

Development of Species Profiles for UK Emissions of VOCs

A report produced for the Department of the
Environment, Transport & the Regions

M E Jenkin, N R Passant & H J Rudd

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E6 Culham
 Abingdon
 Oxon
 OX14 3ED
 Telephone 01235 463977
 Facsimile 01235 463001

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	Name	Signature	Date
Author	Michael Jenkin Neil Passant Howard Rudd		
Reviewed by	John Branson		
Approved by	Mike Woodfield		

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1 Introduction

This report details work carried out as part of the DETR research programme 'Emission Factors and Cost Curves for Air Pollutants', reference EPG 1/3/134. The work programme includes research aimed at further improving the speciation of the inventory for NMVOC included in the National Atmospheric Emissions Inventory (NAEI). This report gives details of speciation work completed in the 1999/2000 financial year, the results of which have been incorporated in the latest NAEI (the '1998 NAEI').

Speciation of the NMVOC inventory has developed over a period of years. Speciated emission factors for the NAEI were first given in Marlowe *et al*, 1992 and were subsequently revised in Rudd, 1995. Further revisions were described in Passant & Lymberidi, 1998. This report outlines those changes made since publication of these reports and should be viewed as supplementary material.

The speciated NMVOC inventory was reviewed in 1999 and a schedule of research drawn up aimed at generating better species profiles for use in the NAEI (Passant & Wenborn, 1999). The work detailed here includes the first phase of that research. The final phase of research, which will be carried out in the 2000/2001 financial year, will be detailed in a subsequent report.

Although, the species profiles presented in this report have been developed for use in the UK, they could also be used for other inventories. To facilitate this, SNAP (Selected Nomenclature for Air Pollutants) codes have been quoted for each species profile in order to define the sources for which they can be used. Interested parties should also consult the other reports mentioned above for further information on UK speciation.

2 Improvements to Speciation

2.1 OVERVIEW

Improvements to the NAEI speciated NMVOC inventory have been threefold. Firstly, a number of the species profiles used to speciate total NMVOC emissions from a given sector have been revised. Revisions have been made to the following profiles:

- industrial paints
- printing
- textile coating
- rubber processes
- wood preservation
- other solvent use
- agrochemicals
- non-aerosol consumer products
- chemicals manufacture
- refineries

In addition, new profiles have been included for the following:

- petroleum processes

Secondly, the NAEI species database has been enhanced through the inclusion of photochemical ozone creation potentials (POCP) for each chemical species. This will allow the generation of POCP weighted emission estimates for each source of NMVOC.

Thirdly, a number of other contacts have been made which, although these have not yet resulted in new information, are expected to yield useful information in the future. This includes further discussions with the Solvent Industry Association (SIA) regarding types and quantities of solvents used in the UK, and discussion with the Institute of Petroleum regarding the development of a protocol for estimating speciated VOC emissions at refineries.

2.2 CHANGES TO SPECIES PROFILES

2.2.1 Solvent xylene

The chemical compound xylene exists in three isomers. Previously, where xylene is used as a solvent, it had been assumed that these isomers were present in equal quantities in the mixture. In reality, solvent xylene contains different quantities of each of the three isomers and also contains large quantities of a fourth compound – ethyl benzene.

The SIA have provided a breakdown, typical for solvent xylene as follows:

ortho-xylene	12%
para-xylene	13%
meta-xylene	55%
ethyl-benzene	20%

Species profiles that contain solvent xylene have been updated to take account of this information. They include industrial paints, textile coating, rubber processes, wood preservation, other solvent use, and non-aerosol consumer products. New species profiles are shown in Appendix 1.

2.2.2 Industrial paints

As described above, the species profiles for industrial paints have been revised to take account of new information regarding the composition of solvent xylene. At the same time, it was decided to revise the methodology slightly for the generation of these profiles.

The profiles are based on information provided by the British Coating Federation (BCF). This information consisted of listings of solvents used in each painting sector, together with an estimate of the usage of each class of solvent (e.g. aliphatic hydrocarbons, esters, chlorinated hydrocarbons etc.) as well as an indication of whether the usage of each individual solvent was significant or not. In order to convert this information into emission estimates for each individual species, then it has been assumed that where use of a solvent is listed as significant in the BCF data, then the level of usage is four times higher than those solvents which are not significant. For example, the BCF have estimated that 400 tonnes of alcohols are used in marine paints as follows:

ethanol	not significant
i-butanol	not significant
n-butanol	significant

We have assumed the following usage of the individual alcohols:

ethanol	67 tonnes (i.e. 1/6th of the total)
i-butanol	67 tonnes (i.e. 1/6th of the total)
n-butanol	267 tonnes (i.e. 4/6ths of the total)

The BCF data contains reference to various mixtures, including white spirit, SBP solvent, solvent xylene, 160–180°C boiling point aromatic solvent and 180–220°C boiling point aromatic solvent, and Bisol K. The speciation used for white spirit has been published elsewhere (Rudd & Marlowe, 1998), while the profiles used for other solvents are given in Appendix 2.

The final profiles for industrial paints are given in Appendix 1.

2.2.3 Printing processes

The British Coatings Federation (BCF) have, after consultation with members, provided species profiles for the various printing processes. However, these contain some undifferentiated

mixtures and BCF are seeking further information to clarify these. The BCF data are given in Appendix 3, together with the provisional profiles used in the NAEI database.

2.2.4 Agrochemicals

Solvents used in agrochemicals are known to consist mainly of aromatic hydrocarbons with lesser quantities of aliphatic hydrocarbons. The aromatic hydrocarbons have previously been reported (Rudd, 1995) to be 85% of total VOC emissions with aliphatic hydrocarbons making up the balance, based on SIA data. The aromatic component was assumed to be a mixture of toluene and xylene and the aliphatic hydrocarbon component was assumed to be hexane. However, discussions with the British Agrochemicals Association have indicated that toluene and xylene are not used at all because they are toxic to plants. The solvents used are actually higher molecular weight aromatics (typically C₉ mixtures). The aromatic component has therefore been assumed to be C₉ aromatic compounds (equal quantities of each isomer). We are currently in discussion with the BAA for more information about which aliphatic compounds are used. A new profile for the sector is given in Appendix 1.

2.2.5 Revisions to benzene and 1,3-butadiene contents of profiles

The species profiles for chemical manufacture, and oil refineries contain reference to benzene. The profile for chemicals manufacture also makes mention to 1,3-butadiene. Data on benzene and 1,3-butadiene emissions from these industries is also available from other sources: the United Kingdom Petroleum Industry Association (UKPIA) have provided estimates of benzene emissions from UK refineries, and the Pollution Inventory provides data on emissions of both compounds from chemical processes. The profiles for both sectors have been revised to take account of these data.

The refinery profile is based on the data given in Rudd, 1995. However, whereas that profile gives a benzene emission of 2.6% of total NMVOC, a figure of 2.9% has been used instead based on the UKPIA estimates. Emissions of other compounds have then been revised downward accordingly.

Emissions of benzene and 1,3-butadiene given in the Pollution Inventory for chemical processes are, as with emissions data for total VOC, assumed to be releases from point sources only. Similar data are available for Scottish processes from SEPA and the total emission from point sources has been adjusted to take account of fugitive releases as described in Passant & Lymberidi, 1998. These new emission estimates for benzene and 1,3-butadiene have been incorporated into the species profiles for chemicals manufacturing with emissions of other compounds adjusted accordingly in order to preserve the original total.

The new profiles are given in Appendix 1.

2.2.6 Petroleum processes

The 1998 NAEI includes a number of industrial sources that have been included for the first time. These sources are listed in the Pollution Inventory as 'petroleum processes', yet are not covered by any of the existing categories in the NAEI, such as 'refineries' or 'offshore oil and gas'. Most of the processes are probably related to the onshore production of crude oil or the processing of crude oil. The Pollution Inventory contains data on benzene emissions from these

processes but the remaining emissions are not fully speciated. The sector is therefore speciated using the existing NAEI profile for crude oil production with the benzene content adjusted to achieve consistency with the Pollution Inventory. The new profile is given in Appendix 1.

2.3 ADDITION OF POCP VALUES TO THE DATABASE

POCP values have been added to the database for all of the NMVOC compounds which are emitted. The POCP values fall into three categories:

1. POCPs determined by the standard methodology using a photochemical trajectory model containing fully developed chemical schemes and NAEI speciated VOC emissions. The values are published in the open literature (Derwent *et al*, 1998; Jenkin & Hayman, 1999).
2. POCPs estimated by a documented methodology. This allows assignment of POCPs on the basis of consideration of how the values determined using the standard methodology vary with structure and reactivity, i.e. this method is optimised on the basis of the determined values, and then used to calculate POCPs for additional VOCs within the same classes (i.e., hydrocarbons, oxygenates and halocarbons). The methodology is described more fully elsewhere (Jenkin, 1998; Jenkin *et al*, 1997)
3. POCPs which have been assigned on the basis of an educated guess, and fall into three sub-categories:
 - a. Unspecific species or mixtures. Some entries cannot rigorously be assigned POCPs because there is insufficient information on the species identity, or because the entry is not a unique VOC. Thus, some assumption has to be made. An example of the former is 'ethyl dimethylbenzene' for which there are 6 isomers that will have different POCPs. In this case, a particular isomer (for which a POCP determined using the standard methodology is available) is assumed. An important example of the latter is 'kerosene' which is a complex hydrocarbon mixture. The assigned POCP is based on an average of the range observed for 'determined' POCPs of alkanes and aromatic hydrocarbons. Of the 541 speciated entries, 125 are unspecific species or mixtures for which assumptions are necessary.
 - b. Indefinable - assigned average. Of the 541 speciated entries, 63 VOCs cannot be defined POCPs because there is insufficient information on the kinetics and/or mechanism of their atmospheric degradation. These are generally VOCs containing heteroatoms such as N, Na, Si, S, K. Of these, 35 are assigned a value of 51.3, which is the average of all the 'determined' POCPs. These are those containing Na, K and some of the N-containing species. The 'unspeciated' category is also assumed to have a value of 51.3.
 - c. Indefinable - assumed zero. The remaining 27 are assigned a zero value because it is suspected that a value of 51.3 is likely to be a severe overestimate. These are all the species containing S and Si (for which there is limited evidence that their oxidation may even remove ozone) and some N-containing species that are probably very unreactive.

In total, there are 113 'determined' POCPs, 240 'estimated' POCPs and 188 'guessed' POCPs. Most of the 'determined' POCPs are for compounds that are emitted in the greatest quantities, whereas most of the 'guessed' POCPs are for compounds that are emitted in the smallest quantities.

POCP values assigned to each chemical species are shown in Appendix 4.

