub>3</sub> / gm VOC)			Probable Reason
	Old	New	Change	
CARB Hydrocarbon Bin 19	0.88	0.61	-31%	8
CARB Hydrocarbon Bin 11	0.91	0.63	-31%	8
3,4-Dimethylhexyl acetate	1.16	0.81	-30%	

Discussion of probable reasons for MIR changes:

- 1 The OH radical rate constant used in SAPRC-99 was found to be low by a factor of 10.
- 2 New amine mechanisms developed. Note that amines without hydrogens on groups adjacent to amino groups are now estimated to be inhibitors. Note also that the magnitudes of the amine MIRs could be significantly lower if loss of amines by reaction with HNO<sub>3</sub> is important. See Carter (2008a).
- 3 Chlorinated aldehyde and ketone products are now assumed to be much more photoreactive.
- 4 The approximate method used to represent bromine-containing compounds was changed. SAPRC-99 used a highly approximate "placeholder" mechanism. SAPRC-07 represents them using the mechanism for the corresponding Cl-containing compound.
- 5 These compounds are now represented by the model species used to represent the lumped C<sub>5</sub> isoprene product IPRD. The estimated mechanisms used in SAPRC-99, derived using the mechanism generation system, are now considered to be too uncertain to use.
- 6 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.
- 7 Furan is now represented explicitly. Previously it was represented by m-xylene using the lumped molecule method.
- 8 See the "Hydrocarbon Bin MIR Calculation" section of this report for a discussion of the calculations of the MIRs for the CARB hydrocarbon bin categories. The "old" values are those given by Kwok et al (2000) and were derived based on correlations between boiling points and SAPRC-99 MIRs for various types of hydrocarbons. The "new" values are calculated using the SAPRC-07 mechanism and chemical compositions derived for each bin, as described in the text. The changes in MIR values reflect both a change in mechanism and a change in methodology.
- 9 The compounds assigned to this mixture were changed and more classes of higher aromatics were added to take into account isomeric differences.

## 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 3. (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 3. 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 3 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 4. The type distribution assumptions are somewhat arbitrary but are consistent with the definitions on Table 3 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 3.

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 4:

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

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

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

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 2. 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 4. 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).

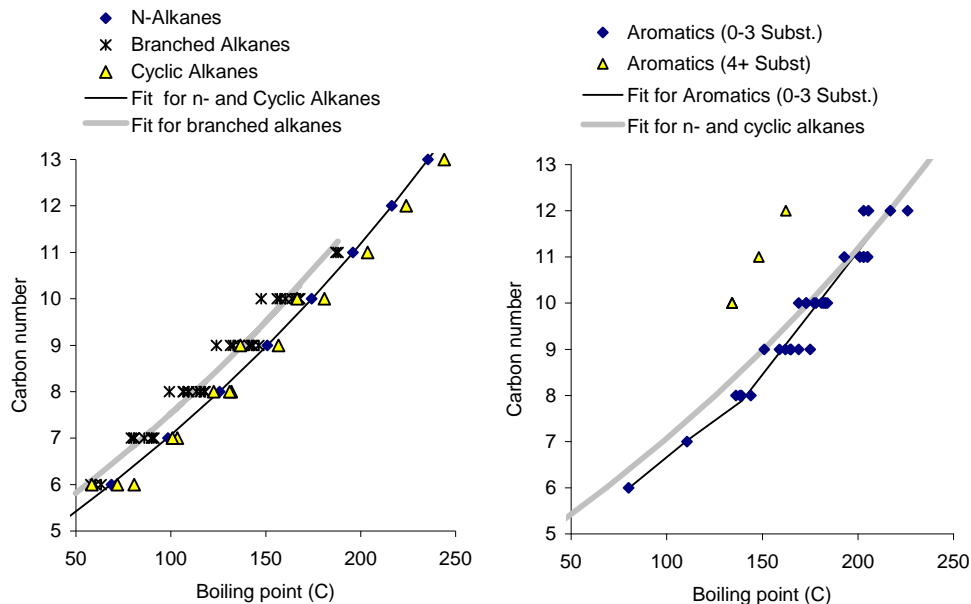


Figure 2. Plots of carbon numbers against boiling points for various alkanes and aromatic hydrocarbons (from Carter and Malkina, 2005).

$nC_{avg}$  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 4, 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 5 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 5 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 4, 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 5 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 6, 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 6. 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 5. 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 6. 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 5. 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 5, and the C<sub>12+</sub> aromatics are assigned compositions based on assuming increasing naphthalene content as shown on Table 6. 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>2</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 4, 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 7. 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 7:

- 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 aromatics. For this reason, the solvents falling into the high aromatics bins (5, 10, 15 and 20-24)

<sup>2</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 7. 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 7 (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	-	-	1.24
7-C	Bin 7 solvent "C"	A	250-320	9.2	-	100	-	-	-	0.82
7-D	Bin 7 solvent "D"	A	320-332	10.0	-	100	-	-	-	1.01
7-E	Bin 7 solvent "E"	A	204-218	8.0	-	100	-	-	-	0.86
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	-	1.23
9-A	Bin 9 solvent "A"	A	240-250	8.0	27	33	37	3	-	1.30
9-B	Bin 9 solvent "B"	A	158-270	6.7	28	41	28	3	-	1.31
CP12	Mineral Spirits	B	300-365	10.0	24	33	40	3	0	1.26
CP11	Mineral Spirits	B	300-365	9.9	20	30	47	3	0	1.09
CP30	VM&P naphtha	B	240-285	8.5	22	43	28	6	-	1.07
CARB Bin 10										
CP35	VM&P naphtha	B	247-282	8.4	17	29	45	10	-	1.47
CP01	VM&P naphtha	B	240-305	8.4	37	28	13	23	-	1.88
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	-	0.70
11-L	Bin 11 solvent "L"	A	415-450	12.6	2	58	40	0	-	0.71
11-J	Bin 11 solvent "J"	A	380-410	10.9	2	28	70	0	-	0.60
11-A	Bin 11 solvent "A"	A	380-410	10.9	24	12	64	-	-	0.82
11-C	Bin 11 solvent "C"	A	315-390	9.9	18	24	58	-	-	0.77
11-D	Bin 11 solvent "D"	A	324-394	10.8	14	29	57	-	-	0.94
11-E	Bin 11 solvent "E"	A	370-408	11.9	20	29	51	-	-	0.79
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	-	-	0.65
11-H	Bin 11 solvent "H"	A	370-405	11.5	-	89	11	-	-	0.59
CP16	aliphatic petroleum dist.	B	351-415	11.3	31	42	27	-	-	0.64
CP18	aliphatic petroleum dist.	B	312-387	11.3	30	43	27	-	-	0.67
CP33	Mineral Spirits	B	324-402	10.4	24	42	34	1	-	0.68
<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>	0.84
CARB Bin 12										
12-A	Bin 12 solvent "A"	A	357-408	11.5	-	100	-	-	-	0.79
12-B	Bin 12 solvent "B"	A	388-459	12.2	-	100	-	-	-	0.55
12-C	Bin 12 solvent "C"	A	434-472	13.3	-	100	-	-	-	0.62
12-D	Bin 12 solvent "D"	A	355-400	11.8	-	100	-	-	-	0.58
12-E	Bin 12 solvent "E"	A	352-370	11.0	-	96	4	-	-	0.52
12-F	Bin 12 solvent "F"	A	354-385	11.5	-	97	3	-	-	0.60
12-G	Bin 12 solvent "G"	A	372-426	11.5	99	1	-	-	-	0.68
12-H	Bin 12 solvent "H"	A	432-469	13.2	99	1	-	-	-	0.63
<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>	0.53

Table 7 (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	1.58
CP25	Mineral Spirits	B	318-380	10.2	11	32	47	11	2	1.60
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	1.79
CP15	aliphatic petroleum dist.	B	351-415	10.1	13	27	44	15	1	1.71
CP02	300-66 solvent, M.S. 66	B	310-400	9.9	21	32	30	17	0	2.03
CP39	paraffinic petroleum dist.	B	315-397	9.9	21	29	32	18	1	2.01
<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>	1.80
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 7 (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 3

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 7 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 4, and Table 7. Table 4 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 4 and Figure 3, and Figure 4a. 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 unspiciated  $C_6$  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.

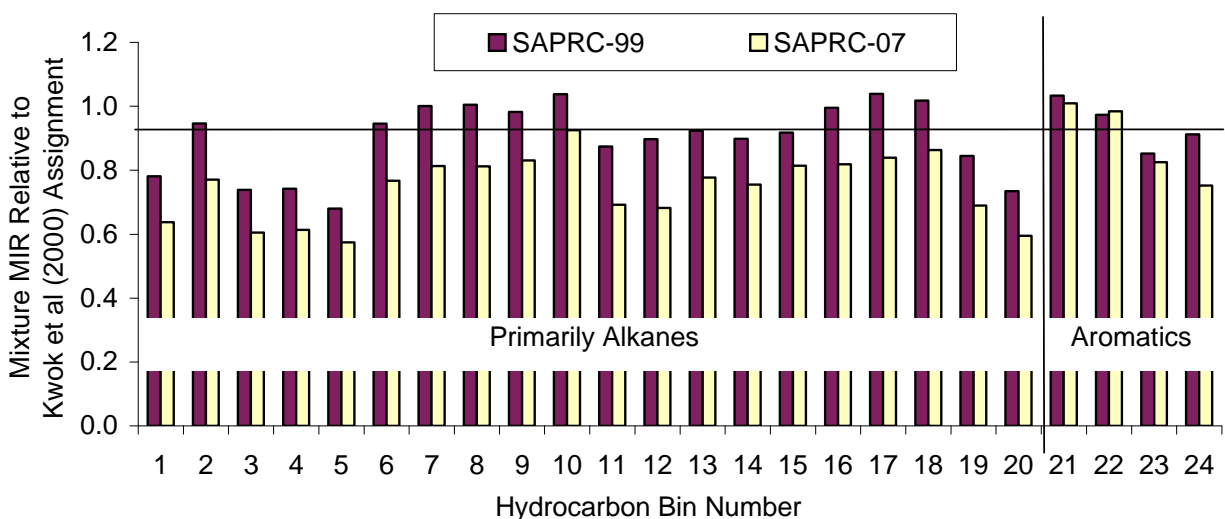


Figure 3. Changes in bin MIR values calculated using the mixture compositions in Table B-1 relative to the initial assignments of Kwok et al (2000). The SAPRC-99 data show the effects of changing the methodology only, and the SAPRC-07 data show the combined effects of changing the methodology and mechanism.

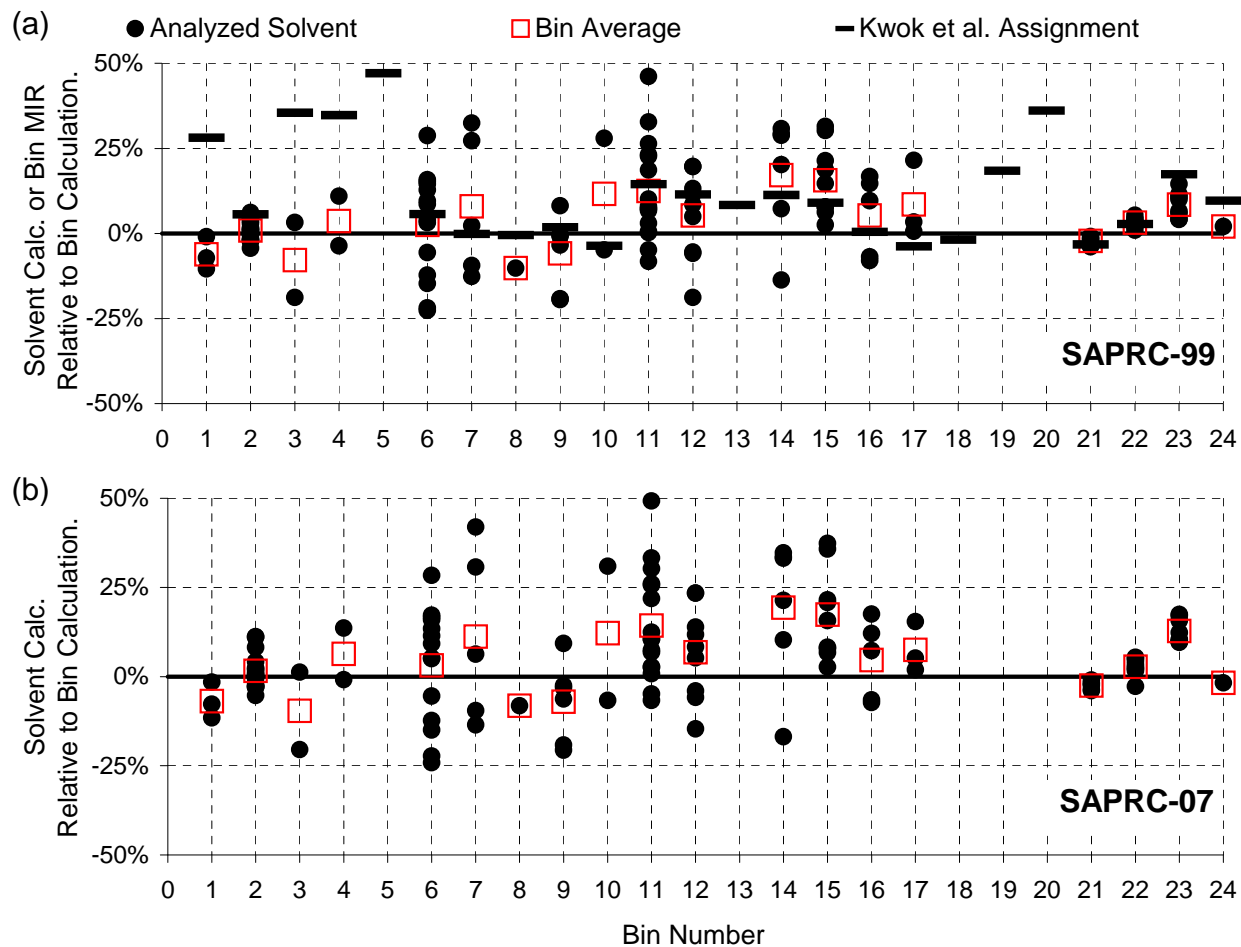


Figure 4. Plots of differences between assigned bin MIRs and explicitly calculated MIRs for the analyzed solvents. (a) Comparisons using SAPRC-99 MIRs, with bin assignments made by Kwok et al (2000) also shown. (b) Comparisons using SAPRC-07 MIRs.

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 7). 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 5 and Table 6). It is likely that they assumed much lower naphthalene fractions for the heaviest aromatics than we assume (see Table 6), 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 7 are shown on Figure 4a. 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 4b 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 4. 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 3 (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 3, 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 3 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.



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

Table A-1. Updated table of MIR values and uncertainty classifications. Previously tabulated MIR values from Carter (2003) are also shown for comparison.