2.4 ONGOING DEVELOPMENTS

2.4.1 Speciation of kerosene

Following the speciation of white spirit (Rudd & Marlowe, 1998), we have collaborated with the Solvent Industries Association (SIA) to produce an industry average species profile for kerosene. This is reproduced in appendix 5. Kerosene is the second largest unspciated mixture after white spirit in the VOC inventory.

Kerosene is a complex mixture of hydrocarbons from a variety of chemical processes, the most important of which is crude oil distillation, blended to meet standardised product specifications. Composition varies greatly and includes C₉ to C₁₆ hydrocarbons with a boiling range of about 150-290°C. Functional and performance additives may also be present at concentrations below reporting thresholds.

The species profile was produced by analysis of a representative sample of kerosene. The analysis was done by GCMS by a solvent supplier. The analysis has at least one surprising aspect: there are no aromatic compounds identified. Although, kerosene was expected to predominantly consist of aliphatic hydrocarbons, some aromatic compounds were anticipated. Some 14% of the kerosene consisted of compounds that could not be identified by the analysis and it is possible that at least some of these compounds are aromatic. We intend to hold further discussions with the SIA in order to resolve this question. For the time being the kerosene profile has not been included in the inventory.

POCPs have been assigned to the speciated component of kerosene using the methodology as described in section 2.3 above. These values are given in Appendix 5.

2.4.2 Discussions with Solvent Industry Association

NETCEN and, before that, Warren Spring Laboratory have maintained contact with the SIA since 1989. During that time, SIA have provided the results of surveys of members' estimates of the markets of various solvents in various end user sectors. The SIA present this in the form of a table of solvent against industry and these data have been used in the NAEI. The SIA activity is continuing and they are currently working on an updated version covering 1999. This should be available in time for inclusion in the 1999 NAEI.

2.4.3 Development of a refinery protocol

Since 1993 the United Kingdom Petroleum Industry Association (UKPIA) has annually submitted estimates of total VOC emissions from UK refineries. These are calculated by individual refineries, using a protocol derived by the Institute of Petroleum (IoP). The IoP

have indicated that they wish to widen this protocol to include speciation and have asked AEA Technology to help them. To date, two meetings have been held with representatives of the IoP - an initial scoping discussion and a meeting of the IoP's emissions working group.

3 References

- Derwent R.G., Jenkin, M.E., Saunders, S.M., and Pilling, M.J. (1998), Photochemical Ozone Creation Potentials for Organic Compounds in North West Europe Calculated with a Master Chemical Mechanism. *Atmospheric Environment*, 32, 2419-2441.
- Jenkin M E, (1998), Photochemical ozone and PAN creation potentials for organic compounds: rationalisation and methods of estimation, Report AEAT-4182/20150/003 Issue 1, prepared for the Department of the Environment, Transport and the Regions on Contract PECD 1/3/70.
- Jenkin M.E. and Hayman, G.D. (1999) Photochemical ozone creation potentials for oxygenated organic compounds: sensitivity to variations in kinetic and mechanistic parameters. *Atmospheric Environment*, 33, 1275-1293.
- Jenkin M.E., Hayman G.D., Derwent R.G., Saunders S.M. and Pilling M.J., (1997), Tropospheric Chemistry Modelling: Improvements to Current Models and Application to Policy Issues. First Annual Report (Reference AEA/RAMP/20150/R001 Issue 1) prepared for the Department of the Environment on Contract PECD 1/3/70.
- Marlowe, I T, Richardson, S J, Dowsett, R, Passant, N R, Coleman, P, Loader, A, Giddings, T, Warde-Jones, S, Richardson, J L, Lethlean, J, & McAlister, R, (1992), Emissions of Volatile Organic Compounds from Stationary Sources in the United Kingdom: A Review of Emission Factors by Species and Process, Warren Spring Laboratory, Report No LR882
- Passant, N R & Lymberidi, E, (1998), Emissions of Non Methane Volatile Organic Compounds from Processes and Solvent Use, AEA Technology, Report No AEAT-2837, Issue 1
- Passant, N R & Wenborn, M, (1999), Options for Improvement of the National Atmospheric Emissions Inventory, AEA Technology, Report No AEAT-5015 Issue 1
- Rudd, H J (1995), Emissions of Volatile Organic Compounds from Stationary Sources in the United Kingdom: Speciation, AEA Technology, Report No AEA/CS/16419033/REMA-029/ISSUE 1
- Rudd, H.J. & Marlowe, I.T., (1998), Improvements to the VOC Inventory through Speciation of White Spirit, AEA Technology, Report No AEAT-3221/20011001, Issue 1

Appendices

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Appendix 2	Species profiles for solvent mixtures
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Appendix 1

New Species Profiles

New profiles are shown in Tables 1.1 to 1.6.

SNAP codes for the various profiles are as follows:

Agrochemicals use	No separate SNAP code, in UK inventory included in 060412
Other solvent use	060412
Wood preservation	060406
Rubber processes	060305
Textile coating	060312
Household products	060408
OEM	060101
Refinishing	060102
Wood coating	060107
Coil coating	060105
Marine paints	060106
Heavy duty paints	060109
General industrial coatings	060108
Packaging coatings	060108
Paint manufacture	060307
Refineries	040101, 040104
Petroleum processes	050201
Chemicals manufacturing	040500

Table 1.1 Species profiles for agrochemicals use.

species	%
hexane	15.0
1,2,3-trimethylbenzene	10.6
1,2,4-trimethylbenzene	10.6
1,3,5-trimethylbenzene	10.6
2-ethyltoluene	10.6
3-ethyltoluene	10.6
4-ethyltoluene	10.6
isopropylbenzene	10.6
propylbenzene	10.6

Table 1.2 Species profiles for solvent use sectors (figures are percentages)

species	Other solvent use	Wood preservation	Rubber processes	Textile coating	Household products
(1-methylethyl)cyclohexane	0.154	0.345	0.520	0.523	0.039
(1-methylpropyl)cyclohexane	0.277	0.621	0.940	0.943	0.071
(2-methylbutyl)cyclohexane	0.020	0.045	0.070	0.069	0.005
(2-methylpropyl)cyclohexane	0.150	0.337	0.510	0.512	0.039
1,1,1-trichloroethane	1.100				
1,1,2-trimethylcyclohexane	0.063	0.140	0.210	0.213	0.016
1,1,3-trimethylcyclohexane	0.071	0.159	0.240	0.242	0.018
1,1,4,4-tetramethylcyclohexane	0.044	0.098	0.150	0.150	0.011
1,1-dimethylcyclohexane	0.005	0.011	0.020	0.017	0.001
1,2,3,4-tetrahydro-naphthalene	0.027	0.059	0.090	0.090	0.007
1,2,3,4-tetramethylbenzene	0.034	0.076	0.120	0.116	0.009
1,2,3,5-tetramethylbenzene	0.043	0.096	0.150	0.146	0.011
1,2,3,5-tetramethylcyclohexane	0.069	0.155	0.240	0.236	0.018
1,2,3-trimethylbenzene	0.197	0.442	0.670	0.671	0.051
1,2,3-trimethylcyclohexane	0.130	0.292	0.440	0.443	0.033
1,2,3-trimethylcyclopentane	0.003	0.008	0.010	0.012	0.001
1,2,4,4-tetramethylcyclopentane	0.012	0.027	0.040	0.040	0.003
1,2,4,5-tetramethylbenzene	0.032	0.071	0.110	0.108	0.008
1,2,4-trimethylcyclopentane	0.002	0.004	0.010	0.006	0.000
1,2,4-trimethylbenzene	0.455	1.019	1.550	1.548	0.117
1,2,4-trimethylcyclohexane	0.041	0.091	0.140	0.138	0.010
1,2-dimethyl-3-isopropylcyclopentane	0.024	0.053	0.080	0.081	0.006
1,2-dimethylcyclohexane	0.032	0.072	0.110	0.109	0.008
1,2-ethylmethylcyclopentane	0.005	0.011	0.020	0.017	0.001
1,3,5-trimethylbenzene	0.220	0.493	0.750	0.748	0.056
1,3-diethylbenzene	0.063	0.142	0.220	0.215	0.016
1,3-dimethyl-4-ethylbenzene	0.063	0.142	0.220	0.215	0.016
1,3-dimethyl-5-propylbenzene	0.008	0.017	0.030	0.026	0.002
1,3-dimethylcyclohexane	0.029	0.064	0.100	0.098	0.007

species	Other solvent use	Wood preservation	Rubber processes	Textile coating	Household products
1,3-ethylmethylcyclopentane	0.003	0.008	0.010	0.012	0.001
1,4-diethylbenzene	0.064	0.144	0.220	0.219	0.017
1,4-dimethyl-2-isopropylbenzene	0.010	0.023	0.030	0.034	0.003
1,4-dimethylcyclohexane	0.073	0.163	0.250	0.247	0.019
1-butanol	0.700	5.403			9.459
1-ethyl-1,4-dimethylcyclohexane	0.030	0.068	0.100	0.104	0.008
1-ethyl-2,2,6-trimethylcyclohexane	0.078	0.174	0.260	0.265	0.020
1-ethyl-2,3-dimethylbenzene	0.052	0.116	0.180	0.176	0.013
1-ethyl-2,3-dimethylcyclohexane	0.036	0.080	0.120	0.121	0.009
1-ethyl-2-propylbenzene	0.016	0.037	0.060	0.056	0.004
1-ethyl-2-propylcyclohexane	0.032	0.072	0.110	0.109	0.008
1-ethyl-3,5-dimethylbenzene	0.071	0.159	0.240	0.241	0.018
1-ethyl-3-methylcyclohexane	0.230	0.515	0.780	0.782	0.059
1-ethyl-4-methylcyclohexane	0.098	0.220	0.330	0.334	0.025
1-ethylpropylbenzene	0.019	0.042	0.060	0.065	0.005
1-methyl-1-phenylcyclopropane	0.014	0.031	0.050	0.047	0.004
1-methyl-1-propylbenzene	0.076	0.170	0.260	0.258	0.019
1-methyl-1-propylcyclopentane	0.039	0.087	0.130	0.132	0.010
1-methyl-2-isopropylbenzene	0.064	0.144	0.220	0.219	0.017
1-methyl-3-(isopropyl)benzene	0.076	0.170	0.260	0.258	0.019
1-methyl-3-isopropylcyclopentane	0.002	0.004	0.010	0.006	0.000
1-methyl-3-propylbenzene	0.150	0.337	0.510	0.512	0.039
1-methyl-4-isopropylbenzene	0.258	0.577	0.880	0.877	0.066
1-methyl-4-isopropylcyclohexane	0.267	0.598	0.910	0.909	0.069
1-methyl-4-tertbutylbenzene	0.043	0.096	0.150	0.146	0.011
1-methylbutylbenzene	0.042	0.093	0.140	0.142	0.011
1-methylindan	0.019	0.042	0.060	0.065	0.005
1-methylindene	0.002	0.004	0.010	0.006	0.000
1-propanol	3.200		1.040	1.042	9.459
2,2,3,3-tetramethylhexane	0.101	0.227	0.350	0.345	0.026
2,2,5-trimethylhexane	0.007	0.015	0.020	0.023	0.002

species	Other solvent use	Wood preservation	Rubber processes	Textile coating	Household products
2,3,3,4-tetramethylpentane	0.002	0.004	0.010	0.006	0.000
2,3,4-trimethylhexane	0.007	0.015	0.020	0.023	0.002
2,3,5-trimethylhexane	0.002	0.004	0.010	0.006	0.000
2,3-dimethylheptane	0.086	0.193	0.290	0.293	0.022
2,3-dimethylnonane	0.064	0.144	0.220	0.219	0.016
2,3-dimethyloctane	0.027	0.061	0.090	0.092	0.007
2,3-dimethylundecane	0.015	0.034	0.050	0.052	0.004
2,4-dimethyl-1-(1-methylethyl)benzene	0.051	0.113	0.170	0.172	0.013
2,4-dimethylheptane	0.014	0.030	0.050	0.046	0.003
2,5-dimethyldecane	0.034	0.076	0.120	0.115	0.009
2,5-dimethylheptane	0.041	0.091	0.140	0.138	0.010
2,5-dimethylhexane	0.002	0.004	0.010	0.006	0.000
2,5-dimethyloctane	0.108	0.242	0.370	0.368	0.028
2,6-dimethyldecane	0.042	0.095	0.140	0.144	0.011
2,6-dimethylheptane	0.044	0.098	0.150	0.150	0.011
2,6-dimethyloctane	0.323	0.723	1.100	1.099	0.083
2,6-dimethylundecane	0.010	0.023	0.030	0.035	0.003
2,7-dimethyloctane	0.064	0.144	0.220	0.219	0.016
2-butanol	0.700	5.403			
2-butanone	5.300	2.875			2.703
2-butoxyethanol	1.600	4.196			6.757
2-c9-unidentifiediso-paraffins	0.003	0.008	0.010	0.012	0.001
2-ethoxyethanol	1.600	4.196			
2-ethoxyethyl acetate	1.100	2.797			
2-ethyl-1,3-dimethylbenzene	0.082	0.184	0.280	0.280	0.021
2-methyl-1-butylbenzene	0.005	0.011	0.020	0.017	0.001
2-methyl-2-propanol	0.700				
2-methyl-5-ethyloctane	0.090	0.201	0.300	0.305	0.023
2-methyldecalin	0.063	0.140	0.210	0.213	0.016
2-methyldecane	0.257	0.575	0.870	0.874	0.066
2-methylheptane	0.014	0.030	0.050	0.046	0.003

species	Other solvent use	Wood preservation	Rubber processes	Textile coating	Household products
2-methylnonane	0.345	0.772	1.170	1.173	0.088
2-methyloctane	0.118	0.265	0.400	0.403	0.030
2-methylundecane	0.042	0.095	0.140	0.144	0.011
2-propanol	3.200		1.040	1.042	9.459
2-propyl acetate		5.594			0.901
3,3,4-trimethylhexane	0.002	0.004	0.010	0.006	0.000
3,3,5-trimethylheptane	0.008	0.019	0.030	0.029	0.002
3,3-dimethylheptane	0.010	0.023	0.030	0.035	0.003
3,3-dimethyloctane	0.091	0.204	0.310	0.311	0.023
3,4-dimethylheptane	0.107	0.239	0.360	0.362	0.027
3,4-dimethylhexane	0.002	0.004	0.010	0.006	0.000
3,5-dimethyloctane	0.029	0.064	0.100	0.098	0.007
3,6-dimethyloctane	0.079	0.178	0.270	0.270	0.020
3,7-dimethylnonane	0.090	0.201	0.300	0.305	0.023
3-ethyl-2-methylheptane	0.391	0.875	1.330	1.329	0.100
3-ethyl-2-methylhexane	0.007	0.015	0.020	0.023	0.002
3-ethylheptane	0.086	0.193	0.290	0.293	0.022
3-ethylhexane	0.002	0.004	0.010	0.006	0.000
3-ethyloctane	0.068	0.151	0.230	0.230	0.017
3-ethyltoluene	0.231	0.518	0.790	0.787	0.059
3-methyldecane	0.289	0.647	0.980	0.984	0.074
3-methylheptane	0.010	0.023	0.030	0.035	0.003
3-methylhexane	0.002	0.004	0.010	0.006	0.000
3-methylnonane	0.399	0.893	1.360	1.358	0.102
3-methyloctane	0.107	0.239	0.360	0.362	0.027
3-methylundecane	0.049	0.110	0.170	0.167	0.013
4 methyl-2-pentanone			7.980	7.979	
4,4-dimethylheptane	0.003	0.008	0.010	0.012	0.001
4,5-dimethylnonane	0.063	0.140	0.210	0.213	0.016
4,6-dimethylindan	0.006	0.014	0.020	0.022	0.002
4,7-dimethylindan	0.003	0.006	0.010	0.009	0.001

species	Other solvent use	Wood preservation	Rubber processes	Textile coating	Household products
4-ethyl-1,2-dimethylbenzene	0.056	0.125	0.190	0.189	0.014
4-ethyloctane	0.030	0.068	0.100	0.104	0.008
4-ethyltoluene	0.096	0.215	0.330	0.327	0.025
4-methyl-2-pentanone		5.148			2.703
4-methyl-4-hydroxy-2-pentanone		1.399			
4-methyldecane	0.484	1.083	1.650	1.645	0.124
4-methylheptane	0.005	0.011	0.020	0.017	0.001
4-methylnonane	0.272	0.610	0.930	0.926	0.070
4-methyloctane	0.122	0.273	0.410	0.414	0.031
4-propylheptane	0.005	0.011	0.020	0.017	0.001
5-methyldecane	0.130	0.292	0.440	0.443	0.033
5-methylundecane	0.041	0.091	0.140	0.138	0.010
6-ethyl-2-methyldecane	0.005	0.011	0.020	0.017	0.001
6-ethyl-2-methyloctane	0.015	0.034	0.050	0.052	0.004
6-methylundecane	0.032	0.072	0.110	0.109	0.008
acetone	1.300	7.945	3.010	3.009	2.703
butyl acetate	2.100	4.196			0.901
butylbenzene	0.066	0.147	0.220	0.224	0.017
butylcyclohexane	0.254	0.568	0.860	0.863	0.065
C ₁₀ -cyclo-paraffin	0.301	0.674	1.020	1.024	0.077
C ₁₀ -iso-paraffin	0.238	0.534	0.810	0.811	0.061
C ₁₁ -aromatic	0.003	0.006	0.010	0.009	0.001
C ₁₁ -cyclo-paraffin	0.020	0.045	0.070	0.069	0.005
C ₁₁ -iso-paraffin	0.279	0.625	0.950	0.949	0.072
C ₁₁ -unidentified	0.012	0.027	0.040	0.040	0.003
C ₁₂ -cyclo-paraffin	0.008	0.019	0.030	0.029	0.002
C ₁₂ -iso-paraffin	0.090	0.201	0.300	0.305	0.023
C ₁₃ -iso-paraffin	0.002	0.004	0.010	0.006	0.000
C ₉ -cyclo-paraffin	0.017	0.038	0.060	0.058	0.004
C ₉ -iso-paraffin	0.014	0.030	0.050	0.046	0.003
coeluting-2-aromatics-1-iso-paraffin	0.025	0.057	0.090	0.086	0.007

species	Other solvent use	Wood preservation	Rubber processes	Textile coating	Household products
coeluting aromatic, cyclo-and iso-paraffin	0.014	0.030	0.050	0.046	0.003
coeluting aromatic and iso-paraffin	0.034	0.076	0.120	0.115	0.009
cyclo-paraffin	0.010	0.023	0.030	0.035	0.003
cycloheptane	0.002	0.004	0.010	0.006	0.000
decalin	0.088	0.197	0.300	0.299	0.023
decane	1.587	3.555	5.400	5.401	0.407
dichloromethane	12.600		1.390	1.389	7.432
dimethylnonane	0.034	0.076	0.120	0.115	0.009
dodecane	0.096	0.216	0.330	0.328	0.025
ethanol	21.000				9.459
ethyl acetate		2.797			0.901
ethylbenzene	0.987	1.349	3.300	3.303	2.577
ethylcyclohexane	0.092	0.204	0.310	0.311	0.023
ethylene glycol	10.500				
ethylisopropylbenzene	0.003	0.006	0.010	0.009	0.001
heptane	0.003	0.008	0.010	0.012	0.001
hexylcyclohexane	0.002	0.004	0.010	0.006	0.000
indan	0.058	0.130	0.200	0.198	0.015
isopentylbenzene	0.010	0.023	0.030	0.034	0.003
isopropylbenzene	0.063	0.142	0.220	0.215	0.016
m-xylene	2.645	3.558	8.850	8.852	7.069
methanol	5.300				
methylcyclodecane	0.014	0.030	0.050	0.046	0.003
methylcyclohexane	0.015	0.034	0.050	0.052	0.004
methyltetralin	0.004	0.008	0.010	0.013	0.001
naphthalene	0.009	0.020	0.030	0.030	0.002
nonane	0.916	2.052	3.120	3.118	0.235
o-xylene	0.657	0.955	2.200	2.204	1.563
octahydro-indan	0.046	0.102	0.160	0.155	0.012
octane	0.066	0.148	0.220	0.224	0.017
p-xylene	0.648	0.891	2.170	2.169	1.677

species	Other solvent use	Wood preservation	Rubber processes	Textile coating	Household products
pentylbenzene	0.003	0.006	0.010	0.009	0.001
pentylcyclohexane	0.063	0.140	0.210	0.213	0.016
propylbenzene	0.144	0.323	0.490	0.490	0.037
propylcyclohexane	0.330	0.738	1.120	1.122	0.085
propylcyclopentane	0.002	0.004	0.010	0.006	0.000
tertbutylcyclopropane	0.002	0.004	0.010	0.006	0.000
tertpentylbenzene	0.025	0.057	0.090	0.086	0.006
tetramethylcyclohexane	0.049	0.110	0.170	0.167	0.013
toluene	4.760	6.357	15.920	15.925	12.840
trichloroethene					7.432
undecane	0.830	1.859	2.820	2.824	0.213
unidentified C ₈ -paraffin	0.002	0.004	0.010	0.006	0.000
unidentified iso-paraffin	0.020	0.045	0.070	0.069	0.005
unspeciated	3.220	0.044	0.070	0.066	0.005