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
1	carbon monoxide	630-08-0	28.01	0.053	0.057	-8%	1	2	0	1
2	methane	74-82-8	16.04	0.014	0.014	-1%	1		0	6
3	ethane	74-84-0	30.07	0.26	0.31	-13%	1	3	0	1
4	propane	74-98-6	44.10	0.46	0.56	-18%	1	3	0	1
5	n-butane	106-97-8	58.12	1.08	1.32	-18%	1	2	0	1
6	n-pentane	109-66-0	72.15	1.23	1.53	-20%	1		0	6
7	n-hexane	110-54-3	86.18	1.15	1.43	-19%	1	3	0	2
8	n-heptane	142-82-5	100.20	0.99	1.26	-22%	1		0	6
9	n-octane	111-65-9	114.23	0.82	1.09	-25%	1	1	0	2
10	n-nonane	111-84-2	128.26	0.71	0.93	-24%	1		0,+	6b
11	n-decane	124-18-5	142.28	0.62	0.81	-24%	1		0,+	6b
12	n-undecane	1120-21-4	156.31	0.55	0.72	-23%	1		0,+	6b
13	n-dodecane	112-40-3	170.33	0.50	0.64	-22%	1	2	0,+	3b
14	n-tridecane	629-50-5	184.36	0.47	0.60	-21%	1		0,+	6b
15	n-tetradecane	629-59-4	198.39	0.46	0.56	-18%	1	2	0,+	3b
16	n-pentadecane	629-62-9	212.41	0.44	0.53	-17%	1	4	0,+	3b
17	n-C16	544-76-3	226.44	0.39	0.50	-21%	1	3	0,+	3b
18	n-C17	629-78-7	240.47	0.37	0.47	-21%			0,+	7b
19	n-C18	593-45-3	254.49	0.35	0.44	-21%			0,+	7b
20	n-C19	629-92-5	268.52	0.33	0.42	-21%			0,+	7b
21	n-C20	112-95-8	282.55	0.31	0.40	-21%			0,+	7b
22	n-C21	629-94-7	296.57	0.30	0.38	-21%			0,+	7b
23	n-C22	629-97-0	310.60	0.29	0.36	-21%			0,+	7b
24	isobutane	75-28-5	58.12	1.17	1.34	-13%	1	3	0	2
25	branched C5 alkanes		72.15	1.36	1.67	-18%			0	8
26	neopentane	463-82-1	72.15	0.64	0.69	-7%	1		0	6
27	iso-pentane	78-78-4	72.15	1.36	1.67	-18%	1		0	6
28	branched C6 alkanes		86.18	1.23	1.52	-19%			0	8
29	2,2-dimethyl butane	75-83-2	86.18	1.11	1.33	-16%	1		0	6
30	2,3-dimethyl butane	79-29-8	86.18	0.91	1.13	-19%	1		0	6
31	2-methyl pentane	107-83-5	86.18	1.41	1.78	-21%	1		0	6
32	3-methyl pentane	96-14-0	86.18	1.70	2.06	-17%	1		0	6
33	branched C7 alkanes		100.20	1.39	1.62	-14%			0	8
34	2,2,3-trimethyl butane	464-06-2	100.20	1.06	1.32	-20%	1		0	6
35	2,2-dimethyl pentane	590-35-2	100.20	1.05	1.21	-13%	1		0	6
36	2,3-dimethyl pentane	565-59-3	100.20	1.26	1.53	-18%			0	7
37	2,4-dimethyl pentane	108-08-7	100.20	1.46	1.63	-10%	1		0	6
38	2-methyl hexane	591-76-4	100.20	1.10	1.36	-19%			0	7
39	3,3-dimethyl pentane	562-49-2	100.20	1.13	1.32	-15%			0	7
40	3-methyl hexane	589-34-4	100.20	1.51	1.84	-18%			0	7
41	3-ethylpentane	617-78-7	100.20	1.79					0	7
42	branched C8 alkanes		114.23	1.35	1.55	-13%			0	8

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k	a	Expt	Bias
43	2,2,3,3-tetramethyl butane	594-82-1	114.23	0.31	0.44	-31%	1		0	6
44	2,2,4-trimethyl pentane	540-84-1	114.23	1.20	1.43	-17%	1	3	0	2
45	2,2-dimethyl hexane	590-73-8	114.23	0.95	1.12	-15%	1		0	6
46	2,3,4-trimethyl pentane	565-75-3	114.23	0.96	1.22	-21%	1		0	6
47	2,3-dimethyl hexane	584-94-1	114.23	1.11	1.32	-16%			0	7
48	2,4-dimethyl hexane	589-43-5	114.23	1.62	1.79	-9%			0	7
49	2,5-dimethyl hexane	592-13-2	114.23	1.36	1.66	-18%			0	7
50	2-methyl heptane	592-27-8	114.23	0.99	1.18	-16%			0	7
51	3-methyl heptane	589-81-1	114.23	1.15	1.33	-14%			0	7
52	4-methyl heptane	589-53-7	114.23	1.16	1.46	-20%			0	7
53	2,3,3-trimethylpentane	560-21-4	114.23	0.95					0	7
54	3,3-dimethylhexane	563-16-6	114.23	1.16					0	7
55	2,2,3-trimethyl-pentane	564-02-3	114.23	1.15					0	7
56	3,4-dimethylhexane	583-48-2	114.23	1.41					0	7
57	3-ethyl 2-methyl pentane	609-26-7	114.23	1.25					0	7
58	branched C9 alkanes		128.26	1.05	1.23	-14%			0	8b
59	2,2,5-trimethyl hexane	3522-94-9	128.26	1.06	1.31	-19%			0	7b
60	2,3,5-trimethyl hexane	1069-53-0	128.26	1.14	1.31	-13%	1		0	6b
61	2,4-dimethyl heptane	2213-23-2	128.26	1.29	1.46	-12%			0	7b
62	2-methyl octane	3221-61-2	128.26	0.75	0.94	-20%	1		0,+	6b
63	3,3-diethyl pentane	1067-20-5	128.26	1.14	1.34	-15%	1		0,+	6b
64	3,5-dimethyl heptane	926-82-9	128.26	1.45	1.61	-10%			0	7b
65	4-ethyl heptane	2216-32-2	128.26	1.13	1.42	-20%			0	7b
66	4-methyl octane	2216-34-4	128.26	0.87	1.05	-17%	1		0,+	6b
67	2,4,4-trimethylhexane	16747-30-1	128.26	1.26					0	7b
68	3,3-dimethylheptane	4032-86-4	128.26	1.05					0	7b
69	4,4-dimethylheptane	1068-19-5	128.26	1.19					0	7b
70	2,2-dimethylheptane	1071-26-7	128.26	0.93					0	7b
71	2,2,4-trimethylhexane	16747-26-5	128.26	1.19					0	7b
72	2,6-dimethylheptane	1072-05-5	128.26	0.96					0	7b
73	2,3-dimethylheptane	3074-71-3	128.26	1.01					0	7b
74	2,5-dimethylheptane	2216-30-0	128.26	1.25					0	7b
75	3-methyloctane	2216-33-3	128.26	0.91					0	7b
76	3,4-dimethylheptane	922-28-1	128.26	1.15					0	7b
77	3-ethylheptane	15869-80-4	128.26	1.01					0	7b
78	branched C10 alkanes		142.28	0.86	1.07	-20%			0	8b
79	2,4,6-trimethyl heptane	2613-61-8	142.28	1.20					0	7b
80	2,4-dimethyl octane	4032-94-4	142.28	0.95	1.07	-11%			0	7b
81	2,6-dimethyl octane	2051-30-1	142.28	1.00	1.24	-20%	1	2	0,+	2b
82	2-methyl nonane	871-83-0	142.28	0.65	0.83	-21%	1	2	0,+	2b
83	3,4-diethyl hexane	19398-77-7	142.28	0.83	1.18	-30%	1	2	0,+	2b
84	3-methyl nonane	5911-04-6	142.28	0.68	0.86	-21%			0	7b
85	4-methyl nonane	17301-94-9	142.28	0.78	0.96	-19%			0	7b
86	4-propyl heptane	3178-29-8	142.28	0.94	1.22	-23%			0	7b
87	2,4,4-trimethylheptane		142.28	1.23					0	7b
88	2,5,5-trimethylheptane		142.28	1.17					0	7b
89	3,3-dimethyloctane	4110-44-5	142.28	1.01					0	7b
90	4,4-dimethyloctane	15869-95-1	142.28	1.06					0	7b
91	2,2-dimethyloctane	15869-87-1	142.28	0.77					0	7b

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
92	2,2,4-trimethylheptane	14720-74-2	142.28	1.09					0	7b
93	2,2,5-trimethylheptane		142.28	1.18					0	7b
94	2,3,6-trimethylheptane	4032-93-3	142.28	0.82					0	7b
95	2,3-dimethyloctane	7146-60-3	142.28	0.79					0	7b
96	2,5-dimethyloctane		142.28	0.94					0	7b
97	2-methyl-3-ethylheptane	14676-29-0	142.28	0.91					0	7b
98	4-ethyloctane	15869-86-0	142.28	0.71					0	7b
99	branched C11 alkanes		156.31	0.66	0.84	-22%			0	8b
100	2,3,4,6-tetramethyl heptane	61868-54-0	156.31	1.03	1.26	-18%			0	7b
101	2,6-dimethyl nonane	17302-28-2	156.31	0.72	0.92	-22%			0	7b
102	3,5-diethyl heptane	61869-02-1	156.31	1.02	1.18	-13%			0	7b
103	3-methyl decane	13151-34-3	156.31	0.58	0.74	-22%			0	7b
104	4-methyl decane	2847-72-5	156.31	0.61	0.78	-21%			0	7b
105	branched C12 alkanes		170.33	0.56	0.77	-27%			0	8b
106	2,3,5,7-tetramethyl octane	62199-32-0	170.33	0.84	1.06	-21%			0	7b
107	2,6-diethyl octane	62183-94-2	170.33	0.89	1.07	-17%			0	7b
108	3,6-dimethyl decane	17312-53-7	170.33	0.62	0.85	-27%			0	7b
109	3-methyl undecane	1002-43-3	170.33	0.53	0.68	-22%			0	7b
110	5-methyl undecane	1632-70-8	170.33	0.49	0.69	-30%			0	7b
111	branched C13 alkanes		184.36	0.54	0.70	-24%			0	8b
112	2,3,6-trimethyl 4-isopropyl heptane		184.36	0.85	1.24	-31%			0	7b
113	2,4,6,8-tetramethyl nonane	14638-54-1	184.36	0.69	0.94	-26%			0	7b
114	3,6-dimethyl undecane	17301-28-9	184.36	0.62	0.79	-21%			0	7b
115	3,7-diethyl nonane		184.36	0.81	1.05	-22%			0	7b
116	3-methyl dodecane	17312-57-1	184.36	0.49	0.61	-21%			0	7b
117	5-methyl dodecane	17453-93-9	184.36	0.41	0.62	-33%			0	7b
118	branched C14 alkanes		198.39	0.49	0.64	-24%			0	8b
119	2,4,5,6,8-pentamethyl nonane		198.39	0.87	1.11	-22%			0	7b
120	2-methyl 3,5-diisopropyl heptane		198.39	0.49	0.78	-37%			0	7b
121	3,7-dimethyl dodecane	82144-67-0	198.39	0.56	0.71	-22%			0	7b
122	3,8-diethyl decane	6224-52-8	198.39	0.53	0.66	-19%			0	7b
123	3-methyl tridecane	6418-41-3	198.39	0.45	0.55	-18%			0	7b
124	6-methyl tridecane	13287-21-3	198.39	0.40	0.59	-33%			0	7b
125	branched C15 alkanes		212.41	0.45	0.58	-22%			0	8b
126	2,6,8-trimethyl 4-isopropyl nonane		212.41	0.57	0.76	-25%			0	7b
127	3,7-dimethyl tridecane		212.41	0.50	0.62	-20%			0	7b
128	3,9-diethyl undecane	13286-72-1	212.41	0.46	0.59	-22%			0	7b
129	3-methyl tetradecane	18435-22-8	212.41	0.43	0.51	-17%			0	7b
130	6-methyl tetradecane	26730-16-5	212.41	0.37	0.55	-33%			0	7b
131	branched C16 alkanes		226.44	0.42	0.52	-19%			0	8b
132	2,7-dimethyl 3,5-diisopropyl heptane		226.44	0.47	0.69	-33%			0	7b
133	3-methyl pentadecane	2882-96-4	226.44	0.41	0.48	-15%			0	7b
134	4,8-dimethyl tetradecane	175032-36-7	226.44	0.44	0.55	-21%			0	7b
135	7-methyl pentadecane	6165-40-8	226.44	0.40	0.49	-18%			0	7b
136	branched C17 alkanes		240.47	0.40	0.49	-19%			0	8b
137	branched C18 alkanes		254.49	0.37	0.46	-19%			0	8b