Table 1.3 Species profiles for industrial paints (figures are percentages)

species	OEM	Refinishing	Wood	Coil	Marine	Heavy duty	Gen. industrial	Packaging	Manufacture
(1-methylethyl)cyclohexane	0.039	0.106	0.006	0.117	0.156	0.148	0.093	0.010	0.081
(1-methylpropyl)cyclohexane	0.070	0.191	0.011	0.211	0.281	0.267	0.168	0.018	0.147
(2-methyl-1-propyl)acetate			1.900				0.417	1.286	0.444
(2-methylbutyl)cyclohexane	0.005	0.014	0.001	0.015	0.021	0.020	0.012	0.001	0.011
(2-methylpropyl)cyclohexane	0.038	0.104	0.006	0.114	0.152	0.145	0.091	0.010	0.080
1,1,1-trichloroethane							0.306		0.154
1,1,2-trimethylcyclohexane	0.016	0.043	0.002	0.048	0.063	0.060	0.038	0.004	0.033
1,1,3-trimethylcyclohexane	0.018	0.049	0.003	0.054	0.072	0.068	0.043	0.004	0.038
1,1,4,4-tetramethylcyclohexane	0.011	0.030	0.002	0.033	0.045	0.042	0.027	0.003	0.023
1,1-dimethylcyclohexane	0.001	0.004	0.000	0.004	0.005	0.005	0.003	0.000	0.003
1,2,3,4-tetrahydro-naphthalene	0.007	0.018	0.001	0.020	0.027	0.026	0.016	0.002	0.014
1,2,3,4-tetramethylbenzene	0.708	0.054	0.027	0.615	0.133	0.085	0.292	0.655	0.312
1,2,3,5-tetramethylbenzene	1.764	0.061	0.027	1.509	0.142	0.094	0.585	1.639	0.681
1,2,3,5-tetramethylcyclohexane	0.018	0.048	0.003	0.053	0.070	0.067	0.042	0.004	0.037
1,2,3-trimethylbenzene	1.973	0.460	0.278	1.770	1.231	0.738	1.482	1.808	1.319
1,2,3-trimethylcyclohexane	0.033	0.090	0.005	0.099	0.132	0.125	0.079	0.008	0.069
1,2,3-trimethylcyclopentane	0.001	0.002	0.000	0.003	0.003	0.003	0.002	0.000	0.002
1,2,4,4-tetramethylcyclopentane	0.003	0.008	0.000	0.009	0.012	0.011	0.007	0.001	0.006
1,2,4,5-tetramethylbenzene	1.159	0.053	0.027	0.994	0.130	0.083	0.414	1.076	0.467
1,2,4-trimethylcyclopentane	0.000	0.001	0.000	0.001	0.002	0.002	0.001	0.000	0.001
1,2,4-trimethylbenzene	6.289	1.750	1.214	5.548	5.029	2.867	5.670	5.791	4.808
1,2,4-trimethylcyclohexane	0.010	0.028	0.002	0.031	0.041	0.039	0.025	0.003	0.021
1,2-dimethyl-3-isopropylcyclopentane	0.006	0.016	0.001	0.018	0.024	0.023	0.014	0.001	0.013
1,2-dimethylcyclohexane	0.008	0.022	0.001	0.024	0.033	0.031	0.020	0.002	0.017
1,2-ethanedioldiacetate							0.417		0.209
1,2-ethylmethylcyclopentane	0.001	0.004	0.000	0.004	0.005	0.005	0.003	0.000	0.003
1,3,5-trimethylbenzene	1.523	0.522	0.317	1.403	1.402	0.838	1.491	1.383	1.251
1,3-diethylbenzene	0.016	0.044	0.002	0.048	0.064	0.061	0.038	0.004	0.033

species	OEM	Refinishing	Wood	Coil	Marine	Heavy duty	Gen. industrial	Packaging	Manufacture
1,3-dimethyl-4-ethylbenzene	0.016	0.044	0.002	0.048	0.064	0.061	0.038	0.004	0.033
1,3-dimethyl-5-propylbenzene	0.002	0.005	0.000	0.006	0.008	0.007	0.005	0.000	0.004
1,3-dimethylcyclohexane	0.007	0.020	0.001	0.022	0.029	0.028	0.017	0.002	0.015
1,3-ethylmethylcyclopentane	0.001	0.002	0.000	0.003	0.003	0.003	0.002	0.000	0.002
1,3-propanediol		0.545			0.133			0.286	0.089
1,3-propanediol diacetate								1.300	0.100
1,4-diethylbenzene	0.016	0.045	0.002	0.049	0.065	0.062	0.039	0.004	0.034
1,4-dimethyl-2-isopropylbenzene	0.003	0.007	0.000	0.008	0.010	0.010	0.006	0.001	0.005
1,4-dimethylcyclohexane	0.018	0.050	0.003	0.055	0.074	0.070	0.044	0.005	0.039
1-butanol	4.000	2.000	4.889	1.667	3.333	2.182	3.048	7.200	3.438
1-ethoxy-2-propanol			0.500	2.400				1.300	0.175
1-ethoxy-2-propyl acetate		0.250	0.500	2.400					0.103
1-ethyl-1,4-dimethylcyclohexane	0.008	0.021	0.001	0.023	0.031	0.029	0.018	0.002	0.016
1-ethyl-2,2,6-trimethylcyclohexane	0.020	0.054	0.003	0.059	0.079	0.075	0.047	0.005	0.041
1-ethyl-2,3-dimethylbenzene	0.013	0.036	0.002	0.039	0.052	0.050	0.031	0.003	0.027
1-ethyl-2,3-dimethylcyclohexane	0.009	0.025	0.001	0.027	0.036	0.034	0.022	0.002	0.019
1-ethyl-2-propylbenzene	0.004	0.011	0.001	0.012	0.017	0.016	0.010	0.001	0.009
1-ethyl-2-propylcyclohexane	0.008	0.022	0.001	0.024	0.033	0.031	0.020	0.002	0.017
1-ethyl-3,5-dimethylbenzene	0.018	0.049	0.003	0.054	0.072	0.068	0.043	0.004	0.037
1-ethyl-3-methylcyclohexane	0.058	0.159	0.009	0.175	0.233	0.221	0.140	0.015	0.122
1-ethyl-4-methylcyclohexane	0.025	0.068	0.004	0.074	0.099	0.094	0.060	0.006	0.052
1-ethylpropylbenzene	0.005	0.013	0.001	0.014	0.019	0.018	0.012	0.001	0.010
1-methoxy-2-propanol	0.600	0.250		2.400		1.000	1.067		0.733
1-methoxy-2-propyl acetate	0.600	1.000		2.400	1.000	1.000	0.267		0.457
1-methyl-1-phenylcyclopropane	0.004	0.010	0.001	0.011	0.014	0.013	0.008	0.001	0.007
1-methyl-1-propylcyclopentane	0.010	0.027	0.001	0.030	0.039	0.037	0.024	0.002	0.021
1-methyl-2-isopropylbenzene	0.016	0.045	0.002	0.049	0.065	0.062	0.039	0.004	0.034
1-methyl-2-propylbenzene	0.019	0.052	0.003	0.058	0.077	0.073	0.046	0.005	0.040
1-methyl-3-(isopropyl)benzene	0.019	0.052	0.003	0.058	0.077	0.073	0.046	0.005	0.040
1-methyl-3-isopropylcyclopentane	0.000	0.001	0.000	0.001	0.002	0.002	0.001	0.000	0.001

species	OEM	Refinishing	Wood	Coil	Marine	Heavy duty	Gen. industrial	Packaging	Manufacture
1-methyl-3-propylbenzene	0.038	0.104	0.006	0.114	0.152	0.145	0.091	0.010	0.080
1-methyl-4-isopropylbenzene	0.065	0.178	0.010	0.196	0.261	0.248	0.157	0.016	0.137
1-methyl-4-isopropylcyclohexane	0.068	0.184	0.010	0.203	0.270	0.257	0.162	0.017	0.142
1-methyl-4-tertbutylbenzene	0.011	0.030	0.002	0.033	0.044	0.041	0.026	0.003	0.023
1-methylbutylbenzene	0.011	0.029	0.002	0.032	0.042	0.040	0.025	0.003	0.022
1-methylindan	0.005	0.013	0.001	0.014	0.019	0.018	0.012	0.001	0.010
1-methylindene	0.000	0.001	0.000	0.001	0.002	0.002	0.001	0.000	0.001
2,2,3,3-tetramethylhexane	0.026	0.070	0.004	0.077	0.103	0.098	0.062	0.006	0.054
2,2,5-trimethylhexane	0.002	0.005	0.000	0.005	0.007	0.007	0.004	0.000	0.004
2,3 dimethylbutane	0.010	0.109	0.024			0.038	0.024	0.010	0.030
2,3,3,4-tetramethylpentane	0.000	0.001	0.000	0.001	0.002	0.002	0.001	0.000	0.001
2,3,4-trimethylhexane	0.002	0.005	0.000	0.005	0.007	0.007	0.004	0.000	0.004
2,3,5-trimethylhexane	0.000	0.001	0.000	0.001	0.002	0.002	0.001	0.000	0.001
2,3-dimethylheptane	0.022	0.060	0.003	0.065	0.087	0.083	0.052	0.005	0.046
2,3-dimethylnonane	0.016	0.044	0.002	0.049	0.065	0.062	0.039	0.004	0.034
2,3-dimethyloctane	0.007	0.019	0.001	0.021	0.027	0.026	0.016	0.002	0.014
2,3-dimethylundecane	0.004	0.011	0.001	0.012	0.015	0.015	0.009	0.001	0.008
2,4-dimethyl-1-(1-methylethyl)benzene	0.013	0.035	0.002	0.038	0.051	0.049	0.031	0.003	0.027
2,4-dimethylheptane	0.003	0.009	0.001	0.010	0.014	0.013	0.008	0.001	0.007
2,5-dimethyldecane	0.009	0.023	0.001	0.026	0.034	0.033	0.021	0.002	0.018
2,5-dimethylheptane	0.010	0.028	0.002	0.031	0.041	0.039	0.025	0.003	0.021
2,5-dimethylhexane	0.000	0.001	0.000	0.001	0.002	0.002	0.001	0.000	0.001
2,5-dimethyloctane	0.027	0.075	0.004	0.082	0.110	0.104	0.066	0.007	0.057
2,6-dimethyldecane	0.011	0.029	0.002	0.032	0.043	0.041	0.026	0.003	0.022
2,6-dimethylheptane	0.011	0.030	0.002	0.033	0.045	0.042	0.027	0.003	0.023
2,6-dimethyloctane	0.082	0.223	0.012	0.245	0.327	0.311	0.196	0.020	0.171
2,6-dimethylundecane	0.003	0.007	0.000	0.008	0.010	0.010	0.006	0.001	0.005
2,7-dimethyloctane	0.016	0.044	0.002	0.049	0.065	0.062	0.039	0.004	0.034
2-(1-hexoxy)ethanol								1.300	0.100
2-(2-butoxyethoxy)ethanol	0.600			2.400			0.267	1.300	0.347