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]				
				New	Old	Chg	k	a	Expt	Bias	Unc
138	branched C19 alkanes		268.52	0.35						0	8 b
139	branched C20 alkanes		282.55	0.34						0	8 b
140	branched C21 alkanes		296.57	0.32						0	8 b
141	branched C22 alkanes		310.60	0.31						0	8 b
142	cyclopropane	75-19-4	42.08	0.082	0.103	-20%	1			0	6
143	cyclobutane	287-23-0	56.11	1.12	1.04	8%	1			0	6
144	cyclopentane	287-92-3	70.13	2.25	2.67	-16%	1			0	6
145	C6 cycloalkanes		84.16	1.16	1.44	-20%				0	8
146	cyclohexane	110-82-7	84.16	1.16	1.44	-20%	1	2		0	2
147	isopropyl cyclopropane	3638-35-5	84.16	1.15	1.51	-24%	1			0	6
148	methylcyclopentane	96-37-7	84.16	2.06	2.40	-14%				0	7
149	1,1-dimethylcyclopentane	1638-26-2	98.19	1.01						0	7
150	1,2-dimethylcyclopentane	2452-99-5	98.19	1.87						0	7
151	C7 cycloalkanes		98.19	1.58	1.97	-20%				0	7
152	1,3-dimethyl cyclopentane	2453-00-1	98.19	1.82	2.13	-14%				0	7
153	cycloheptane	291-64-5	98.19	1.83	2.23	-18%	1			0	6
154	ethyl cyclopentane	1640-89-7	98.19	1.89	2.25	-16%				0	7
155	methylcyclohexane	108-87-2	98.19	1.58	1.97	-20%	1			0	6
156	C8 bicycloalkanes		110.20	1.41	1.75	-20%				0	8
157	1,1,2-trimethylcyclopentane	4259-00-1	112.21	1.04						0	7
158	1,1,3-trimethylcyclopentane	4516-69-2	112.21	0.94						0	7
159	1,1-dimethyl cyclohexane	590-66-9	112.21	1.13						0	7
160	1,2,3-trimethylcyclopentane		112.21	1.52						0	7
161	1,2,4-trimethylcyclopentane		112.21	1.43						0	7
162	1-methyl-3-ethylcyclopentane		112.21	1.53						0	7
163	1,2-dimethylcyclohexane	583-57-3	112.21	1.30						0	7
164	1,4-dimethylcyclohexane	589-90-2	112.21	1.51						0	7
165	C8 cycloalkanes		112.21	1.37	1.72	-20%				0	8
166	1,3-dimethyl cyclohexane	591-21-9	112.21	1.41	1.69	-16%				0	7
167	cyclooctane	292-64-8	112.21	1.35	1.70	-21%	1			0	6
168	ethylcyclohexane	1678-91-7	112.21	1.37	1.72	-20%				0	7
169	propyl cyclopentane	2040-96-2	112.21	1.57	1.89	-16%				0	7
170	cis-hydrindane; bicyclo[4.3.0]nonane	496-10-6	124.22	1.20						0	7 b
171	C9 bicycloalkanes		124.22	1.28	1.54	-17%				0	8 b
172	1,2,3-trimethylcyclohexane	1678-97-3	126.24	1.12						0	7 b
173	1,3,5-trimethylcyclohexane	1839-63-0	126.24	1.06						0	7 b
174	C9 cycloalkanes		126.24	1.26	1.52	-17%				0	8 b
175	1,1,3-trimethyl cyclohexane	3073-66-3	126.24	1.11	1.34	-18%	1			0	6 b
176	1-ethyl-4-methyl cyclohexane	3728-56-1	126.24	1.33	1.59	-16%				0	7 b
177	propyl cyclohexane	1678-92-8	126.24	1.19	1.45	-18%				0	7 b
178	C10 bicycloalkanes		138.25	1.00	1.26	-21%				0	8 b
179	isobutylcyclohexane; (2- methylpropyl) cyclohexane	1678-98-4	140.27	0.90						0	8 b
180	sec-butylcyclohexane	7058-01-7	140.27	0.90						0	8 b
181	C10 cycloalkanes		140.27	0.99	1.24	-21%				0	8 b
182	1,3-diethyl-cyclohexane	1678-99-5	140.27	1.16	1.31	-11%				0	7 b
183	1,4-diethyl-cyclohexane	1679-00-1	140.27	1.14	1.46	-22%				0	7 b

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
184	1-methyl-3-isopropyl cyclohexane	16580-24-8	140.27	0.92	1.23	-25%			0	7b
185	butyl cyclohexane	1678-93-9	140.27	0.90	1.05	-14%	1		0	6b
186	C11 bicycloalkanes		152.28	0.83	0.98	-15%			0	8b
187	C11 cycloalkanes		154.29	0.82	0.96	-15%			0	8b
188	1,3-diethyl-5-methyl cyclohexane	164259-42-1	154.29	0.96	1.08	-11%			0	7b
189	1-ethyl-2-propyl cyclohexane	62238-33-9	154.29	0.73	0.92	-21%			0	7b
190	pentyl cyclohexane	4292-92-6	154.29	0.77	0.89	-14%			0	7b
191	C12 tricycloalkanes		164.29	0.74					0	8b
192	C12 bicycloalkanes		166.30	0.73	0.86	-15%			0	8b
193	C12 cycloalkanes		168.32	0.72	0.85	-15%			0	8b
194	1,3,5-triethyl cyclohexane	164259-43-2	168.32	0.94	1.03	-8%			0	7b
195	1-methyl-4-pentyl cyclohexane	75736-67-3	168.32	0.65	0.80	-18%			0	7b
196	hexyl cyclohexane	4292-75-5	168.32	0.57	0.72	-21%	1	2	0	2b
197	C13 tricycloalkanes		178.31	0.64					0	8b
198	C13 bicycloalkanes		180.33	0.64	0.76	-17%			0	8b
199	C13 cycloalkanes		182.35	0.63	0.75	-17%			0	8b
200	1,3-diethyl-5-propyl cyclohexane		182.35	0.89	0.96	-7%			0	7b
201	1-methyl-2-hexyl-cyclohexane	92031-93-1	182.35	0.52	0.67	-23%			0	7b
202	heptyl cyclohexane	5617-41-4	182.35	0.49	0.63	-23%			0	7b
203	C14 tricycloalkanes		192.34	0.60					0	8b
204	C14 bicycloalkanes		194.36	0.59	0.70	-15%			0	8b
205	C14 cycloalkanes		196.37	0.59	0.69	-15%			0	8b
206	1,3-dipropyl-5-ethyl cyclohexane		196.37	0.84	0.91	-8%			0	7b
207	trans 1-methyl-4-heptyl cyclohexane	205324-73-8	196.37	0.47	0.58	-19%			0	7b
208	octyl cyclohexane	1795-15-9	196.37	0.45	0.58	-21%		2	0	7b
209	C15 tricycloalkanes		206.37	0.56					0	8b
210	C15 bicycloalkanes		208.38	0.56	0.66	-15%			0	8b
211	C15 cycloalkanes		210.40	0.55	0.65	-15%			0	8b
212	1,3,5-tripropyl cyclohexane		210.40	0.81	0.87	-7%			0	7b
213	1-methyl-2-octyl cyclohexane		210.40	0.45	0.58	-22%			0	7b
214	nonyl cyclohexane	2883-02-5	210.40	0.41	0.52	-21%			0	7b
215	C16 tricycloalkanes		220.39	0.53					0	8b
216	C16 bicycloalkanes		222.41	0.52					0	8b
217	C16 cycloalkanes		224.43	0.49	0.58	-15%			0	8b
218	1,3-propyl-5-butyl cyclohexane		224.43	0.69	0.75	-8%			0	7b
219	1-methyl-4-nonyl cyclohexane	39762-40-8	224.43	0.41	0.53	-21%			0	7b
220	decyl cyclohexane	1795-16-0	224.43	0.38	0.48	-21%			0	7b
221	C17 tricycloalkanes		234.42	0.50					0	8b
222	C17 bicycloalkanes		236.44	0.49					0	8b
223	C17 cycloalkanes		238.45	0.46					0	8b
224	C18 tricycloalkanes		248.45	0.47					0	8b
225	C18 bicycloalkanes		250.46	0.46					0	8b
226	C18 cycloalkanes		252.48	0.44					0	8b
227	C19 tricycloalkanes		262.47	0.44					0	8b
228	C19 bicycloalkanes		264.49	0.44					0	8b
229	C19 cycloalkanes		266.51	0.42					0	8b

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]				
				New	Old	Chg	k	a	Expt	Bias	Unc
230	C20 tricycloalkanes		276.50	0.42						0	8 b
231	C20 bicycloalkanes		278.52	0.42						0	8 b
232	C20 cycloalkanes		280.53	0.39						0	8 b
233	C21 tricycloalkanes		290.53	0.40						0	8 b
234	C21 bicycloalkanes		292.54	0.40						0	8 b
235	C21 cycloalkanes		294.56	0.38						0	8 b
236	C22 tricycloalkanes		304.55	0.38						0	8 b
237	C22 bicycloalkanes		306.57	0.38						0	8 b
238	C22 cycloalkanes		308.58	0.36						0	8 b
239	ethene	74-85-1	28.05	8.76	9.07	-3%	1	1	0	0	3 d
240	propene	115-07-1	42.08	11.37	11.57	-2%	1	1	0	0	3 d
241	1-butene	106-98-9	56.11	9.42	10.22	-8%	1	3	0	0	3 d
242	C4 terminal alkenes		56.11	9.42	10.22	-8%			0	0	7
243	1-pentene	109-67-1	70.13	6.97	7.73	-10%	1		0	0	6 d
244	3-methyl-1-butene	563-45-1	70.13	6.76	6.95	-3%	1		0	0	6 d
245	C5 terminal alkenes		70.13	6.97	7.73	-10%			0	0	7
246	1-hexene	592-41-6	84.16	5.28	6.12	-14%	1	4	0	0	4 d
247	3,3-dimethyl-1-butene	558-37-2	84.16	5.61	6.02	-7%	1		0	0	8 d
248	3-methyl-1-pentene	760-20-3	84.16	5.93	6.17	-4%			0	0	8
249	4-methyl-1-pentene	691-37-2	84.16	5.48	6.21	-12%			0	0	8
250	C6 terminal alkenes		84.16	5.28	6.12	-14%			0	0	8
251	1-heptene	592-76-7	98.19	4.25	4.20	1%	1		0	0	8 d
252	3,4-dimethyl-1-pentene	7385-78-6	98.19	4.66					0	0	8
253	3-methyl-1-hexene	3404-61-3	98.19	4.24					0	0	8
254	1-octene	111-66-0	112.21	3.12	3.42	-9%			0	0	8
255	C8 terminal alkenes		112.21	3.12	3.42	-9%			0	0	8
256	2,4,4-trimethyl-1-pentene	107-39-1	112.21	3.24					0	0	8
257	1-nonene	124-11-8	126.24	2.48	2.73	-9%			0	0	8
258	C9 terminal alkenes		126.24	2.48	2.73	-9%			0	0	8
259	1-decene	872-05-9	140.27	2.07	2.25	-8%			0	0	8
260	C10 terminal alkenes		140.27	2.07	2.25	-8%			0	0	8
261	1-undecene	821-95-4	154.29	1.78	1.93	-8%			0	0	8
262	C11 terminal alkenes		154.29	1.78	1.93	-8%			0	0	8
263	C12 terminal alkenes		168.32	1.56	1.74	-10%			0	0	8
264	1-dodecene	112-41-4	168.32	1.56	1.74	-10%			0	0	8
265	1-tridecene	2437-56-1	182.35	1.41	1.52	-8%			0	0	8
266	C13 terminal alkenes		182.35	1.41	1.52	-8%			0	0	8
267	1-tetradecene	1120-36-1	196.37	1.27	1.38	-8%			0	0	8
268	C14 terminal alkenes		196.37	1.27	1.38	-8%			0	0	8
269	1-pentadecene	13360-61-7	210.40	1.19	1.27	-6%			0	0	8
270	C15 terminal alkenes		210.40	1.19	1.27	-6%			0	0	8
271	isobutene	115-11-7	56.11	6.14	6.31	-3%	1	3	0	0	3
272	2-methyl-1-butene	563-46-2	70.13	6.23	6.47	-4%	1		0	0	8
273	2,3-dimethyl-1-butene	563-78-0	84.16	4.61	4.75	-3%			0	0	8
274	2-ethyl-1-butene	760-21-4	84.16	4.93	5.01	-2%			0	0	8
275	2-methyl-1-pentene	763-29-1	84.16	5.12	5.15	-1%	1		0	0	8
276	2,4-dimethyl-1-pentene	2213-32-3	98.19	5.81					0	0	8
277	2,3-dimethyl-1-pentene	3404-72-6	98.19	4.97					0	0	8
278	3,3-dimethyl-1-pentene	3404-73-7	98.19	4.71					0	0	8



Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
279	2-methyl-1-hexene	6094-02-6	98.19	4.92					0	8
280	2,3,3-trimethyl-1-butene	594-56-9	98.19	4.33	4.59	-6%			0	8
281	C7 terminal alkenes		98.19	4.25	4.20	1%			0	8
282	3-methyl-2-isopropyl-1-butene	111823-35-9	112.21	3.17	3.26	-3%			0	8
283	4,4-dimethyl-1-pentene	762-62-9	126.24	3.00					0	8
284	cis-2-butene	590-18-1	56.11	13.89	13.22	5%	1		0	6
285	trans-2-butene	624-64-6	56.11	14.79	13.90	6%	1	1	0	3
286	C4 internal alkenes		56.11	14.34	13.56	6%			0	7
287	2-methyl-2-butene	513-35-9	70.13	13.72	14.44	-5%	1		0	6
288	cis-2-pentene	627-20-3	70.13	10.07	10.23	-2%	1		0	6
289	trans-2-pentene	646-04-8	70.13	10.25	10.23	0%	1		0	6
290	2-pentenes		70.13	10.16	10.23	-1%			0	7
291	C5 internal alkenes		70.13	10.16	10.23	-1%			0	7
292	3-methyl-trans-2-pentene	616-12-6	84.16	11.32					0	7
293	2,3-dimethyl-2-butene	563-79-1	84.16	12.13	13.32	-9%	1		0	8
294	2-methyl-2-pentene	625-27-4	84.16	10.70	11.87	-10%	1		0	8
295	cis 4-methyl-2-pentene		84.16	7.88					0	8
296	cis-2-hexene	7688-21-3	84.16	8.06	8.35	-3%			0	8
297	cis-3-hexene	7642-09-3	84.16	7.33	8.13	-10%			0	8
298	cis-3-methyl-2-pentene	922-62-3	84.16	12.15	12.84	-5%			0	8
299	trans 3-methyl-2-pentene	20710-38-7	84.16	12.81	13.54	-5%			0	8
300	trans 4-methyl-2-pentene	674-76-0	84.16	7.88	7.82	1%	1		0	8
301	trans-2-hexene	4050-45-7	84.16	8.37	8.35	0%			0	8
302	trans-3-hexene	13269-52-8	84.16	7.30	8.07	-10%			0	8
303	2-hexenes	592-43-8	84.16	8.21	8.35	-2%			0	8
304	C6 internal alkenes		84.16	8.21	8.35	-2%			0	8
305	4,4-dimethyl-cis-2-pentene	762-63-0	98.19	6.45					0	8
306	2,4-dimethyl-2-pentene	625-65-0	98.19	9.03					0	8
307	2-methyl-2-hexene	2738-19-4	98.19	9.22					0	8
308	3-ethyl-2-pentene	816-79-5	98.19	9.49					0	8
309	3-methyl-trans-3-hexene	3899-36-3	98.19	9.44					0	8
310	cis-2-heptene	6443-92-1	98.19	6.94					0	8
311	2-methyl-trans-3-hexene	692-24-0	98.19	6.03					0	8
312	3-methyl-cis-3-hexene	4914-89-0	98.19	9.44					0	8
313	3,4-dimethyl-cis-2-pentene	4914-91-4	98.19	8.91					0	8
314	2,3-dimethyl-2-pentene	10574-37-5	98.19	9.45	10.40	-9%	1		0	8
315	cis-3-heptene	7642-10-6	98.19	6.10	6.88	-11%			0	8
316	trans 4,4-dimethyl-2-pentene	690-08-4	98.19	6.45	6.92	-7%	1		0	8
317	trans-2-heptene	14686-13-6	98.19	6.92	7.26	-5%	1		0	8
318	trans-3-heptene	14686-14-7	98.19	6.09	6.88	-12%			0	8
319	2-heptenes		98.19	6.09	6.88	-12%			0	8
320	C7 internal alkenes		98.19	6.09	6.88	-12%			0	8
321	trans-2-octene	13389-42-9	112.21	5.81					0	8
322	2-methyl-2-heptene	627-97-4	112.21	8.10					0	8
323	cis-4-octene	7642-15-1	112.21	4.55	5.86	-22%			0	8
324	trans 2,2-dimethyl 3-hexene	690-93-7	112.21	4.81	5.90	-19%			0	8
325	trans 2,5-dimethyl 3-hexene	692-70-6	112.21	4.63	5.37	-14%			0	8
326	trans-3-octene	14919-01-8	112.21	5.14	6.06	-15%			0	8
327	trans-4-octene	14850-23-8	112.21	4.63	5.83	-21%	1		0	8

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
328	3-octenes		112.21	5.14	6.06	-15%			0	8
329	C8 internal alkenes		112.21	4.63	5.83	-21%			0	8
330	2,4,4-trimethyl-2-pentene	107-40-4	112.21	6.13	8.52	-28%			0	8
331	4-nonene	2198-23-4	126.24	4.37					0	8
332	3-nonenes		126.24	4.37	5.24	-17%			0	8
333	C9 internal alkenes		126.24	4.37	5.24	-17%			0	8
334	trans-4-nonene	10405-85-3	126.24	4.37	5.24	-17%			0	8
335	3,4-diethyl-2-hexene	59643-70-8	140.27	3.25	3.90	-17%			0	8
336	cis-5-decene	7433-78-5	140.27	3.52	4.83	-27%			0	8
337	trans-4-decene	19398-89-1	140.27	3.72	4.44	-16%			0	8
338	C10 3-alkenes		140.27	3.72	4.44	-16%			0	8
339	C10 internal alkenes		140.27	3.72	4.44	-16%			0	8
340	trans-5-undecene	764-97-6	154.29	3.46	4.18	-17%			0	8
341	C11 3-alkenes		154.29	3.46	4.18	-17%			0	8
342	C11 internal alkenes		154.29	3.46	4.18	-17%			0	8
343	C12 2-alkenes		168.32	3.02	3.70	-18%			0	8
344	C12 3-alkenes		168.32	3.02	3.70	-18%			0	8
345	C12 internal alkenes		168.32	3.02	3.70	-18%			0	8
346	trans-5-dodecene	7206-16-8	168.32	3.02	3.70	-18%			0	8
347	trans-5-tridecene	23051-84-5	182.35	2.49	3.34	-26%			0	8
348	C13 3-alkenes		182.35	2.49	3.34	-26%			0	8
349	C13 internal alkenes		182.35	2.49	3.34	-26%			0	8
350	trans-5-tetradecene	41446-66-6	196.37	2.26	3.03	-25%			0	8
351	C14 3-alkenes		196.37	2.26	3.03	-25%			0	8
352	C14 internal alkenes		196.37	2.26	3.03	-25%			0	8
353	trans-5-pentadecene	74392-33-9	210.40	2.08	2.78	-25%			0	8
354	C15 3-alkenes		210.40	2.08	2.78	-25%			0	8
355	C15 internal alkenes		210.40	2.08	2.78	-25%			0	8
356	C4 alkenes		56.11	11.88	11.89	0%			0	8
357	C5 alkenes		70.13	8.57	8.98	-5%			0	8
358	C6 alkenes		84.16	6.59	6.63	-1%			0	8
359	C7 alkenes		98.19	5.17	5.54	-7%			0	8
360	C8 alkenes		112.21	3.88	4.63	-16%			0	8
361	C9 alkenes		126.24	3.43	3.99	-14%			0	8
362	C10 alkenes		140.27	3.17	3.34	-5%			0	8
363	C11 alkenes		154.29	2.62	3.05	-14%			0	8
364	C12 alkenes		168.32	2.29	2.72	-16%			0	8
365	C13 alkenes		182.35	1.95	2.43	-20%			0	8
366	C14 alkenes		196.37	1.77	2.21	-20%			0	8
367	C15 alkenes		210.40	1.63	2.03	-19%			0	8
368	cyclopentene	142-29-0	68.12	6.55	7.32	-11%	1		0	8
369	3-methylcyclopentene	1120-62-3	82.14	4.92					0	8
370	1-methyl cyclopentene	693-89-0	82.14	12.11	13.44	-10%			0	8
371	cyclohexene	110-83-8	82.14	4.81	5.40	-11%	1	4	0	4
372	1-methyl cyclohexene	591-49-1	96.17	6.41	7.70	-17%	1		0	8
373	4-methyl cyclohexene	591-47-9	96.17	4.02	4.44	-9%			0	8
374	1,2-dimethyl cyclohexene	1674-10-8	110.20	5.43	6.66	-18%			0	8
375	1,2-propadiene (allene)	463-49-0	40.06	8.11			1		0	11
376	1-buten-3-yne (vinyl acetylene)	689-97-4	52.07	10.15					0	11

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k	a	Expt	Bias
377	1,2-butadiene	590-19-2	54.09	9.03			1		0	11
378	1,3-butadiene	106-99-0	54.09	12.21	13.47	-9%	1		0	6
379	trans 1,3-pentadiene	2004-70-8	68.12	12.10					0	8
380	cis 1,3-pentadiene	1574-41-0	68.12	12.10					0	8
381	1,4-pentadiene	591-93-5	68.12	8.92			1		0	8
382	1,2-pentadiene	591-95-7	68.12	7.59			1		0	11
383	3-methyl-1,2-butadiene	598-25-4	68.12	9.95			1		0	11
384	isoprene	78-79-5	68.12	10.28	10.68	-4%	1	2	0	1
385	trans,trans-2,4-hexadiene	5194-51-4	82.14	8.57					0	8
386	trans 1,3-hexadiene	20237-34-7	82.14	10.03					0	8
387	trans 1,4-hexadiene	7319-00-8	82.14	8.36			1		0	8
388	C6 cyclic or di-olefins		82.14	8.41	8.55	-2%			0	8
389	C7 cyclic or di-olefins		96.17	7.07	7.41	-5%			0	8
390	C8 cyclic or di-olefins		110.20	4.71	5.94	-21%			0	8
391	C9 cyclic or di-olefins		124.22	4.44	5.33	-17%			0	8
392	C10 cyclic or di-olefins		138.25	3.78	4.50	-16%			0	8
393	C11 cyclic or di-olefins		152.28	3.50	4.23	-17%			0	8
394	C12 cyclic or di-olefins		166.30	3.05	3.75	-18%			0	8
395	C13 cyclic or di-olefins		180.33	2.51	3.38	-25%			0	8
396	C14 cyclic or di-olefins		194.36	2.29	3.06	-25%			0	8
397	C15 cyclic or di-olefins		208.38	2.10	2.81	-25%			0	8
398	cyclopentadiene	542-92-7	66.10	6.75	7.55	-11%			0	8
399	3-carene	13466-78-9	136.23	3.13	3.21	-3%	1	3	0	4
400	$\alpha$ -pinene	80-56-8	136.23	4.38	4.29	2%	1	2	0	4
401	$\beta$ -pinene	127-91-3	136.23	3.38	3.28	3%	1	2	0	4
402	<i>d</i> -limonene	5989-27-5	136.23	4.40	3.99	11%	1	2	0	4
403	sabinene	3387-41-5	136.23	4.01	3.66	10%	1	3	0	4
404	terpene		136.23	3.91	3.78	3%			0	8
405	terpinolene	586-62-9	136.23	6.16					0	8
406	styrene	100-42-5	104.15	1.65	1.94	-15%	1	2	0	2
407	allylbenzene	300-57-2	118.18	1.45					0	8
408	$\alpha$ -methyl styrene	98-83-9	118.18	1.45	1.71	-15%			0	8
409	C9 styrenes		118.18	1.45	1.71	-15%			0	8
410	$\beta$ -methyl styrene	637-50-3	118.18	0.95			1		0	8
411	C10 styrenes		132.20	1.30	1.53	-15%			0	8
412	benzene	71-43-2	78.11	0.69	0.81	-15%	1	2	0?	4
413	toluene	108-88-3	92.14	3.88	3.97	-2%	1	2	0	4
414	ethyl benzene	100-41-4	106.17	2.93	2.79	5%	1	3	0	4
415	C9 monosubstituted benzenes		120.19	1.95	2.20	-11%			0	8
416	n-propyl benzene	103-65-1	120.19	1.95	2.20	-11%	1		0	8
417	isopropyl benzene (cumene)	98-82-8	120.19	2.43	2.32	5%	1		0	8
418	C10 monosubstituted benzenes		134.22	2.27	1.97	15%			0	8
419	n-butyl benzene	104-51-8	134.22	2.27	1.97	15%			0	8
420	sec-butyl benzene	135-98-8	134.22	2.27	1.97	15%			0	8
421	t-butyl benzene	98-06-6	134.22	1.89			1		0	8
422	n-pentylbenzene	538-68-1	148.24	2.04					0	8
423	C11 monosubstituted benzenes		148.24	2.04	1.78	14%			0	8
424	C12 monosubstituted benzenes		162.27	1.83	1.63	12%			0	8
425	C13 monosubstituted benzenes		176.30	1.67	1.50	12%			0	8

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]				
				New	Old	Chg	k	a	Expt	Bias	Unc
426	C14 monosubstituted benzenes		190.32	1.53						0	8
427	C15 monosubstituted benzenes		204.35	1.42						0	8
428	C16 monosubstituted benzenes		218.38	1.32						0	8
429	C17 monosubstituted benzenes		232.40	1.24						0	8
430	C18 monosubstituted benzenes		246.43	1.17						0	8
431	C19 monosubstituted benzenes		260.46	1.11						0	8
432	C20 monosubstituted benzenes		274.48	1.05						0	8
433	C21 monosubstituted benzenes		288.51	1.00						0	8
434	C22 monosubstituted benzenes		302.54	0.96						0	8
435	C8 disubstituted benzenes	1330-20-7	106.17	7.57	7.48	1%				0	8
436	m-xylene	108-38-3	106.17	9.52	10.61	-10%	1	1	0	4	
437	o-xylene	95-47-6	106.17	7.44	7.48	-1%	1	2	0	4	
438	p-xylene	106-42-3	106.17	5.69	4.24	34%	1	3	0	4	
439	C9 disubstituted benzenes		120.19	5.65	6.60	-15%				0	8
440	m-ethyl toluene	620-14-4	120.19	7.21	9.37	-23%	1		0	8	
441	o-ethyl toluene	611-14-3	120.19	5.43	6.61	-18%	1		0	8	
442	p-ethyl toluene	622-96-8	120.19	4.32	3.75	15%	1		0	8	
443	o-cymene; 1-methyl-2-(1-methylethyl)benzene	527-84-4	134.22	5.34						0	8
444	1-methyl-2-n-propylbenzene	1074-17-5	134.22	5.34						0	8
445	m-cymene; 1-methyl-3-(1-methylethyl)benzene	535-77-3	134.22	6.92						0	8
446	1-methyl-3-n-propylbenzene	1074-43-7	134.22	6.92						0	8
447	1-methyl-4-n-propylbenzene	1074-55-1	134.22	4.31						0	8
448	C10 disubstituted benzenes		134.22	5.53	5.92	-7%				0	8
449	m-C10 disubstituted benzenes		134.22	6.92						0	8
450	o-C10 disubstituted benzenes		134.22	5.34						0	8
451	p-C10 disubstituted benzenes		134.22	4.31						0	8
452	m-diethyl benzene	141-93-5	134.22	6.92	8.39	-18%				0	8
453	o-diethyl benzene	135-01-3	134.22	5.34	5.92	-10%				0	8
454	1-methyl-4-isopropylbenzene (p-cymene)	99-87-6	134.22	4.32			1		0	8	
455	p-diethyl benzene	105-05-5	134.22	4.31	3.36	28%				0	8
456	m-C11 disubstituted benzenes		148.24	5.98						0	8
457	o-C11 disubstituted benzenes		148.24	4.60						0	8
458	p-C11 disubstituted benzenes		148.24	3.77						0	8
459	1-butyl-2-methylbenzene		148.24	4.60						0	8
460	1-ethyl-2-n-propylbenzene		148.24	4.60						0	8
461	o-t-butyl toluene; 1-(1,1-dimethylethyl)-2-methylbenzene	1074-92-6	148.24	4.60						0	8
462	1-methyl-3-n-butylbenzene	1595-04-6	148.24	5.98						0	8
463	p-isobutyl toluene; 1-methyl-4(2-methylpropyl) benzene	5161-04-6	148.24	3.77						0	8
464	C11 disubstituted benzenes		148.24	4.79	5.35	-11%				0	8
465	m-C12 disubstituted benzenes		162.27	5.35						0	8
466	o-C12 disubstituted benzenes		162.27	4.11						0	8
467	p-C12 disubstituted benzenes		162.27	3.38						0	8
468	1,3-di-n-propylbenzene		162.27	4.11						0	8
469	1,4 diisopropyl benzene		162.27	3.38						0	8

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
470	3-isopropyl cumene; 1,3-diisopropyl benzene	99-62-7	162.27	5.35					0	8
471	C12 disubstituted benzenes		162.27	4.28	4.89	-13%			0	8
472	m-C13 disubstituted benzenes		176.30	4.80					0	8
473	o-C13 disubstituted benzenes		176.30	3.67					0	8
474	p-C13 disubstituted benzenes		176.30	3.03					0	8
475	C13 disubstituted benzenes		176.30	3.84	4.50	-15%			0	8
476	m-C14 disubstituted benzenes		190.32	4.32					0	8
477	o-C14 disubstituted benzenes		190.32	3.30					0	8
478	p-C14 disubstituted benzenes		190.32	2.75					0	8
479	C14 disubstituted benzenes		190.32	3.46					0	8
480	C15 disubstituted benzenes		204.35	3.15					0	8
481	m-C15 disubstituted benzenes		204.35	3.93					0	8
482	o-C15 disubstituted benzenes		204.35	3.00					0	8
483	p-C15 disubstituted benzenes		204.35	2.51					0	8
484	m-C16 disubstituted benzenes		218.38	3.60					0	8
485	o-C16 disubstituted benzenes		218.38	2.74					0	8
486	p-C16 disubstituted benzenes		218.38	2.30					0	8
487	C16 disubstituted benzenes		218.38	2.88					0	8
488	C17 disubstituted benzenes		232.40	2.71					0	8
489	C18 disubstituted benzenes		246.43	2.55					0	8
490	C19 disubstituted benzenes		260.46	2.42					0	8
491	C20 disubstituted benzenes		274.48	2.29					0	8
492	C21 disubstituted benzenes		288.51	2.18					0	8
493	C22 disubstituted benzenes		302.54	2.08					0	8
494	isomers of ethylbenzene		106.17	6.39	5.16	24%			0	8
495	isomers of propylbenzene		120.19	6.06	6.12	-1%			0	8
496	C9 trisubstituted benzenes	25551-13-7	120.19	10.58	9.90	7%			0	8
497	1,2,3-trimethyl benzene	526-73-8	120.19	11.66	11.25	4%	1	2	0	4
498	1,2,4-trimethyl benzene	95-63-6	120.19	8.64	7.18	20%	1	2	0	4
499	1,3,5-trimethyl benzene	108-67-8	120.19	11.44	11.22	2%	1	2	0	4
500	1,2,3-C10 trisubstituted benzenes		134.22	9.89					0	8
501	1,2,4-C10 trisubstituted benzenes		134.22	7.35					0	8
502	1,3,5-C10 trisubstituted benzenes		134.22	9.80					0	8
503	1,2,3,4-tetramethylbenzene	488-23-3	134.22	9.01					0	8
504	1,2,4,5-tetramethylbenzene	95-93-2	134.22	9.01					0	8
505	1,2-dimethyl-3-ethylbenzene	933-98-2	134.22	9.89					0	8
506	1,2-dimethyl-4-ethylbenzene	934-80-5	134.22	7.35					0	8
507	1,3-dimethyl-2-ethylbenzene	2870-04-4	134.22	9.89					0	8
508	1,3-dimethyl-4-ethylbenzene	874-41-9	134.22	7.35					0	8
509	1,3-dimethyl-5-ethylbenzene	934-74-7	134.22	9.80					0	8
510	1,4-dimethyl-2-ethylbenzene	1758-88-9	134.22	7.35					0	8
511	1,2,3,5 tetramethyl benzene	527-53-7	134.22	9.01	8.25	9%			0	8
512	isomers of butylbenzene		134.22	5.60	5.48	2%			0	8
513	C10 trisubstituted benzenes		134.22	9.01	8.86	2%			0	8
514	C10 tetrasubstituted benzenes		134.22	9.01	8.86	2%			0	8
515	1,2,3-C11 trisubstituted benzenes		148.24	8.64					0	8
516	1,2,4-C11 trisubstituted benzenes		148.24	6.44					0	8
517	1,3,5-C11 trisubstituted benzenes		148.24	8.65					0	8