species	OEM	Refinishing	Wood	Coil	Marine	Heavy duty	Gen. industrial	Packaging	Manufacture
2-(2-butoxyethoxy)ethyl acetate				2.400					0.039
2-(2-ethoxyethoxy)ethanol				2.400			0.267	1.300	0.273
2-(2-ethoxyethoxy)ethyl acetate				2.400					0.039
2-butanol		0.500	1.222	1.667		0.545	3.048	1.800	1.870
2-butanone	5.167	4.449	6.000			1.333	2.560	5.091	3.319
2-butanone oxime	0.400	0.545			0.133		0.216		0.225
2-butoxyethanol	0.600	1.000	0.500	2.400			1.067	1.300	0.897
2-butoxyethyl acetate	0.600	0.250		2.400			0.267	1.300	0.375
2-c9-unidentifiediso-paraffins	0.001	0.002	0.000	0.003	0.003	0.003	0.002	0.000	0.002
2-ethoxyethanol		0.250	0.500	2.400	1.000	1.000	0.267	1.300	0.434
2-ethoxyethyl acetate				9.600	1.000	1.000	0.267	1.300	0.488
2-ethyl-1,3-dimethylbenzene	0.021	0.057	0.003	0.062	0.083	0.079	0.050	0.005	0.044
2-methyl-1-butylbenzene	0.001	0.003	0.000	0.004	0.005	0.005	0.003	0.000	0.003
2-methyl-1-propanol	1.000	2.000	4.889	1.667		0.545	3.048	1.800	2.425
2-methyl-2,4-pentanediol	0.400	0.545			0.133			0.286	0.138
2-methyl-5-ethyloctane	0.023	0.062	0.003	0.068	0.091	0.086	0.054	0.006	0.047
2-methyldecalin	0.016	0.043	0.002	0.048	0.063	0.060	0.038	0.004	0.033
2-methyldecane	0.065	0.177	0.010	0.195	0.260	0.247	0.156	0.016	0.136
2-methylheptane	0.003	0.009	0.001	0.010	0.014	0.013	0.008	0.001	0.007
2-methylnonane	0.087	0.238	0.013	0.262	0.349	0.332	0.210	0.022	0.183
2-methyloctane	0.030	0.082	0.004	0.090	0.120	0.114	0.072	0.007	0.063
2-methylpentane	0.100	1.091	0.240			0.380	0.240	0.100	0.302
2-methylundecane	0.011	0.029	0.002	0.032	0.043	0.041	0.026	0.003	0.022
2-propanol	1.000	2.000	4.889	1.667	0.833	0.545	0.762	1.800	1.312
2-propyl acetate		0.278	1.900				0.577	1.286	0.556
3,3,4-trimethylhexane	0.000	0.001	0.000	0.001	0.002	0.002	0.001	0.000	0.001
3,3,5-trimethylheptane	0.002	0.006	0.000	0.006	0.009	0.008	0.005	0.001	0.004
3,3-dimethylheptane	0.003	0.007	0.000	0.008	0.010	0.010	0.006	0.001	0.005
3,3-dimethyloctane	0.023	0.063	0.003	0.069	0.092	0.088	0.055	0.006	0.048
3,4-dimethylheptane	0.027	0.074	0.004	0.081	0.108	0.102	0.065	0.007	0.056

species	OEM	Refinishing	Wood	Coil	Marine	Heavy duty	Gen. industrial	Packaging	Manufacture
3,4-dimethylhexane	0.000	0.001	0.000	0.001	0.002	0.002	0.001	0.000	0.001
3,5-dimethyloctane	0.007	0.020	0.001	0.022	0.029	0.028	0.017	0.002	0.015
3,6,9-trioxa-1-undecanol								1.300	0.100
3,6-dimethyloctane	0.020	0.055	0.003	0.060	0.080	0.076	0.048	0.005	0.042
3,7-dimethylnonane	0.023	0.062	0.003	0.068	0.091	0.086	0.054	0.006	0.047
3-ethyl-2-methylheptane	0.099	0.270	0.015	0.297	0.395	0.376	0.237	0.025	0.207
3-ethyl-2-methylhexane	0.002	0.005	0.000	0.005	0.007	0.007	0.004	0.000	0.004
3-ethylheptane	0.022	0.060	0.003	0.065	0.087	0.083	0.052	0.005	0.046
3-ethylhexane	0.000	0.001	0.000	0.001	0.002	0.002	0.001	0.000	0.001
3-ethyloctane	0.017	0.047	0.003	0.051	0.068	0.065	0.041	0.004	0.036
3-ethyltoluene	0.059	0.160	0.009	0.176	0.234	0.223	0.141	0.015	0.123
3-methyldecane	0.073	0.200	0.011	0.220	0.293	0.278	0.176	0.018	0.153
3-methylheptane	0.003	0.007	0.000	0.008	0.010	0.010	0.006	0.001	0.005
3-methylhexane	0.000	0.001	0.000	0.001	0.002	0.002	0.001	0.000	0.001
3-methylnonane	0.101	0.275	0.015	0.303	0.404	0.384	0.242	0.025	0.211
3-methyloctane	0.027	0.074	0.004	0.081	0.108	0.102	0.065	0.007	0.056
3-methylpentane	0.090	0.982	0.216			0.342	0.216	0.090	0.272
3-methylundecane	0.012	0.034	0.002	0.037	0.050	0.047	0.030	0.003	0.026
4,4-dimethylheptane	0.001	0.002	0.000	0.003	0.003	0.003	0.002	0.000	0.002
4,5-dimethylnonane	0.016	0.043	0.002	0.048	0.063	0.060	0.038	0.004	0.033
4,6-dimethylindan	0.002	0.004	0.000	0.005	0.006	0.006	0.004	0.000	0.003
4,7-dimethylindan	0.001	0.002	0.000	0.002	0.003	0.002	0.002	0.000	0.001
4,8-dioxa-1-dodecane							0.267		0.134
4-ethyl-1,2-dimethylbenzene	0.014	0.038	0.002	0.042	0.056	0.054	0.034	0.004	0.029
4-ethyloctane	0.008	0.021	0.001	0.023	0.031	0.029	0.018	0.002	0.016
4-ethyltoluene	0.024	0.066	0.004	0.073	0.097	0.092	0.058	0.006	0.051
4-methyl-1,3-dioxol-2-one				0.167	0.133				0.008
4-methyl-2-pentanol		0.500							0.056
4-methyl-2-pentanone	20.667	3.580	6.000		1.500	1.333	0.560	5.091	4.184
4-methyl-4-hydroxy-2-pentanone	1.000	0.500	1.222	1.667		0.545	3.048	1.800	1.993

species	OEM	Refinishing	Wood	Coil	Marine	Heavy duty	Gen. industrial	Packaging	Manufacture
4-methyldecane	0.122	0.334	0.018	0.367	0.490	0.465	0.294	0.031	0.256
4-methylheptane	0.001	0.004	0.000	0.004	0.005	0.005	0.003	0.000	0.003
4-methylnonane	0.069	0.188	0.010	0.207	0.276	0.262	0.165	0.017	0.144
4-methyloctane	0.031	0.084	0.005	0.092	0.123	0.117	0.074	0.008	0.064
4-propylheptane	0.001	0.004	0.000	0.004	0.005	0.005	0.003	0.000	0.003
5-methyl-2-hexanone			1.500				0.500		0.359
5-methyldecane	0.033	0.090	0.005	0.099	0.132	0.125	0.079	0.008	0.069
5-methylundecane	0.010	0.028	0.002	0.031	0.041	0.039	0.025	0.003	0.021
6-ethyl-2-methyldecane	0.001	0.004	0.000	0.004	0.005	0.005	0.003	0.000	0.003
6-ethyl-2-methyloctane	0.004	0.011	0.001	0.012	0.015	0.015	0.009	0.001	0.008
6-methylundecane	0.008	0.022	0.001	0.024	0.033	0.031	0.020	0.002	0.017
8-methyl-1-nonanol							0.762		0.383
acetone	5.167	4.171	6.000				2.400	1.273	2.838
benzyl alcohol						0.545		1.800	0.169
bis(2-hydroxyethyl)ether				0.167	0.133				0.008
butoxyl		1.250							0.141
butyl acetate	3.200	5.000	7.600		1.000		1.667	1.286	2.479
butyl glycolate		1.250							0.141
butyl lactate		1.250							0.141
butylbenzene	0.017	0.045	0.002	0.050	0.067	0.063	0.040	0.004	0.035
butylcyclohexane	0.064	0.175	0.010	0.193	0.257	0.244	0.154	0.016	0.134
butyrolactone				0.167	0.133			0.286	0.030
C ₁₀ -cyclo-paraffin	0.076	0.208	0.011	0.229	0.305	0.289	0.183	0.019	0.159
C ₁₀ -iso-paraffin	0.060	0.165	0.009	0.181	0.241	0.229	0.145	0.015	0.126
C ₁₁ -aromatic	0.001	0.002	0.000	0.002	0.003	0.002	0.002	0.000	0.001
C ₁₁ -cyclo-paraffin	0.005	0.014	0.001	0.015	0.021	0.020	0.012	0.001	0.011
C ₁₁ -iso-paraffin	0.071	0.193	0.011	0.212	0.282	0.268	0.169	0.018	0.148
C ₁₁ -unidentified	0.003	0.008	0.000	0.009	0.012	0.011	0.007	0.001	0.006
C ₁₂ -cyclo-paraffin	0.002	0.006	0.000	0.006	0.009	0.008	0.005	0.001	0.004
C ₁₂ -iso-paraffin	0.023	0.062	0.003	0.068	0.091	0.086	0.054	0.006	0.047

species	OEM	Refinishing	Wood	Coil	Marine	Heavy duty	Gen. industrial	Packaging	Manufacture
C ₁₃ -iso-paraffin	0.000	0.001	0.000	0.001	0.002	0.002	0.001	0.000	0.001
C ₉ -cyclo-paraffin	0.004	0.012	0.001	0.013	0.017	0.016	0.010	0.001	0.009
C ₉ -iso-paraffin	0.003	0.009	0.001	0.010	0.014	0.013	0.008	0.001	0.007
coeluting-2-aromatics-1-iso-paraffin	0.006	0.018	0.001	0.019	0.026	0.024	0.015	0.002	0.013
coeluting aromatic, cyclo-and iso-paraffin	0.003	0.009	0.001	0.010	0.014	0.013	0.008	0.001	0.007
coeluting aromatic and iso-paraffin	0.009	0.023	0.001	0.026	0.034	0.033	0.021	0.002	0.018
cyclo-paraffin	0.003	0.007	0.000	0.008	0.010	0.010	0.006	0.001	0.005
cycloheptane	0.000	0.001	0.000	0.001	0.002	0.002	0.001	0.000	0.001
cyclohexane	0.095	1.036	0.228			0.361	0.228	0.095	0.287
cyclohexanol							0.762		0.383
cyclohexanone		0.869	1.500	0.600	1.500	1.333	0.500	1.273	0.701
decalin	0.022	0.061	0.003	0.067	0.089	0.085	0.053	0.006	0.047
decane	0.402	1.096	0.060	1.206	1.608	1.527	0.965	0.100	0.841
dichloromethane		0.636					0.306		0.225
diethyl ketone		0.834					0.480		0.335
diethylbenzene	0.593	0.093	0.077	0.499	0.295	0.157	0.401	0.553	0.362
dimethyl esters				3.000					0.049
dimethylcyclohexane	0.045	0.491	0.108			0.171	0.108	0.045	0.136
dimethylformamide				0.167	0.133			0.286	0.030
dimethylnonane	0.009	0.023	0.001	0.026	0.034	0.033	0.021	0.002	0.018
dimethylpentane	0.045	0.491	0.108			0.171	0.108	0.045	0.136
dodecane	0.024	0.067	0.004	0.073	0.098	0.093	0.059	0.006	0.051
ethanol	1.000	0.500	4.889	1.667	0.833	0.545	0.762	1.800	1.143
ethyl acetate	0.800	1.667	7.600				1.907	5.143	2.184
ethyl hexanol	1.000								0.123
ethyl lactate							0.417		0.209
ethylbenzene	2.779	3.545	2.935	2.361	11.237	5.991	3.051	2.587	3.519
ethylcyclohexane	0.023	0.063	0.003	0.069	0.092	0.088	0.055	0.006	0.048
ethyldimethylbenzene	4.783	0.324	0.270	4.030	1.032	0.549	2.145	4.464	2.203
ethylisopropylbenzene	0.001	0.002	0.000	0.002	0.003	0.002	0.002	0.000	0.001

species	OEM	Refinishing	Wood	Coil	Marine	Heavy duty	Gen. industrial	Packaging	Manufacture
heptane	0.096	1.039	0.228	0.003	0.003	0.364	0.230	0.095	0.289
hexane	0.260	2.836	0.624			0.988	0.624	0.260	0.785
hexylcyclohexane	0.000	0.001	0.000	0.001	0.002	0.002	0.001	0.000	0.001
indan	0.316	0.040	0.002	0.298	0.059	0.056	0.118	0.285	0.135
isopentylbenzene	0.003	0.007	0.000	0.008	0.010	0.010	0.006	0.001	0.005
isopropylbenzene	0.016	0.044	0.002	0.048	0.064	0.061	0.038	0.004	0.033
isophorone				2.400			0.500	1.273	0.388
limonene	0.400	0.545			0.133		0.216	0.286	0.247
m-xylene	7.624	9.700	8.068	6.442	30.833	16.409	8.349	7.110	9.641
methanol	1.000					0.545	0.762		0.536
methyl indane	0.602			0.507			0.165	0.562	0.208
methylcyclodecane	0.003	0.009	0.001	0.010	0.014	0.013	0.008	0.001	0.007
methylcyclohexane	0.039	0.392	0.085	0.012	0.015	0.148	0.093	0.036	0.114
methylcyclopentane	0.065	0.709	0.156			0.247	0.156	0.065	0.196
methylethylbenzene	4.974	1.389	1.158	4.191	4.421	2.351	4.947	4.643	4.074
methylhexane	0.160	1.745	0.384			0.608	0.384	0.160	0.483
methylpropylbenzene	1.938	0.185	0.154	1.633	0.589	0.313	1.008	1.808	0.984
methyltetralin	0.001	0.003	0.000	0.003	0.004	0.004	0.002	0.000	0.002
n-methyl pyrrolidone				0.167	0.133				0.008
naphthalene	0.755	0.006	0.000	0.641	0.009	0.009	0.211	0.703	0.265
nitropentane					0.133		0.216		0.114
nonane	0.232	0.633	0.035	0.696	0.928	0.882	0.557	0.058	0.485
o-xylene	1.684	2.172	1.763	1.466	6.808	3.657	1.870	1.556	2.146
octahydro-indan	0.012	0.032	0.002	0.035	0.046	0.044	0.028	0.003	0.024
octane	0.017	0.046	0.003	0.050	0.067	0.063	0.040	0.004	0.035
organic amines					0.133		0.216		0.114
p-xylene	1.808	2.308	1.908	1.540	7.311	3.900	1.987	1.682	2.291
pentylbenzene	0.001	0.002	0.000	0.002	0.003	0.002	0.002	0.000	0.001
pentylcyclohexane	0.016	0.043	0.002	0.048	0.063	0.060	0.038	0.004	0.033
phenol				0.167	0.133		0.216		0.117

species	OEM	Refinishing	Wood	Coil	Marine	Heavy duty	Gen. industrial	Packaging	Manufacture
pine oil	0.400				0.133			0.286	0.077
propyl acetate		0.174					0.100		0.070
propylbenzene	0.619	0.285	0.160	0.601	0.735	0.452	0.725	0.553	0.592
propylcyclohexane	0.083	0.228	0.013	0.250	0.334	0.317	0.200	0.021	0.175
propylcyclopentane	0.000	0.001	0.000	0.001	0.002	0.002	0.001	0.000	0.001
propylene oxide					0.133			0.286	0.027
styrene							3.786		1.901
tertbutylcyclopropane	0.000	0.001	0.000	0.001	0.002	0.002	0.001	0.000	0.001
tertpentylbenzene	0.006	0.017	0.001	0.019	0.026	0.024	0.015	0.002	0.013
tetramethylcyclohexane	0.012	0.034	0.002	0.037	0.050	0.047	0.030	0.003	0.026
texanol	0.400				0.133				0.055
toluene	3.464	17.603	14.667	0.008	0.010	29.788	15.149	3.231	12.995
trichloroethene							0.306		0.154
undecane	0.210	0.573	0.032	0.630	0.841	0.799	0.504	0.053	0.440
unidentified C ₈ -paraffin	0.000	0.001	0.000	0.001	0.002	0.002	0.001	0.000	0.001
unidentified iso-paraffin	0.005	0.014	0.001	0.015	0.021	0.020	0.012	0.001	0.011
unspeciated	0.005	0.013	0.001	0.015	0.020	0.019	0.012	0.001	0.010

Table 1.4 Species profile for refineries

species	%
2,2,3,3-tetramethylbutane	0.03
2,2,3-trimethylbutane	0.78
2,2,3-trimethylpentane	0.03
2,2,4-trimethylpentane	0.03
2,2-dimethylbutane	1.39
2,2-dimethylhexane	0.03
2,2-dimethylpentane	0.78
2,3,3-trimethylpentane	0.03
2,3-dimethylbutane	1.39
2,3-dimethylhexane	0.03
2,3-dimethylpentane	0.78
2,4-dimethylhexane	0.03
2,4-dimethylpentane	0.78
2,5-dimethylhexane	0.03
2-methylbutane	6.13
2-methylheptane	0.03
2-methylhexane	0.78
2-methylpentane	1.39
2-methylpropane	10.16
3,3-dimethylhexane	0.03
3,3-dimethylpentane	0.78
3,4-dimethylhexane	0.03
3-ethyl-2-methylpentane	0.03
3-methylheptane	0.03
3-methylhexane	0.78
3-methylpentane	1.39
4-methylheptane	0.03
benzene	2.86
butane	22.72
ethane	2.99
heptane	2.19
hexane	5.18
neopentane	6.13
octane	0.03
pentane	11.06
propane	17.64
toluene	1.49

Table 1.5 Species profile for petroleum processes

species	%
1,2,3-trimethylcyclopentane	0.07
1,2,4-trimethylcyclopentane	0.07
1,2-dimethylcyclohexane	0.07
1,2-dimethylcyclopentane	0.44
1,3-dimethylcyclohexane	0.07
1,3-dimethylcyclopentane	0.44
1,4-dimethylcyclohexane	0.07
1-ethyl-2-methylcyclopentane	0.07
1-ethyl-3-methylcyclopentane	0.07
2,2,3,3-tetramethylbutane	0.80
2,2,3-trimethylbutane	1.99
2,2,3-trimethylpentane	0.80
2,2,4-trimethylpentane	0.80
2,2-dimethylbutane	2.72
2,2-dimethylhexane	0.80
2,2-dimethylpentane	1.99
2,3,3-trimethylpentane	0.80
2,3-dimethylbutane	2.72
2,3-dimethylhexane	0.80
2,3-dimethylpentane	1.99
2,4-dimethylhexane	0.80
2,4-dimethylpentane	1.99
2,5-dimethylhexane	0.80
2-methylbutane	2.57
2-methylheptane	0.80
2-methylhexane	1.99
2-methylpentane	2.72
2-methylpropane	0.55
3,3-dimethylhexane	0.80
3,3-dimethylpentane	1.99
3,4-dimethylhexane	0.80
3-ethyl-2-methylpentane	0.80
3-methylheptane	0.80
3-methylhexane	1.99
3-methylpentane	2.72
4-methylheptane	0.80
benzene	14.37
butane	10.17
cycloheptane	0.44
cyclooctane	0.07
ethane	8.80
ethylcyclohexane	0.07
ethylcyclopentane	0.44
heptane	1.99
hexane	2.72
isopropylcyclopentane	0.07
methylcycloheptane	0.07

species	%
methylcyclohexane	0.44
neopentane	2.57
octane	0.80
pentane	2.57
propane	13.88
propylcyclopentane	0.07