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
518	pentamethylbenzene	700-12-9	148.24	7.91					0	8
519	1-methyl-3,5-diethylbenzene	2050-24-0	148.24	8.65					0	8
520	isomers of pentylbenzene		148.24	4.76	4.96	-4%			0	8
521	C11 trisubstituted benzenes		148.24	7.91	8.02	-1%			0	8
522	C11 tetrasubstituted benzenes		148.24	7.91	8.02	-1%			0	8
523	C11 pentasubstituted benzenes		148.24	7.91	8.02	-1%			0	8
524	1,2,3-C12 trisubstituted benzenes		162.27	7.74					0	8
525	1,2,4-C12 trisubstituted benzenes		162.27	5.78					0	8
526	1,3,5-C12 trisubstituted benzenes		162.27	7.79					0	8
527	1-(1,1-dimethylethyl)-3,5-dimethylbenzene	98-19-1	162.27	7.79					0	8
528	isomers of hexylbenzene		162.27	4.28	4.53	-6%			0	8
529	C12 trisubstituted benzenes		162.27	7.10	7.33	-3%			0	8
530	C12 tetrasubstituted benzenes		162.27	7.10	7.33	-3%			0	8
531	C12 pentasubstituted benzenes		162.27	7.10	7.33	-3%			0	8
532	C12 hexasubstituted benzenes		162.27	7.10	7.33	-3%			0	8
533	1,2,3-C13 trisubstituted benzenes		176.30	6.94					0	8
534	1,2,4-C13 trisubstituted benzenes		176.30	5.20					0	8
535	1,3,5-C13 trisubstituted benzenes		176.30	7.04					0	8
536	C13 trisubstituted benzenes		176.30	6.39	6.75	-5%			0	8
537	1,2,3-C14 trisubstituted benzenes		190.32	6.31					0	8
538	1,2,4-C14 trisubstituted benzenes		190.32	4.75					0	8
539	1,3,5-C14 trisubstituted benzenes		190.32	6.44					0	8
540	C14 trisubstituted benzenes		190.32	5.84					0	8
541	C15 trisubstituted benzenes		204.35	5.35					0	8
542	1,2,3-C15 trisubstituted benzenes		204.35	5.77					0	8
543	1,2,4-C15 trisubstituted benzenes		204.35	4.35					0	8
544	1,3,5-C15 trisubstituted benzenes		204.35	5.92					0	8
545	1,2,3-C16 trisubstituted benzenes		218.38	5.31					0	8
546	1,2,4-C16 trisubstituted benzenes		218.38	4.01					0	8
547	1,3,5-C16 trisubstituted benzenes		218.38	5.47					0	8
548	C16 trisubstituted benzenes		218.38	4.93					0	8
549	C17 trisubstituted benzenes		232.40	4.63					0	8
550	C18 trisubstituted benzenes		246.43	4.37					0	8
551	C19 trisubstituted benzenes		260.46	4.13					0	8
552	C20 trisubstituted benzenes		274.48	3.92					0	8
553	C21 trisubstituted benzenes		288.51	3.73					0	8
554	C22 trisubstituted benzenes		302.54	3.56					0	8
555	indene	95-13-6	116.16	1.48	3.21	-54%			0	10
556	indan	496-11-7	118.18	3.20	3.16	1%			0	10
557	naphthalene	91-20-3	128.17	3.24	3.26	-1%	1	4	+	5
558	methyl indans		132.20	2.86	2.83	1%			0	10
559	tetralin	119-64-2	132.20	2.86	2.83	1%	1	4	+	5
560	methyl naphthalenes	1321-94-4	142.20	2.96	4.61	-36%			+	10
561	1-methyl naphthalene	90-12-0	142.20	2.96	4.61	-36%			+	10
562	2-methyl naphthalene	91-57-6	142.20	2.96	4.61	-36%			+	10
563	C11 tetralin or indan		146.23	2.58	2.55	1%			+	10
564	1-ethylnaphthalene	1127-76-0	156.22	2.69					+	10
565	C12 naphthalenes		156.22	3.76					+	10

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k	a	Expt	Bias
566	C12 monosubstituted naphthalene		156.22	2.69	4.20	-36%			+	10
567	C12 disubstituted naphthalenes		156.22	4.84	5.54	-13%			+	10
568	2,3-dimethyl naphthalene	581-40-8	156.22	4.84	5.54	-13%	1	4	+	5
569	dimethyl naphthalenes		156.22	4.84	5.54	-13%			+	10
570	C12 tetralin or indan		160.26	2.36	2.33	1%			0	10
571	C13 naphthalenes		170.25	3.45					0	10
572	C13 monosubstituted naphthalene		170.25	2.47	3.85	-36%			0	10
573	C13 disubstituted naphthalenes		170.25	4.44	5.08	-13%			0	10
574	C13 trisubstituted naphthalenes		170.25	4.44	5.08	-13%			0	10
575	C13 tetralin or indan		174.28	2.17					0	10
576	C14 naphthalenes		184.28	3.19					0	10
577	C14 tetralin or indan		188.31	2.01					0	10
578	C15 naphthalenes		198.30	2.97					0	10
579	C15 tetralin or indan		202.34	1.87					0	10
580	C16 naphthalenes		212.33	2.77					0	10
581	C16 tetralin or indan		216.36	1.75					0	10
582	C17 naphthalenes		226.36	2.60					0	10
583	C17 tetralin or indan		230.39	1.64					0	10
584	C18 naphthalenes		240.38	2.45					0	10
585	C18 tetralin or indan		244.41	1.55					0	10
586	C19 naphthalenes		254.41	2.31					0	10
587	C19 tetralin or indan		258.44	1.46					0	10
588	C20 naphthalenes		268.44	2.19					0	10
589	C20 tetralin or indan		272.47	1.39					0	10
590	C21 naphthalenes		282.46	2.08					0	10
591	C21 tetralin or indan		286.49	1.32					0	10
592	C22 naphthalenes		296.49	1.98					0	10
593	C22 tetralin or indan		300.52	1.26					0	10
594	acetylene	74-86-2	26.04	0.93	1.24	-25%	1	2	-	3
595	methyl acetylene	74-99-7	40.06	6.57	6.44	2%	1		-	7
596	1,3-butadiyne	460-12-8	50.06	5.53					0	11
597	2-butyne	503-17-3	54.09	15.95	16.32	-2%	1		0	10
598	ethyl acetylene	107-00-6	54.09	5.95	6.18	-4%	1		-	7
599	methanol	67-56-1	32.04	0.65	0.69	-6%	1	3	0	2
600	ethanol	64-17-5	46.07	1.45	1.69	-14%	1	3	0	2
601	isopropyl alcohol	67-63-0	60.10	0.59	0.71	-17%	1	2	0	2
602	n-propyl alcohol	71-23-8	60.10	2.38	2.73	-13%	1		0	6
603	isobutyl alcohol	78-83-1	74.12	2.41	2.23	8%	1		0	6
604	n-butyl alcohol	71-36-3	74.12	2.76	3.33	-17%	1		0	6
605	sec-butyl alcohol	78-92-2	74.12	1.30	1.59	-18%	1		0	6
606	t-butyl alcohol	75-65-0	74.12	0.39	0.45	-13%	1	2	+	2
607	cyclopentanol	96-41-3	86.13	1.65	1.94	-15%	1		0	6
608	2-pentanol	6032-29-7	88.15	1.54	1.73	-11%	1		0	6
609	3-pentanol	584-02-1	88.15	1.56	1.73	-10%	1		0	6
610	pentyl alcohol	71-41-0	88.15	2.71	3.33	-19%	1		0	6
611	isoamyl alcohol (3-methyl-1-butanol)	123-51-3	88.15	3.04	2.73	11%	1		0	6

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
612	2-methyl-1-butanol	137-32-6	88.15	2.30	2.60	-12%			0	7
613	cyclohexanol	108-93-0	100.16	1.84	2.23	-18%	1		0	6
614	1-hexanol	111-27-3	102.17	2.56	2.72	-6%	1		0	6
615	2-hexanol	626-93-7	102.17	1.97	2.45	-20%	1		0	6
616	4-methyl-2-pentanol (methyl isobutyl carbinol)	108-11-2	102.17	2.52	2.89	-13%			0	7
617	1-heptanol	111-70-6	116.20	1.75	2.19	-20%	1		0	6
618	dimethylpentanol (2,3-dimethyl-1-pentanol)	10143-23-4	116.20	2.13	2.51	-15%			0	7
619	1-octanol	111-87-5	130.23	1.35	1.99	-32%	1	2	+	2
620	2-ethyl-1-hexanol	104-76-7	130.23	1.90	2.18	-13%			0	7
621	2-octanol	4128-31-8	130.23	1.86	2.13	-13%	1	2	+	2
622	3-octanol	20296-29-1	130.23	2.16	2.53	-15%	1	2	+	2
623	4-octanol	589-62-8	130.23	2.10	3.04	-31%	1		0	6
624	5-methyl-1-heptanol	7212-53-5	130.23	1.70	1.95	-13%			0	7
625	trimethylcyclohexanol	1321-60-4	142.24	1.75	2.17	-19%			0	7
626	dimethylheptanol (2,6-dimethyl-2-heptanol)	13254-34-7	144.25	0.88	1.07	-18%			0	7
627	2,6-dimethyl-4-heptanol	108-82-7	144.25	1.98	2.37	-17%			0	7
628	menthol	89-78-1	156.27	1.35	1.70	-20%			0	7
629	8-methyl-1-nonanol (isodecyl alcohol)	25339-17-7	158.28	0.99	1.21	-18%			0	7
630	1-decanol	112-30-1	158.28	1.00	1.22	-18%			0	7
631	3,7-dimethyl-1-octanol	106-21-8	158.28	1.13	1.42	-20%			0	7
632	trimethylnonanol threo/erythro; 2,6,8-trimethyl-4-nonanol	123-17-1	186.33	1.24	1.55	-20%			0	7
633	ethylene glycol	107-21-1	62.07	3.01	3.36	-10%	1	2	0	2
634	propylene glycol	57-55-6	76.09	2.48	2.74	-9%	1	2	0	2
635	glycerol	56-81-5	92.09	3.05	3.26	-7%			0	7
636	1,3-butanediol	107-88-0	90.12	3.21			1		0	6
637	1,2-butandiol	584-03-2	90.12	2.43	2.20	10%	1		0	6
638	1,4-butanediol	110-63-4	90.12	2.61	3.22	-19%			0	7
639	2,3-butanediol		90.12	4.23			1		0	6
640	pentaerythritol	115-77-5	136.15	2.09	2.42	-14%			0	7
641	1,2-dihydroxy hexane	6920-22-5	118.17	2.45	2.73	-10%			0	7
642	2-methyl-2,4-pentanediol	107-41-5	118.17	1.39	1.03	35%	1		0	6
643	2-ethyl-1,3-hexanediol	94-96-2	146.23	1.95	2.62	-25%			0	7
644	dimethyl ether	115-10-6	46.07	0.76	0.93	-18%	1	3	0	2
645	trimethylene oxide	503-30-0	58.08	4.32	5.19	-17%	1		0	6
646	1,3-dioxolane	646-06-0	74.08	4.73	5.47	-14%			0	7
647	dimethoxy methane	109-87-5	76.09	0.89	1.04	-14%	1		0	6
648	tetrahydrofuran	109-99-9	72.11	4.10	4.91	-17%	1		0	6
649	diethyl ether	60-29-7	74.12	3.61	4.01	-10%	1	2	0	2
650	1,4-dioxane	123-91-1	88.11	2.48	2.71	-9%			0	7
651	alpha-methyltetrahydrofuran	96-47-9	86.13	3.78	4.59	-18%	1		0	6
652	tetrahydropyran	142-68-7	86.13	3.05	3.78	-19%	1		0	6
653	ethyl isopropyl ether	625-54-7	88.15	3.61	3.86	-6%			0	7
654	methyl n-butyl ether	628-28-4	88.15	2.99	3.63	-18%	1		0	6
655	methyl t-butyl ether	1634-04-4	88.15	0.70	0.78	-10%	1	3	0	2



Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
656	2,2-dimethoxy propane	77-76-9	104.15	0.46	0.52	-12%			0	7
657	di n-propyl ether	111-43-3	102.17	2.93	3.23	-9%	1		0	6
658	ethyl n-butyl ether	628-81-9	102.17	3.33	3.84	-13%	1		0	6
659	ethyl t-butyl ether	637-92-3	102.17	1.93	2.11	-9%	1		0	6
660	methyl t-amyl ether	994-05-8	102.17	1.61	2.14	-25%	1		0	6
661	diisopropyl ether	108-20-3	102.17	3.39	3.56	-5%			0	7
662	ethylene glycol diethyl ether; 1,2-diethoxyethane	629-14-1	118.17	2.81	2.84	-1%			0	7
663	acetal (1,1-diethoxyethane)	105-57-7	118.17	3.43	3.68	-7%			0	7
664	4,4-dimethyl-3-oxahexane	919-94-8	116.20	1.86	2.03	-8%			0	7
665	2-butyl tetrahydrofuran	1004-29-1	128.21	2.00	2.49	-20%			0	7
666	di-isobutyl ether	628-55-7	130.23	1.12	1.29	-13%	1		0	6
667	di-n-butyl ether	142-96-1	130.23	2.70	3.14	-14%	1		0	6
668	2-methoxy-1-(2-methoxy-1- methylethoxy)-propane; dipropylene glycol dimethyl ether	89399-28-0	162.23	1.91	2.09	-9%			0	7
669	di-n-pentyl ether	693-65-2	158.28	2.02	2.60	-22%	1		0	6
670	2-methoxyethanol	109-86-4	76.09	2.83	2.97	-5%	1		0	6
671	1-methoxy-2-propanol	107-98-2	90.12	2.33	2.60	-10%	1	2	0	2
672	2-ethoxyethanol	110-80-5	90.12	3.57	3.76	-5%	1	3	0	2
673	2-methoxy-1-propanol	1589-47-5	90.12	2.92	3.00	-3%			0	7
674	3-methoxy-1-propanol	1320-67-8	90.12	3.71	4.01	-7%			0	7
675	diethylene glycol	111-46-6	106.12	3.23	3.53	-8%			0	7
676	tetrahydro-2-furanmethanol	97-99-4	102.13	3.19	3.54	-10%			0	7
677	1-ethoxy-2-propanol	1569-02-4	104.15	2.96	3.23	-8%			0	7
678	2-propoxyethanol	2807-30-9	104.15	3.17	3.50	-9%			0	7
679	3-ethoxy-1-propanol	111-35-3	104.15	3.94	4.22	-7%	1		0	6
680	3-methoxy-1-butanol	2517-43-3	104.15	3.75	0.97	287%	1		0	6
681	2-(2-methoxyethoxy) ethanol	111-77-3	120.15	2.54	2.88	-12%			0	7
682	1-propoxy-2-propanol (propylene glycol n-propyl ether)	1569-01-3	118.17	2.56	2.84	-10%			0	7
683	2-butoxyethanol	111-76-2	118.17	2.78	2.88	-4%	1	2	0	2
684	3 methoxy -3 methyl-butanol	56539-66-3	118.17	1.46	1.73	-15%			0	7
685	n-propoxypropanol	30136-13-1	118.17	3.62	3.84	-6%			0	7
686	2-(2-ethoxyethoxy) ethanol	111-90-0	134.17	3.11	3.34	-7%	1	3	0	2
687	dipropylene glycol isomer (1-[2- hydroxypropyl]-2-propanol)	110-98-5	134.17	2.20	2.47	-11%			0	7
688	triethylene glycol	112-27-6	150.17	3.11	3.41	-9%			0	7
689	1-tert-butoxy-2-propanol	57018-52-7	132.20	1.53	1.70	-10%			0	7
690	2-tert-butoxy-1-propanol	94023-15-1	132.20	1.75	1.79	-2%			0	7
691	n-butoxy-2-propanol (propylene glycol n-butyl ether)	5131-66-8	132.20	2.59	2.73	-5%			0	7
692	2-(2-propoxyethoxy) ethanol	6881-94-3	148.20	2.71	2.97	-9%			0	7
693	dipropylene glycol methyl ether isomer (1-methoxy-2-[2- hydroxypropoxy]-propane)		148.20	1.87	2.19	-14%			0	7
694	dipropylene glycol methyl ether isomer (2-[2-methoxypropoxy]- 1-propanol)	13588-28-8	148.20	2.46	2.70	-9%			0	7

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
695	2-[2-(2-methoxyethoxy) ethoxy] ethanol	112-35-6	164.20	2.44	2.59	-6%			0	7
696	2-hexyloxyethanol	112-25-4	146.23	1.98	2.43	-19%			0	7
697	2,2,4-trimethyl-1,3-pentanediol	144-19-4	146.23	1.46	1.76	-17%			0	7
698	2-(2-butoxyethoxy)-ethanol	112-34-5	162.23	2.26	2.87	-21%	2		0	7
699	dipropylene glycol ethyl ether	15764-24-6	162.23	2.60	2.75	-5%			0	7
700	2-[2-(2-ethoxyethoxy) ethoxy] ethanol	112-50-5	178.23	2.33	2.64	-11%			0	7
701	tetraethylene glycol	112-60-7	194.23	2.38	2.84	-16%			0	7
702	1-(butoxyethoxy)-2-propanol	124-16-3	176.25	1.82	2.08	-12%			0	7
703	2-[2-(2-propoxyethoxy) ethoxy] ethanol	23305-64-8	192.25	2.05	2.43	-16%			0	7
704	tripropylene glycol	24800-44-0	192.25	2.07					0	7
705	2,5,8,11-tetraoxatridecan-13-ol	23783-42-8	208.25	1.86	2.13	-13%			0	7
706	2-(2-ethylhexyloxy) ethanol	1559-35-9	174.28	1.45	1.68	-14%			0	7
707	2-(2-hexyloxyethoxy) ethanol	112-59-4	190.28	1.73	2.00	-14%			0	7
708	glycol ether dpnb {1-(2-butoxy-1-methylethoxy)-2-propanol}	29911-28-2	190.28	1.73	1.96	-12%			0	7
709	2-[2-(2-butoxyethoxy) ethoxy] ethanol	143-22-6	206.28	1.85	2.21	-16%			0	7
710	tripropylene glycol monomethyl ether	25498-49-1	206.28	1.81	1.88	-3%			0	7
711	diethylene glycol mono(2-ethylhexyl) ether	1559-36-0	218.33	1.46					0	7
712	3,6,9,12-tetraoxahexadecan-1-ol	1559-34-8	250.33	1.62	1.86	-13%			0	7
713	tripropylene glycol n-butyl ether	55934-93-5	248.36	1.55					0	7
714	methyl formate	107-31-3	60.05	0.054	0.064	-16%	1		0	6
715	ethyl formate	109-94-4	74.08	0.45	0.52	-13%	1		0	6
716	methyl acetate	79-20-9	74.08	0.067	0.073	-7%	1	2	0	2
717	gamma-butyrolactone	96-48-0	86.09	0.90	1.15	-21%			0	7
718	ethyl acetate	141-78-6	88.11	0.59	0.64	-7%	1	2	0	3
719	methyl propionate	554-12-1	88.11	0.63	0.71	-11%	1		0	6
720	n-propyl formate	110-74-7	88.11	0.73	0.92	-20%	1		0	6
721	isopropyl formate	625-55-8	88.11	0.35	0.42	-18%			0	7
722	ethyl propionate	105-37-3	102.13	0.73	0.79	-8%	1		0	6
723	isopropyl acetate	108-21-4	102.13	1.03	1.12	-8%	1	2	0	2
724	methyl butyrate	623-42-7	102.13	1.04	1.16	-10%	1		0	6
725	methyl isobutyrate	547-63-7	102.13	0.58	0.69	-16%	1	2	0	2
726	n-butyl formate	592-84-7	102.13	0.77	0.94	-18%	1		0	6
727	propyl acetate	109-60-4	102.13	0.73	0.86	-15%	1		0	6
728	ethyl butyrate	105-54-4	116.16	1.11	1.24	-10%	1		0	6
729	isobutyl acetate	110-19-0	116.16	0.58	0.67	-13%			0	7
730	methyl pivalate	598-98-1	116.16	0.33	0.39	-15%	1	2	0	2
731	n-butyl acetate	123-86-4	116.16	0.78	0.88	-11%	1	2	0,+	2
732	n-propyl propionate	106-36-5	116.16	0.79	0.92	-14%	1		0	6
733	sec-butyl acetate	105-46-4	116.16	1.25	1.43	-13%	1		0	6
734	t-butyl acetate	540-88-5	116.16	0.172	0.204	-16%	1	3	0	2
735	butyl propionate	590-01-2	130.18	0.79	0.87	-10%			0	7
736	amyl acetate	628-63-7	130.18	0.78	0.94	-17%			0	7

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
737	n-propyl butyrate	105-66-8	130.18	0.99	1.15	-14%	1	0	6	
738	isoamyl acetate (3-methylbutyl acetate)	123-92-2	130.18	1.02	1.18	-14%		0	7	
739	2-methyl-1-butyl acetate	624-41-9	130.18	1.01	1.17	-13%		0	7	
740	ethyl 3-ethoxy propionate	763-69-9	146.18	3.46	3.59	-4%		0	7	
741	hexyl acetates		144.21	0.74				0	7	
742	2,3-dimethylbutyl acetate		144.21	0.70	0.84	-17%		0	7	
743	2-methylpentyl acetate		144.21	0.91	1.11	-17%		0	7	
744	3-methylpentyl acetate		144.21	1.00	1.31	-24%		0	7	
745	4-methylpentyl acetate		144.21	0.76	0.91	-17%		0	7	
746	isobutyl isobutyrate	97-85-8	144.21	0.55	0.61	-9%		0	7	
747	n-butyl butyrate	109-21-7	144.21	1.02	1.10	-8%	1	0	6	
748	n-hexyl acetate	142-92-7	144.21	0.63	0.87	-27%		0	7	
749	methyl amyl acetate (4-methyl-2-pentanol acetate)	108-84-9	144.21	1.28	1.46	-12%		0	7	
750	n-pentyl propionate	624-54-4	144.21	0.66	0.79	-17%		0	7	
751	2,4-dimethylpentyl acetate		158.24	0.85	0.98	-13%		0	7	
752	2-methylhexyl acetate		158.24	0.64	0.89	-29%		0	7	
753	3-ethylpentyl acetate		158.24	1.03	1.24	-17%		0	7	
754	3-methylhexyl acetate		158.24	0.83	1.01	-18%		0	7	
755	4-methylhexyl acetate		158.24	0.76	0.90	-16%		0	7	
756	5-methylhexyl acetate		158.24	0.54	0.79	-32%		0	7	
757	isoamyl isobutyrate	2050-01-3	158.24	0.76	0.88	-13%		0	7	
758	n-heptyl acetate	112-06-1	158.24	0.59	0.73	-19%		0	7	
759	2,4-dimethylhexyl acetate		172.26	0.70	0.92	-24%		0	7	
760	2-ethyl-hexyl acetate	103-09-3	172.26	0.60	0.77	-22%		0	7	
761	3,4-dimethylhexyl acetate		172.26	0.81	1.16	-30%		0	7	
762	3,5-dimethylhexyl acetate		172.26	0.92	1.08	-15%		0	7	
763	3-ethylhexyl acetate		172.26	0.84	1.03	-18%		0	7	
764	3-methylheptyl acetate		172.26	0.61	0.75	-18%		0	7	
765	4,5-dimethylhexyl acetate		172.26	0.63	0.85	-27%		0	7	
766	4-methylheptyl acetate		172.26	0.60	0.72	-17%		0	7	
767	5-methylheptyl acetate		172.26	0.55	0.73	-24%		0	7	
768	n-octyl acetate	112-14-1	172.26	0.52	0.64	-19%		0	7	
769	2,3,5-teimethylhexyl acetate		186.29	0.79	0.86	-8%		0	7	
770	2,3-dimethylheptyl acetate		186.29	0.65	0.84	-23%		0	7	
771	2,4-dimethylheptyl acetate		186.29	0.62	0.87	-29%		0	7	
772	2,5-dimethylheptyl acetate		186.29	0.72	0.86	-17%		0	7	
773	2-methyloctyl acetate		186.29	0.47	0.62	-25%		0	7	
774	3,5-dimethylheptyl acetate		186.29	0.74	1.01	-26%		0	7	
775	3,6-dimethylheptyl acetate		186.29	0.71	0.87	-18%		0	7	
776	3-ethylheptyl acetate		186.29	0.57	0.70	-18%		0	7	
777	4,5-dimethylheptyl acetate		186.29	0.63	0.96	-34%		0	7	
778	4,6-dimethylheptyl acetate		186.29	0.72	0.83	-13%		0	7	
779	4-methyloctyl acetate		186.29	0.56	0.68	-18%		0	7	
780	5-methyloctyl acetate		186.29	0.50	0.67	-25%		0	7	
781	n-nonyl acetate	143-13-5	186.29	0.47	0.58	-19%		0	7	
782	3,6-dimethyloctyl acetate		200.32	0.72	0.88	-17%		0	7	
783	3-isopropylheptyl acetate		200.32	0.49	0.71	-32%		0	7	

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k	a	Expt	Bias
784	4,6-dimethyloctyl acetate		200.32	0.70	0.85	-17%			0	7
785	3,5,7-trimethyloctyl acetate		214.34	0.60	0.82	-28%			0	7
786	3-ethyl-6-methyloctyl acetate		214.34	0.57	0.80	-29%			0	7
787	4,7-dimethylnonyl acetate		214.34	0.45	0.63	-29%			0	7
788	methyl dodecanoate {methyl laurate}	111-82-0	214.34	0.42	0.53	-20%			0	7
789	2,3,5,7-tetramethyloctyl acetate		228.37	0.57	0.74	-23%			0	7
790	3,5,7-trimethylnonyl acetate		228.37	0.56	0.76	-26%			0	7
791	3,6,8-trimethylnonyl acetate		228.37	0.53	0.72	-26%			0	7
792	2,4,6,8-tetramethylnonyl acetate		242.40	0.46	0.63	-27%			0	7
793	3-ethyl-6,7-dimethylnonyl acetate		242.40	0.55	0.76	-28%			0	7
794	4,7,9-trimethyldecyl acetate		242.40	0.37	0.55	-32%			0	7
795	methyl myristate {methyl tetradecanoate}	124-10-7	242.40	0.39	0.47	-18%			0	7
796	2,3,5,6,8-pentamethylnonyl acetate		256.42	0.59	0.74	-20%			0	7
797	3,5,7,9-tetramethyldecyl acetate		256.42	0.43	0.58	-27%			0	7
798	5-ethyl-3,6,8-trimethylnonyl acetate		256.42	0.71	0.77	-7%			0	7
799	dimethyl carbonate	616-38-6	90.08	0.055	0.059	-6%	1	2	0	2
800	propylene carbonate	108-32-7	102.09	0.27	0.25	6%	1	2	+	2
801	methyl lactate	547-64-8	104.10	2.59	2.76	-6%	1		0	6
802	2-methoxyethyl acetate	110-49-6	118.13	1.08	1.18	-9%			0	7
803	ethyl lactate	97-64-3	118.13	2.39	2.72	-12%	1		0	6
804	methyl isopropyl carbonate	51729-83-0	118.13	0.59	0.69	-14%	1	2	0	2
805	1-methoxy-2-propyl acetate	108-65-6	132.16	1.62	1.69	-4%	1	2	0,+	2
806	2-ethoxyethyl acetate	111-15-9	132.16	1.75	1.88	-7%			0	7
807	2-methoxy-1-propyl acetate	70657-70-4	132.16	1.06	1.12	-6%			0	7
808	methoxypropanol acetate	84540-57-8	132.16	1.76	1.97	-10%			0	7
809	dimethyl succinate	106-65-0	146.14	0.21	0.23	-8%	1	2	0	2
810	ethylene glycol diacetate	111-55-7	146.14	0.62	0.73	-14%			0	7
811	diisopropyl carbonate	6482-34-4	146.18	0.94	1.04	-10%			0	7
812	1,2-propylene glycol diacetate	623-84-7	160.17	0.58	0.94	-39%			0	7
813	dimethyl glutarate	1119-40-0	160.17	0.39	0.50	-22%	1	2	0	2
814	2-butoxyethyl acetate	112-07-2	160.21	1.53	1.65	-7%			0	7
815	dimethyl adipate	627-93-0	174.19	1.72	1.94	-12%	1		0	6
816	2-(2-ethoxyethoxy) ethyl acetate	112-15-2	176.21	1.39	1.49	-6%			0	7
817	dipropylene glycol n-propyl ether isomer #1		176.25	1.89	2.13	-11%			0	7
818	dipropylene glycol methyl ether acetate isomer #1		190.24	1.30	1.41	-8%			0	7
819	dipropylene glycol methyl ether acetate isomer #2		190.24	1.43	1.58	-9%			0	7
820	dipropylene glycol methyl ether acetate isomers	88917-22-0	190.24	1.37	1.49	-9%			0	7
821	glyceryl triacetate	102-76-1	218.20	0.51	0.57	-11%			0	7
822	2-(2-butoxyethoxy) ethyl acetate	124-17-4	204.26	1.30	1.36	-4%			0	7
823	substituted C7 ester (C12)		216.32	0.76	0.88	-14%			0	7