Table 1.6 Species profile for chemicals manufacturing

species	%
1,1,1-trichloroethane	0.349
1,1-dichloroethene	0.141
1,1-dichloroethene	0.070
1,2-dichlorobenzene	0.001
1,2-dichloroethane	2.017
1,3-butadiene	4.638
1-butanol	0.798
1-butene	0.718
1-chloro-2,3-epoxypropane	0.015
1-chloro-4-nitrobenzene	0.029
1-propanol	0.996
2-butanol	0.569
2-butanone	1.629
2-butene	0.718
2-methyl-1-propanol	0.019
2-methyl-2-butene	0.015
2-methyl-2-propanol	0.569
2-propanol	1.948
2-propyl acetate	0.104
3A,4,7,7A-tetrahydro-4,7-methanoindene	0.001
4-methyl-2-pentanone	1.014
acetaldehyde	0.488
acetic acid	1.516
acetic anhydride	0.179
acetone	4.824
acetyl chloride	0.001
acetylene	0.753
A-chlorotoluene	0.002
acrylic acid	0.004
acrylonitrile	1.297
adiponitrile	0.288
aniline	0.117
benzene	2.976
bromoethene	0.002
bromomethane	0.135
butane	0.512
butyl acetate	0.098
chlorobenzene	0.044

species	%
chloroethane	3.524
chloroethane	0.089
chloroethene	0.952
chloroethene	0.191
chloromethane	1.141
chloroprene	0.695
cyclohexane	0.441
cyclohexanol	0.219
cyclohexanone	0.220
dichlorobenzene	0.034
dichloromethane	2.723
difluoromethane	0.031
diisopropyl ether	0.290
dimethyl ether	0.004
ethane	1.108
ethanol	2.988
ethanolamine	0.025
ethyl acetate	0.479
ethylbenzene	0.059
ethylene	9.561
ethylene glycol	0.995
ethylene oxide	0.618
formaldehyde	1.696
formanilide	0.051
glycerol	0.001
hexamethylenediamine	0.013
iodomethane	0.001
isopropanolamine	0.025
isopropylbenzene	0.258
maleic anhydride	0.422
methacrylic acid	0.029
methanol	4.477
methyl acetate	7.253
methyl acrylate	0.011
methyl formate	0.027
methylpropene	0.718
N,N-dimethylformamide	0.104
naphthalene	0.088
nitrobenzene	0.008
o-xylene	0.088
pentafluoroethane	0.001
pentane	0.898
phenol	0.385
phenylacetonitrile	0.001
propane	1.423
propylene	4.705
propylene oxide	0.061
p-xylene	3.465
styrene	3.061

species	%
tert-butylamine	0.004
tetrachloroethene	0.781
tetrafluoroethene	0.046
tetrahydrofuran	0.168
toluene	2.540
trichloroethene	0.355
trichloromethane	0.128
trifluoroethene	0.001
trifluoromethane	0.001
unspeciated hydrocarbons	6.204
vinyl acetate	0.306
xylenes	4.219

Appendix 2

Species profiles for solvent mixtures

The following species profiles have been used for solvents, which are mixtures of compounds. The profiles have been provided by solvent suppliers.

Table 2.1 Composition of SBP solvents

Component	SBP 65/70	SBP 80/110
2,3-dimethyl butane	2%	
2-methyl pentane	20%	
3-methyl pentane	18%	
n-hexane	49%	3%
methylcyclopentane	8%	5%
cyclohexane	3%	16%
dimethylpentanes		9%
methylhexanes		32%
n- heptane		19%
dimethylcyclopentane		9%
methylcyclohexane		7%

Table 2.2 Composition of aromatic hydrocarbon solvents

Component	160–180°C b.p.	180–220°C b.p.
propyl benzene	4%	
methyl ethyl benzene	30%	4%
1,3,5-trimethyl benzene	8%	2%
1,2,4-trimethyl benzene	31%	11%
1,2,3-trimethyl benzene	7%	6%
diethyl benzene	2%	2%
methyl propyl benzene	4%	9%
ethyl dimethyl benzene	7%	25%
indane		2%
tetramethyl benzenes	2%	
1,2,4,5-tetramethyl benzene		7%
1,2,3,5-tetramethyl benzene		11%
1,2,3,4-tetramethyl benzene		4%
methyl indane		4%
naphthalene		5%

Table 2.3 Composition of Bisol K

Component	Bisol K
acetone	20%
ethyl acetate	12%
2-propyl acetate	8%
propyl acetate	5%
2-butanone	28%
4-methyl-2-pentanone	3%
diethyl ketone	24%

Appendix 3

Solvent use in printing

Information received from the BCF on solvents used in printing is tabulated below.

End use/application process category	VOC mix at application (average for the category)	% breakdown	
1	Heatset web offset	high boiling naphthenic and petroleum distillates	100
2	Sheetfed offset lithography	none	-
3	Coldset offset lithography	none	-
4	Letterpress	none	-
5	Publication gravure	toluene low boiling aliphatic distillates	60 40
6	Non-publication gravure	ethanol ethyl acetate iso-propyl acetate n-propyl acetate low boiling aliphatic distillates n-propanol iso-propanol methyl ethyl ketone glycol ethers	50 22 8 8 4 2 2 2 2
7	Flexography	ethanol ethyl acetate n-propanol glycol ethers iso-propanol iso-propyl acetate n-propyl acetate	60 12 8 8 5 4 3
8	Screen printing	aromatic hydrocarbons glycol ethers and glycol ether esters cyclohexanone others (e.g. pentoxone, GBA)	50 30 10 10

This information was used to generate the species profiles listed below.

1. Heatset web offset

No information is available on the speciation of the high boiling point distillates used although the Intergraf report (1999) gives a boiling range of 240–270°C and lists the solvents as aromatic free. For the time being the solvent is assumed to be tetradecane (boiling point of 254°C)

2. Publication gravure

The profile is based on the BCF data assuming that the low boiling point aliphatic distillate is SBP 65/70 (see profile in Appendix 2)

3. Non publication gravure

The profile is based on the BCF data, however a couple of assumptions have to be made. The low boiling point aliphatic distillate is assumed to be SBP 65/70 (see profile in Appendix 2). The glycol ethers are assumed to be equal quantities of 1-methoxy-2-propanol and 1-ethoxy-2-propanol (these solvents are given as typical glycol ethers used in packaging gravure inks in the Intergraf report).

4 Flexography

The profile is based on the BCF data, however the glycol ethers are assumed to equal quantities of 1-methoxy-2-propanol and 1-ethoxy-2-propanol (these solvents are given as typical glycol ethers used in flexography inks in the Intergraf report).

5 Screen printing

The profile is based on the BCF data. The aromatic hydrocarbons are assumed to be equal quantities of toluene and solvent xylene. The glycol ethers are assumed to be equal quantities of 1-methoxy-2-propanol, 1-methoxy-2-propylacetate and 2-butoxyethanol which are given in the Intergraf report as solvents in screen inks.

All of the profiles are for SNAP code 060403 and therefore further information on the emissions from each type of printing process is necessary in order for the profiles to be used accurately.

Reference

Intergraf, Printing and the Environment: Guidance on Best Available Techniques (BAT) in Printing Industries, January 1999

Appendix 4

POCP Values

POCP values for chemical species that are currently contained in the NAEI species database are given in the table below. In this table the methods given are as follows:

1. POCPs determined by the standard methodology using a photochemical trajectory model containing fully developed chemical schemes and NAEI speciated VOC emissions. The values are published in the open literature (Derwent *et al*, 1998; Jenkin & Hayman, 1999).
2. POCPs estimated by a documented methodology. This allows assignment of POCPs on the basis of consideration of how the values determined using the standard methodology vary with structure and reactivity, i.e. this method is optimised on the basis of the determined values, and then used to calculate POCPs for additional VOCs within the same classes (i.e., hydrocarbons, oxygenates and halocarbons). The methodology is described more fully elsewhere (Jenkin, 1998; Jenkin *et al*, 1997)
3. POCPs which have been assigned on the basis of an educated guess.

POCP values have also been calculated for species found in kerosene, although the kerosene speciation has not yet been incorporated in the database. These POCP values are given in appendix 5.

species	POCP	Method	reference (if 1)
(1-methylethyl)cyclohexane	40.5	2	
(1-methylpropyl)cyclohexane	38.5	2	
(2-methyl-1-propyl)acetate	32.8	2	
(2-methylbutyl)cyclohexane	39.8	2	
(2-methylpropyl)cyclohexane	42.7	2	
1,1,1-trichloroethane	0.9	1	Derwent et al., 1998
1,1,1-trichlorotrifluoroethane	0.0	1	By definition
1,1,2-trimethylcyclohexane	41.2	2	
1,1,3-trimethylcyclohexane	41.2	2	
1,1,4,4-tetramethylcyclohexane	34.3	2	
1,1-dichloroethane	9.4	2	
1,1-dichloroethene	52.6	2	
1,1-dichlorotetrafluoroethane	0.0	1	By definition
1,1-dimethylcyclohexane	42.8	2	
1,2,3,4-tetrahydro-naphthalene	115.1	2	
1,2,3,4-tetramethylbenzene	114.6	2	
1,2,3,5-tetramethylbenzene	136.0	2	

species	POCP	Method	reference (if 1)
1,2,3,5-tetramethylcyclohexane	42.7	2	
1,2,3-trimethylbenzene	126.7	1	Derwent et al., 1998
1,2,3-trimethylcyclohexane	45.4	2	
1,2,3-trimethylcyclopentane	43.6	2	
1,2,4,4-tetramethylcyclopentane	37.5	2	
1,2,4,5-tetramethylbenzene	114.6	2	
1,2,4-trimethylcyclopentane	43.6	2	
1,2,4-trimethylbenzene	127.8	1	Derwent et al., 1998
1,2,4-trimethylcyclohexane	45.4	2	
1,2-dichlorobenzene	12.0	2	
1,2-dichloroethane	7.0	2	
1,2-dichloroethene	42.0	1	Derwent et al., 1998 (mean of cis/trans)
1,2-dichlorotetrafluoroethane	0.0	1	By definition
1,2-dimethyl-3-isopropylcyclopentane	39.3	2	
1,2-dimethylcyclohexane	48.2	2	
1,2-dimethylcyclopentane	45.9	2	
1,2-ethanedioldiacetate	16.0	2	
1,2-ethylmethylcyclopentane	44.2	2	
1,3,5-trimethylbenzene	138.1	1	Derwent et al., 1998
1,3-butadiene	85.1	1	Derwent et al., 1998
1,3-diethylbenzene	104.1	2	
1,3-dimethyl-4-ethylbenzene	114.6	2	
1,3-dimethyl-5-propylbenzene	132.5	2	
1,3-dimethylcyclohexane	48.2	2	
1,3-dimethylcyclopentane	45.9	2	
1,3-dioxolane	50.9	2	
1,3-ethylmethylcyclopentane	44.2	2	
1,3-propanediol	44.6	2	
1,3-propanediol diacetate	14.3	2	
1,4-diethylbenzene	89.6	2	
1,4-dimethyl-2-isopropylbenzene	111.7	2	
1,4-dimethylcyclohexane	48.2	2	
1-butanol	62.0	1	Jenkin and Hayman 1999
1-butene	107.9	1	Derwent et al., 1998
1-chloro-2,3-epoxypropane	10.2	2	
1-chloro-4-nitrobenzene	0.0	3	
1-decene	91.7	2	
1-ethoxy-2-propanol	49.7	2	
1-ethoxy-2-propyl acetate	35.2	2	
1-ethyl-1,4-dimethylcyclohexane	38.7	2	
1-ethyl-2,2,6-trimethylcyclohexane	37.2	2	
1-ethyl-2,3-dimethylbenzene	114.6	2	
1-ethyl-2,3-dimethylcyclohexane	42.3	2	
1-ethyl-2-propylbenzene	86.2	2	
1-ethyl-2-propylcyclohexane	40.0	2	
1-ethyl-3,5-dimethylbenzene	136.0	2	
1-ethyl-3-methylcyclohexane	45.6	2	
1-ethyl-4-methylcyclohexane	45.6	2	