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k	a	Expt	Bias
824	1-hydroxy-2,2,4-trimethylpentyl-3-isobutyrate	18491-15-1	216.32	0.84	0.91	-8%			0	7
825	3-hydroxy-2,2,4-trimethylpentyl-1-isobutyrate	77-68-9	216.32	0.72	0.86	-17%			0	7
826	texanol isomers	25265-77-4	216.32	0.76	0.88	-14%	1	2	0	2
827	substituted C9 ester (C12)		216.32	0.76	0.88	-14%			0	7
828	dimethyl sebacate	106-79-6	230.30	0.40	0.48	-17%			0	7
829	diisopropyl adipate	6938-94-9	230.30	1.22	1.42	-14%			0	7
830	triethyl citrate	77-93-0	276.28	0.66					0	8
831	2,2,4-trimethyl-1,3-pentanediol diisobutyrate	6846-50-0	286.41	0.34					0	7
832	ethylene oxide	75-21-8	44.05	0.037	0.044	-17%	1		0	6
833	propylene oxide	75-56-9	58.08	0.28	0.32	-12%	1		0	6
834	1,2-epoxybutane	106-88-7	72.11	0.86	1.01	-15%	1		0	6
835	formic acid	64-18-6	46.03	0.062	0.076	-17%	1		0	6
836	acetic acid	64-19-7	60.05	0.66	0.50	32%	1		0	6
837	glycolic acid	79-14-1	76.05	2.32	2.67	-13%			0	8
838	peroxyacetic acid	79-21-0	76.05	0.52					0	8
839	acrylic acid	79-10-7	72.06	11.10	11.57	-4%			0	8
840	propionic acid	79-09-4	74.08	1.17	0.79	48%			0	7
841	methacrylic acid	79-41-4	86.09	18.04	18.78	-4%			0	8
842	isobutyric acid	79-31-2	88.11	1.15	1.22	-6%			0	7
843	butanoic acid	107-92-6	88.11	1.75	1.78	-2%			0	7
844	malic acid	6915-15-7	134.09	6.77	7.51	-10%			0	8
845	3-methylbutanoic acid	503-74-2	102.13	4.11	4.26	-4%			0	7
846	adipic acid	124-04-9	146.14	2.94	3.37	-13%			0	8
847	2-ethyl hexanoic acid	149-57-5	144.21	3.19	3.49	-9%			0	7
848	methyl acrylate	96-33-3	86.09	11.21	12.10	-7%			0	8
849	vinyl acetate	108-05-4	86.09	3.11	3.26	-5%			0	8
850	2-methyl-3-butene-2-ol	115-18-4	86.13	4.73	5.08	-7%	1		0	8
851	ethyl acrylate	140-88-5	100.12	7.55	8.73	-14%			0	8
852	methyl methacrylate	80-62-6	100.12	15.22	15.84	-4%			0	8
853	ethyl methacrylate	97-63-2	114.14	12.15					0	8
854	hydroxypropyl acrylate	2918-23-2	130.14	4.74	5.56	-15%			0	8
855	n-butyl acrylate	141-32-2	128.17	4.87	5.52	-12%			0	8
856	isobutyl acrylate	106-63-8	128.17	4.57	5.05	-10%			0	8
857	butyl methacrylate	97-88-1	142.20	8.47	9.08	-7%			0	8
858	isobutyl methacrylate	97-86-9	142.20	8.39	8.98	-7%			0	8
859	$\alpha$ -terpineol	98-55-5	154.25	4.50	5.16	-13%			0	8
860	citronellol (3,7-dimethyl-6-octen-1-ol)	106-22-9	154.25	5.63					0	8
861	linalool	78-70-6	156.27	5.28					0	8
862	geraniol	106-24-1	172.26	4.97					0	8
863	2-ethyl-hexyl acrylate	103-11-7	184.28	2.43	2.42	1%			0	8
864	hexyl cinnamal	101-86-0	216.32	2.86					0	10
865	furan	110-00-9	68.07	8.86	16.54	-46%	1	3	-	4
866	2-methyl furan	534-22-5	82.10	8.02			1	3	0	4
867	3-methyl furan	930-27-8	82.10	6.64			1	3	0	4
868	2-ethyl furan	3208-16-0	96.13	6.85					0	8

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
869	2,5-dimethyl furan	625-86-5	96.13	7.60			1	3	0	4
870	formaldehyde	50-00-0	30.03	9.24	8.96	3%	1	1	0	1 b
871	acetaldehyde	75-07-0	44.05	6.34	6.83	-7%	1	2	0	1
872	propionaldehyde	123-38-6	58.08	6.83	7.88	-13%	1		0	6
873	2-methylpropanal	78-84-2	72.11	5.05	5.86	-14%	1		0	7
874	butanal	123-72-8	72.11	5.75	6.68	-14%	1		0	7
875	C4 aldehydes		72.11	5.75	6.68	-14%			0	7
876	2,2-dimethylpropanal (pivaldehyde)	630-19-3	86.13	4.71	5.40	-13%	1		0	8
877	3-methylbutanal (isovaleraldehyde)	590-86-3	86.13	4.79	5.47	-12%	1		0	8
878	pentanal (valeraldehyde)	110-62-3	86.13	4.89	5.71	-14%	1		0	8
879	C5 aldehydes		86.13	4.89	5.71	-14%			0	8
880	glutaraldehyde	111-30-8	100.12	4.14	4.79	-14%			0	8
881	hexanal	66-25-1	100.16	4.18	4.93	-15%	1		0	8
882	C6 aldehydes		100.16	4.18	4.93	-15%			0	8
883	heptanal	111-71-7	114.19	3.54	4.19	-16%	1		0	8
884	C7 aldehydes		114.19	3.54	4.19	-16%			0	8
885	2-methyl-hexanal	925-54-2	114.19	3.40	3.97	-14%			0	8
886	octanal	124-13-0	128.21	3.03	3.62	-16%			0	8
887	C8 aldehydes		128.21	3.03	3.62	-16%			0	8
888	hydroxycitronellal	107-75-5	154.25	2.50					0	8
889	glyoxal	107-22-2	58.04	12.13	14.22	-15%	1		0	6
890	methyl glyoxal	78-98-8	72.06	16.02	16.21	-1%	1		0	6
891	acrolein	107-02-8	56.06	7.24	7.55	-4%	1	3	0	2
892	crotonaldehyde	4170-30-3	70.09	9.14	9.96	-8%	1		0	8
893	methacrolein	78-85-3	70.09	5.84	6.18	-6%	1	2	0	2
894	hydroxy methacrolein	40364-84-9	86.09	6.04	6.56	-8%			0	8
895	lumped C5+ unsaturated carbonyl species		100.12	6.18					0	8
896	cinnamic aldehyde	104-55-2	132.16	4.68					0	10
897	amyl cinnamal	122-40-7	202.29	3.06					0	10
898	benzaldehyde	100-52-7	106.12	-0.67	-0.61	10%	1	3	0	2
899	tolualdehyde		120.15	-0.59	-0.54	10%			0	7
900	acetone	67-64-1	58.08	0.35	0.43	-19%	1	1	0	2
901	cyclobutanone	1191-95-3	70.09	0.59	0.68	-14%	1		0	8
902	methyl ethyl ketone	78-93-3	72.11	1.43	1.48	-3%	1	2	0	2
903	cyclopentanone	120-92-3	84.12	1.08	1.42	-24%	1		0	8
904	C5 cyclic ketones		84.12	1.08	1.42	-24%			0	8
905	2-pentanone	107-87-9	86.13	2.70	3.06	-12%	1	2	0	2
906	3-pentanone	96-22-0	86.13	1.18	1.44	-18%	1		0	6
907	C5 ketones		86.13	2.70	3.06	-12%			0	7
908	methyl isopropyl ketone	563-80-4	86.13	1.58	1.64	-3%	1		0	6
909	2,4-pentanedione	123-54-6	100.12	0.98	1.02	-4%			0	8
910	cyclohexanone	108-94-1	98.14	1.26	1.59	-21%	1	2	0	2
911	C6 cyclic ketones		98.14	1.26	1.59	-21%			0	7
912	4-methyl-2-pentanone	108-10-1	100.16	3.74	4.28	-13%	1	2	0	3
913	methyl n-butyl ketone	591-78-6	100.16	3.00	3.53	-15%	1		0	8
914	methyl t-butyl ketone	75-97-8	100.16	0.62	0.78	-21%	1		0	8

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
915	C6 ketones		100.16	3.00	3.53	-15%			0	8
916	C7 cyclic ketones		112.17	1.10	1.39	-21%			0	8
917	2-heptanone	110-43-0	114.19	2.24	2.77	-19%	1	3	?	4
918	2-methyl-3-hexanone	7379-12-6	114.19	1.45	1.77	-18%			0	8
919	di-isopropyl ketone	565-80-0	114.19	1.23	1.61	-24%	1		0	8
920	C7 ketones		114.19	2.24	2.77	-19%			0	8
921	5-methyl-2-hexanone	110-12-3	114.19	2.28	2.10	9%	1		0	8
922	3-methyl-2-hexanone	2550-21-2	114.19	2.43	2.81	-14%			0	8
923	C8 cyclic ketones		126.20	0.98	1.24	-21%			0	8
924	2-octanone	111-13-7	128.21	1.31	1.64	-20%	1		0	8
925	C8 ketones		128.21	1.31	1.64	-20%			0	8
926	C9 cyclic ketones		140.22	0.88	1.11	-21%			0	8
927	2-propyl cyclohexanone	94-65-5	140.22	1.43	1.71	-16%			0	8
928	4-propyl cyclohexanone	40649-36-3	140.22	1.74	2.08	-16%			0	8
929	2-nonanone	821-55-6	142.24	1.00	1.28	-22%	1		0	8
930	di-isobutyl ketone (2,6-dimethyl-4-heptanone)	108-83-8	142.24	2.56	2.90	-12%	1		0	8
931	C9 ketones		142.24	1.00	1.28	-22%			0	8
932	camphor	76-22-2	152.23	0.45					0	8
933	C10 cyclic ketones		154.25	0.80	1.01	-21%			0	8
934	2-decanone	693-54-9	156.27	0.82	1.04	-20%	1		0	8
935	C10 ketones		156.27	0.82	1.04	-20%			0	8
936	2,6,8-trimethyl-4-nonanone; isobutyl heptyl ketone	123-18-2	184.32	1.57	1.86	-16%			0	8
937	biacetyl	431-03-8	86.09	19.43	20.73	-6%	1		0	6
938	methylvinyl ketone	78-94-4	70.09	9.39	8.67	8%	1	3	0	2
939	mesityl oxide (2-methyl-2-penten-4-one)	141-79-7	98.14	6.31	17.37	-64%			0	8
940	isophorone {3,5,5-trimethyl-2-cyclohexenone}	78-59-1	138.21	4.48	10.58	-58%			0	8
941	1-nonene-4-one	61168-10-3	140.22	3.03	3.39	-11%			0	8
942	hydroxy acetone	116-09-6	74.08	3.15	3.08	2%	1		0	8
943	dihydroxyacetone	96-26-4	90.08	3.89	4.02	-3%			0	8
944	methoxy acetone	5878-19-3	88.11	1.94	2.13	-9%	1		0	8
945	diacetone alcohol	123-42-2	116.16	0.57	0.68	-17%			0	8
946	phenol	108-95-2	94.11	2.69	1.82	48%			0	8
947	C7 alkyl phenols	1319-77-3	108.14	2.34	2.34	0%			0	5
948	m-cresol	108-39-4	108.14	2.34	2.34	0%		4	-0	5
949	p-cresol	106-44-5	108.14	2.34	2.34	0%		4	0?	5
950	o-cresol	95-48-7	108.14	2.34	2.34	0%	1	4	?	5
951	4-vinylphenol	2628-17-3	120.15	1.43					0	11
952	2,4-dimethyl phenol	105-67-9	122.16	2.07					0	8
953	2,5-dimethyl phenol		122.16	2.07					0	8
954	3,4-dimethyl phenol	95-65-8	122.16	2.07					0	8
955	2,3-dimethyl phenol	526-75-0	122.16	2.07					0	8
956	2,6-dimethyl phenol	576-26-1	122.16	2.07					0	8
957	C8 alkyl phenols		122.16	2.07	2.07	0%			0	8
958	methylparaben (4-hydroxybenzoic acid, methyl ester)	99-76-3	152.15	1.66					0	11

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
959	2,3,5-trimethyl phenol	697-82-5	136.19	1.86					0	8
960	2,3,6-trimethyl phenol	2416-94-6	136.19	1.86					0	8
961	C9 alkyl phenols		136.19	1.86	1.86	0%			0	8
962	C10 alkyl phenols		150.22	1.68	1.68	0%			0	8
963	propylparaben	94-13-3	180.20	1.40					0	11
964	C11 alkyl phenols		164.24	1.54	1.54	0%			0	8
965	C12 alkyl phenols		178.27	1.42	1.42	0%			0	8
966	2,6-di-tert-butyl-p-cresol	128-37-0	220.35	1.15					0	10
967	benzyl alcohol	100-51-6	108.14	4.98			1	2	0	4
968	methoxybenzene; anisole	100-66-3	108.14	6.49			1		0	8
969	beta-phenethyl alcohol	98-85-1	122.16	4.41					-	11
970	2-phenoxyethanol; ethylene glycol phenyl ether	122-99-6	138.16	4.35	3.61	20%			0	8
971	phthalic anhydride	85-44-9	148.12	2.50					0	8
972	cinnamic alcohol	104-54-1	134.18	0.84					-1	10
973	1-phenoxy-2-propanol	770-35-4	152.19	1.54	1.73	-11%			0	8
974	anethol	104-46-1	148.20	0.76					0	11
975	1,2-diacetyl benzene	704-00-7	162.19	2.17			1		0	8
976	diethyl phthalate	84-66-2	222.24	1.56					0	8
977	2-ethylhexyl benzoate	5444-75-7	234.33	0.93					0	10
978	dibutyl phthalate	84-74-2	278.34	1.20					0	8
979	nitrobenzene	98-95-3	123.11	0.054	0.067	-19%	1		0	8
980	m-nitrotoluene	99-08-1	137.14	0.48			1		0	8
981	para toluene isocyanate	622-58-2	133.15	1.03	0.94	10%	1	2	0	5
982	2,4-toluene diisocyanate	584-84-9	174.16	-0.072	-0.133	-46%	1	2	0	5
983	2,6-toluene diisocyanate	91-08-7	174.16	-0.072				4	0	5
984	toluene diisocyanate (mixed isomers)	26471-62-5	174.16	-0.072					0	5
985	methylene diphenylene diisocyanate	101-68-8	250.25	0.87	0.79	9%			0	8
986	methylamine	74-89-5	31.06	7.29			1		+	13 a,n
987	dimethyl amine	124-40-3	45.08	2.95	9.37	-69%	1		+	13 a,n
988	ethyl amine	75-04-7	45.08	5.48	7.79	-30%	1		+	13 a,n
989	trimethyl amine	75-50-3	59.11	6.03	7.06	-15%	1		+	13 a,n
990	isopropylamine	75-31-0	59.11	6.93				4a	+	12 a,n
991	t-butyl amine	75-64-9	73.14	-3.15			1	4a	-	12 a
992	triethyl amine	121-44-8	101.19	3.66					+	13 a,n
993	triethylene diamine	280-57-9	112.17	3.31					+	13 a,n
994	ethanolamine	141-43-5	61.08	6.53	5.96	10%		3a	+	12 a,n
995	dimethylaminoethanol	108-01-0	89.14	5.41	4.75	14%	1		+	13 a,n
996	2-amino-1-butanol	96-20-8	89.14	4.78					+	13 a,n
997	2-amino-2-methyl-1-propanol	124-68-5	89.14	-2.57	4.75	-154%		3a	-	12 a
998	diethanol amine	111-42-2	105.14	2.36	4.05	-42%			+	13 a,n
999	triethanolamine	102-71-6	149.19	4.08	2.75	48%			+	13 a,n
1000	triisopropanolamine	122-20-3	191.27	2.60					+	13 a,n
1001	methyl nitrite	624-91-9	61.04	10.50			1		0	6
1002	acrylonitrile	107-13-1	53.06	2.16			1		0	10
1003	1-nitropropane	108-03-2	89.09	0.20					0	8
1004	ethyl methyl ketone oxime	96-29-7	87.12	1.52					0	10



Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
1005	n-methyl-2-pyrrolidone	872-50-4	99.13	2.28	2.55	-11%	1	2	0	2
1006	lauryl pyrrolidone	2687-96-9	253.42	0.89					0	11
1007	methyl chloride	74-87-3	50.49	0.036	0.034	6%	1		0	10
1008	dichloromethane	75-09-2	84.93	0.039	0.066	-41%	1		0	10
1009	methyl bromide	74-83-9	94.94	0.018	0.017	6%	1		0	10
1010	chloroform	67-66-3	119.38	0.020	0.034	-41%	1		0	10
1011	carbon tetrachloride	56-23-5	153.82	0	0	0%			0	1
1012	methylene bromide	74-95-3	173.83	0	0	0%			0	1
1013	ethyl chloride	75-00-3	64.51	0.27	0.25	10%	1		0	10
1014	1,1-dichloroethane	75-34-3	98.96	0.065	0.101	-35%	1		0	10
1015	1,2-dichloroethane	107-06-2	98.96	0.21	0.10	111%	1		0	10
1016	ethyl bromide	74-96-4	108.97	0.121	0.108	12%	1		0	20
1017	1,1,1-trichloroethane	71-55-6	133.40	0.005	0.004	28%	1		0	10
1018	1,1,2-trichloroethane	79-00-5	133.40	0.082	0.058	42%	1		0	10
1019	1,2-dibromoethane	106-93-4	187.86	0.098	0.046	111%	1		0	20
1020	1,2-dichloropropane	78-87-5	112.99	0.28					0	10
1021	n-propyl bromide	106-94-5	122.99	0.40	0.35	17%	1	2x	-,+2	20n
1022	1-chlorobutane	109-69-3	92.57	1.04					0	10
1023	n-butyl bromide	109-65-9	137.02	0.78	0.60	30%	1	2x	-,+2	20n
1024	3-(chloromethyl)-heptane	123-04-6	148.67	0.88					0	10
1025	vinyl chloride	75-01-4	62.50	2.70	2.92	-8%	1		0	10
1026	1,1-dichloroethene	75-35-4	96.94	1.69					0	10
1027	trans-1,2-dichloroethene	156-60-5	96.94	1.65	0.81	103%	1		0	10
1028	cis-1,2-dichloroethene		96.94	1.65					0	10
1029	trichloroethylene	79-01-6	131.39	0.61	0.60	1%	1	2x	+2	20
1030	perchloroethylene	127-18-4	165.83	0.029	0.040	-27%	1		0	10
1031	3-chloropropene		76.52	11.98					0	10
1032	trans-1,3-dichloropropene	10061-02-6	110.97	4.92			1	2m	0	3
1033	cis-1,3-dichloropropene	10061-01-5	110.97	3.61			1	2m	0	3
1034	1,3-dichloropropene mixture		110.97	4.19			1	2	0	2
1035	trans 1,3,3,3-tetrafluoropropene (HFO 1234ze)	1645-83-6	114.04	0.091			1	2	0	1
1036	2,3,3,3-tetrafluoropropene (HFO 1234yf)	754-12-1	114.04	0.27			1	2	0	1
1037	2-(cl-methyl)-3-cl-propene	1871-57-4	125.00	6.85	3.13	119%	1	4	-	20
1038	monochlorobenzene	108-90-7	112.56	0.31	0.36	-15%	1		0	8
1039	p-dichlorobenzene	106-46-7	147.00	0.171	0.202	-16%			0	10
1040	o-dichlorobenzene	95-50-1	147.00	0.171					0	8
1041	hexafluorobenzene	392-56-3	186.05	0.045			1		0	8
1042	2-chlorotoluene	95-49-8	126.58	2.82					1	8
1043	benzotrifluoride	98-08-8	146.11	0.28	0.26	7%	1		0	8
1044	p-trifluoromethyl-cl-benzene	98-56-6	180.55	0.121	0.113	7%	1		0	8
1045	methyl nonafluorobutyl ether	163702-07-6	234.06	0.052					0	8
1046	methyl nonafluoroisobutyl ether	163702-08-7	234.06	0.052					0	8
1047	ethyl nonafluorobutyl ether	163702-05-4	264.09	0.192					+	8
1048	ethyl nonafluoroisobutyl ether	163702-06-5	264.09	0.192					+	8
1049	chloroacetaldehyde	107-20-0	78.50	12.00			1		0	7
1050	chloroacetone	78-95-5	92.52	9.22			1	3	0	5
1051	chloropicrin	76-06-2	164.38	1.80			1	2	0	1

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
1052	hexamethyldisiloxane	107-46-0	162.38	-0.027			1	3	0	5
1053	hydroxymethyldisiloxane		164.35	-0.131			1	3	0	5
1054	d4 cyclosiloxane	556-67-2	296.62	-0.056			1	3	0	5
1055	d5 cyclosiloxane	541-02-6	370.77	-0.068			1	4	0	5
1056	carbon disulfide	75-15-0	76.14	0.23			1	2	0	2
1057	methyl isothiocyanate	556-61-6	73.12	0.31			1	2	0	2
1058	dimethyl sulfoxide	67-68-5	78.13	6.46	6.83	-5%	1	2	-2,0	4
1059	molinate		187.30	1.43					0	7
1060	eptc (s-ethyl dipropylthiocarbamate)	759-94-4	189.32	1.58			1	2	0	2
1061	pebulate		203.34	1.58					0	7
1062	thiobencarb		257.78	0.65					0	8
1063	methyl iodide	74-88-4	141.94	-0.53					0	3
1064	Base ROG Mixture		14.44	3.50	3.71	-5%			0	7
1065	Final LEV -- RFA		14.03	3.44	3.63	-5%			0	7
1066	TLEV Exhaust -- RFA		14.04	3.89	4.09	-5%			0	7
1067	TLEV Exhaust -- Phase 2		14.12	3.85	4.05	-5%			0	7
1068	Final LEV -- Phase 2		14.22	3.34	3.55	-6%			0	7
1069	TLEV Exhaust -- LPG		14.86	1.99	2.10	-6%			0	7
1070	TLEV Exhaust -- CNG		15.22	0.70	0.75	-6%			0	7
1071	TLEV Exhaust -- E-85		20.74	2.46	2.70	-9%			0	7
1072	TLEV Exhaust -- M-85		27.45	1.53	1.57	-3%			0	7
1073	Composite mineral spirit (naphthas or lactol spirits) (CARB Profile ID 802)		14.06	1.75	2.02	-13%			0	7
1074	Safety-Kleen Mineral Spirits "A" (Type I-B, 91% Alkanes)		14.08	1.11	1.27	-13%		2	0,+	7
1075	Safety-Kleen Mineral Spirits "B" (Type II-C)		14.10	0.65	0.78	-16%		2	0,+	7
1076	Safety-Kleen Mineral Spirits "C" (Type II-C)		14.11	0.65	0.78	-17%		2	0,+	7
1077	Exxon Exxol(r) D95 Fluid		14.11	0.55	0.67	-17%		2	0	7
1078	Safety-Kleen Mineral Spirits "D" (Type II-C)		14.12	0.65	0.78	-17%		2	0,+	7
1079	Exxon Isopar(r) M Fluid		14.15	0.54	0.65	-18%		2	0	7
1080	Thinning Solvent/Mineral Spirits (Cal Poly SLO. 1996)		14.40	1.79	1.99	-10%			0	7
1081	Aromatic 100		13.36	7.38				2	0	7
1082	Kerosene		13.94	1.46				2	0	7
1083	Regular mineral spirits		13.97	1.73				2	0	7
1084	Reduced Aromatics Mineral Spirits		14.05	1.08				2	0	7
1085	Dearomatized Alkanes, mixed, predominately C10-C12		14.09	0.80				2	0	7
1086	VMP Naphtha		14.16	1.12				2	0	7
1087	Synthetic isoparaffinic alkane mixture, predominately C10-C12		14.20	0.68				2	0	7
1088	ASTM-3C1 "Highly Branched" rep'n		14.20	1.03					0	7

Table A-1 (continued)

No.	Description	CAS	MWt	MIR [a]			Unc. Codes [b]			
				New	Old	Chg	k a	Expt	Bias	Unc
1089	Oxo-Tridecyl Acetate		16.19	0.54	0.67	-20%			0	7
1090	Oxo-Dodecyl Acetate		16.30	0.58	0.72	-20%			0	7
1091	Oxo-Decyl Acetate		16.71	0.66	0.83	-20%		2	0	7
1092	Oxo-Nonyl Acetate		16.89	0.69					0	7
1093	Oxo-Octyl Acetate		17.23	0.78					0	7
1094	Oxo-Heptyl Acetate		17.58	0.80					0	7
1095	Oxo-Hexyl Acetate		18.02	0.84					0	7
1096	CARB Hydrocarbon Bin 1		14.25	1.33	2.08	-36%			0	7c
1097	CARB Hydrocarbon Bin 2		14.36	1.23	1.59	-23%			0	7c
1098	CARB Hydrocarbon Bin 3		14.03	1.53	2.52	-39%			0	7c
1099	CARB Hydrocarbon Bin 4		14.19	1.37	2.24	-39%			0	7c
1100	CARB Hydrocarbon Bin 5		14.07	1.47	2.56	-43%			0	7c
1101	CARB Hydrocarbon Bin 6		14.18	1.08	1.41	-23%			0	7c
1102	CARB Hydrocarbon Bin 7		14.26	0.95	1.17	-19%			0	7c
1103	CARB Hydrocarbon Bin 8		14.03	1.34	1.65	-19%			0	7c
1104	CARB Hydrocarbon Bin 9		14.14	1.35	1.62	-17%			0	7c
1105	CARB Hydrocarbon Bin 10		14.05	1.88	2.03	-8%			0	7c
1106	CARB Hydrocarbon Bin 11		14.14	0.63	0.91	-31%			0	7c
1107	CARB Hydrocarbon Bin 12		14.20	0.55	0.81	-32%			0	7c
1108	CARB Hydrocarbon Bin 13		14.03	0.79	1.01	-22%			0	7c
1109	CARB Hydrocarbon Bin 14		14.11	0.91	1.21	-24%			0	7c
1110	CARB Hydrocarbon Bin 15		14.03	1.48	1.82	-19%			0	7c
1111	CARB Hydrocarbon Bin 16		14.11	0.47	0.57	-18%			0	7c
1112	CARB Hydrocarbon Bin 17		14.16	0.43	0.51	-16%			0	7c
1113	CARB Hydrocarbon Bin 18		14.03	0.54	0.63	-14%			0	7c
1114	CARB Hydrocarbon Bin 19		14.07	0.61	0.88	-31%			0	8c
1115	CARB Hydrocarbon Bin 20		13.99	0.89	1.49	-41%			0	10c
1116	CARB Hydrocarbon Bin 21		13.27	7.44	7.37	1%			0	7c
1117	CARB Hydrocarbon Bin 22		13.36	7.39	7.51	-2%			0	8c
1118	CARB Hydrocarbon Bin 23		13.42	6.66	8.07	-17%			0	10c
1119	CARB Hydrocarbon Bin 24		13.28	3.76	5.00	-25%			0	11c

## Notes:

[a] 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" = previous values provided by Carter (2003), calculated using the SAPRC-99 mechanism.

[b] 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).

Table A-1 (continued)

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)

	<u>Chamber data available</u>	<u>No chamber data available</u>
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.

Table A-1 (continued)

- 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  $\pm 1$  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.
- 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.

Table A-1 (continued)

- 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.

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.
- 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 NO<sub>x</sub> is limited. This should affect MIR values but will lead to too high reactivities in lower NO<sub>x</sub> scenarios.
- a This compound may react with HNO<sub>3</sub> 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 HNO<sub>3</sub> 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 HNO<sub>3</sub> 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 HNO<sub>3</sub> 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.

Table A-1 (continued)

- 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 by Carter and Malkina (2005) and in Appendix B of this report. The differences between the two sets reflect differences in the calculation methodology as well as differences in chemical mechanism. See Appendix B 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.

**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		