species	POCP	Method	reference (if 1)
1-ethylpropylbenzene	105.7	3	
1-hexene	87.4	1	Derwent et al., 1998
1-methoxy-2-propanol	35.5	1	Jenkin and Hayman 1999
1-methoxy-2-propyl acetate	32.3	2	
1-methyl-1-phenylcyclopropane	63.7	3	
1-methyl-1-propylcyclohexane	38.5	2	
1-methyl-1-propylcyclopentane	37.9	2	
1-methyl-2-isopropylbenzene	88.4	2	
1-methyl-2-propylbenzene	88.4	2	
1-methyl-3-(isopropyl)benzene	104.1	2	
1-methyl-3-isopropylcyclopentane	39.1	2	
1-methyl-3-propylbenzene	104.1	2	
1-methyl-4-isopropylbenzene	89.6	2	
1-methyl-4-isopropylcyclohexane	43.0	2	
1-methyl-4-tertbutylbenzene	87.3	2	
1-methylbutylbenzene	105.7	3	
1-methylindan	80.0	2	
1-methylindene	136.2	3	
1-nonene	95.6	2	
1-pentanol	59.5	2	
1-pentene	97.7	1	Derwent et al., 1998
1-propanol	56.1	1	Jenkin and Hayman 1999
2 & 3 methylhexane	38.8	3	
2-(1-hexoxy)ethanol	44.7	2	
2-(2-aminoethylamino)ethanol	51.3	3	
2-(2-butoxyethoxy)ethanol	50.2	2	
2-(2-butoxyethoxy)ethyl acetate	40.0	2	
2-(2-ethoxyethoxy)ethanol	49.3	2	
2-(2-ethoxyethoxy)ethyl acetate	34.6	2	
2,2,3,3-tetramethylhexane	19.2	2	
2,2,3-trimethylbutane	38.6	2	
2,2,5-trimethylhexane	37.6	2	
2,2-dimethylbutane	24.1	1	Derwent et al., 1998
2,2-dimethylpentane	38.6	2	
2,2-dimethylpropane	17.3	1	Derwent et al., 1998
2,2'-iminodi(ethylamine)	51.3	3	
2,2'-iminodiethanol	51.3	3	
2,3,3,4-tetramethylpentane	37.2	2	
2,3,4-trimethylhexane	42.9	2	
2,3,5-trimethylhexane	42.6	2	
2,3-dimethylbutane	54.1	1	Derwent et al., 1998
2,3-dimethylheptane	42.6	2	
2,3-dimethylnonane	37.7	2	
2,3-dimethyloctane	40.2	2	
2,3-dimethylpentane	39.1	2	
2,3-dimethylundecane	31.7	2	
2,4-difluoroaniline	0.0	3	
2,4-dimethyl-1-(1-methylethyl)benzene	111.7	2	

species	POCP	Method	reference (if 1)
2,4-dimethyl-1-isopropylbenzene	111.7	2	
2,4-dimethylheptane	42.6	2	
2,4-dimethylpentane	46.6	2	
2,5-dimethyldecane	34.6	2	
2,5-dimethylheptane	51.2	2	
2,5-dimethylhexane	44.6	2	
2,5-dimethyloctane	40.2	2	
2,6-dimethyldecane	35.1	2	
2,6-dimethylheptane	42.3	2	
2,6-dimethyloctane	40.2	2	
2,6-dimethylundecane	31.7	2	
2,7-dimethyloctane	39.9	2	
2-aminoethanol	51.3	3	
2-butanol	44.7	1	Jenkin and Hayman 1999
2-butanone	37.3	1	Derwent et al., 1998
2-butanone oxime	51.3	3	
2-butene	113.9	1	Derwent et al., 1998 (mean of cis/trans)
2-butoxyethanol	48.3	1	Jenkin and Hayman 1999
2-butoxyethyl acetate	35.1	2	
2-c9-unidentifiediso-paraffins	41.4	3	
2-chloroethanol	30.3	2	
2-ethoxyethanol	38.6	1	Jenkin and Hayman 1999
2-ethoxyethyl acetate	34.6	2	
2-ethyl-1,3-dimethylbenzene	114.6	2	
2-ethyltoluene	89.8	1	Derwent et al., 1998
2-methoxyethanol	30.7	1	Jenkin and Hayman 1999
2-methyl-1-butene	77.1	1	Derwent et al., 1998
2-methyl-1-butylbenzene	86.2	2	
2-methyl-1-propanol	36.0	1	Jenkin and Hayman 1999
2-methyl-2,4-pentanediol	46.4	2	
2-methyl-2-butene	84.2	1	Derwent et al., 1998
2-methyl-2-propanol	10.6	1	Jenkin and Hayman 1999
2-methyl-5-ethyloctane	38.0	2	
2-methylbutanal	86.0	2	
2-methyldecalin	41.4	2	
2-methyldecane	37.5	2	
2-methylheptane	44.6	2	
2-methylhexane	41.1	1	Derwent et al., 1998
2-methylnonane	39.9	2	
2-methyloctane	42.8	2	
2-methylpentane	42.0	1	Derwent et al., 1998
2-methylpropanal	51.4	1	Derwent et al., 1998
2-methylundecane	35.2	2	
2-pentanone	54.8	1	Derwent et al., 1998
2-pentene	111.9	1	Derwent et al., 1998 (mean of cis/trans)
2-phenylpropene	14.2	3	
2-propanol	18.8	1	Jenkin and Hayman 1999

species	POCP	Method	reference (if 1)
2-propen-1-ol	74.6	2	
2-propyl acetate	21.1	1	Jenkin and Hayman 1999
2-propyl benzene	50.0	1	Derwent et al., 1998
3,3,4-trimethylhexane	37.6	2	
3,3,5-trimethylheptane	36.2	2	
3,3-dimethylheptane	37.2	2	
3,3-dimethyloctane	35.8	2	
3,3-dimethylpentane	37.8	2	
3,4-dimethylheptane	42.6	2	
3,4-dimethylhexane	45.3	2	
3,5-dimethyloctane	40.5	2	
3,6,9-trioxa-1-undecanol	35.7	2	
3,6-dimethyloctane	40.5	2	
3,7-dimethylnonane	37.9	2	
3A,4,7,7A-tetrahydro-4,7-methanoindene	72.0	3	
3-chloropropene	46.0	2	
3-ethyl-2-methylheptane	39.9	2	
3-ethyl-2-methylhexane	43.1	2	
3-ethylheptane	43.1	2	
3-ethylhexane	41.5	2	
3-ethyloctane	44.4	2	
3-ethyltoluene	101.9	1	Derwent et al., 1998
3-methyl-1-butene	67.1	1	Derwent et al., 1998
3-methyldecane	37.7	2	
3-methylheptane	45.0	2	
3-methylhexane	36.4	1	Derwent et al., 1998
3-methylnonane	40.2	2	
3-methyloctane	42.6	2	
3-methylpentane	47.9	1	Derwent et al., 1998
3-methylundecane	35.1	2	
3-pentanone	41.4	1	Derwent et al., 1998
4 methyl-2-pentanone	49.0	1	Derwent et al., 1998
4,4-dimethylheptane	37.2	2	
4,4'-methylenedianiline	51.3	3	
4,5-dimethylnonane	37.9	2	
4,6-dimethylindan	132.5	3	
4,7-dimethylindan	132.5	3	
4,8-dioxa-1-dodecane	41.3	2	
4-4'-methylenediphenyl diisocyanate	51.3	3	
4-bromophenylacetate	51.3	3	
4-ethyl-1,2-dimethylbenzene	114.6	2	
4-ethylcyclohexane	48.3	2	
4-ethyloctane	44.4	2	
4-ethyltoluene	90.6	1	Derwent et al., 1998
4-isopropyltoluene	89.6	2	
4-methyl-1,3-dioxol-2-one	21.9	2	
4-methyl-2-pentanol	60.9	2	
4-methyl-2-pentanone	49.0	1	Derwent et al., 1998

species	POCP	Method	reference (if 1)
4-methyl-4-hydroxy-2-pentanone	30.7	1	Jenkin and Hayman 1999
4-methyldecane	37.7	2	
4-methylheptane	45.0	2	
4-methylnonane	40.2	2	
4-methyloctane	42.3	2	
4-propylheptane	40.5	2	
5-methyl-2-hexanone	51.6	2	
5-methyldecane	37.7	2	
5-methylundecane	35.1	2	
6-ethyl-2-methyldecane	32.8	2	
6-ethyl-2-methyloctane	38.0	2	
6-methylundecane	35.1	2	
8-methyl-1-nonanol	50.2	2	
acetaldehyde	64.1	1	Derwent et al., 1998
acetic acid	9.7	1	Derwent et al., 1998
acetic anhydride	2.5	2	
acetone	9.4	1	Derwent et al., 1998
acetonitrile	0.0	3	
acetyl chloride	0.2	2	
acetylene	8.5	1	Derwent et al., 1998
A-chlorotoluene	20.1	3	
acrolein	73.0	2	
acrylamide	51.3	3	
acrylic acid	34.4	2	
acrylonitrile	0.0	3	
adiponitrile	51.3	3	
alcohols	34.3	3	
alifates c2-c10	36.7	3	
aliphatic hydrocarbons unspecified	36.8	3	
alkylbenzenes	63.7	3	
aniline	51.3	3	
aromatic hydrocarbons unspecified	95.4	3	
aromatics other	95.4	3	
benzaldehyde	-9.2	1	Derwent et al., 1998
benzene	21.8	1	Derwent et al., 1998
benzene-1,2,4-tricarboxylic acid 1,2-anhydride	51.3	3	
benzenes higher substituted	123.3	3	
benzophenone	51.3	3	
benzyl alcohol	46.9	2	
bis(2-hydroxyethyl)ether	40.2	2	
bromoethane	1.3	2	
bromoethene	12.2	2	
bromomethane	0.6	2	
butanal	79.5	1	Derwent et al., 1998
butane	35.2	1	Derwent et al., 1998
butanethiols	0.0	3	
butene	99.6	3	
butoxyl	51.3	3	

species	POCP	Method	reference (if 1)
butyl acetate	26.9	1	Jenkin and Hayman 1999
butyl acrylate	47.9	2	
butyl benzenes	69.0	3	
butyl glycolate	26.8	2	
butyl lactate	29.1	2	
butylbenzene	69.0	2	
butylcyclohexane	42.5	2	
butylcyclohexanes	42.5	3	
butyrolactone	51.3	3	
C ₁₀ -cyclo-paraffin	38.4	3	
C ₁₀ -iso-paraffin	38.4	3	
C ₁₁ -aromatic	134.2	3	
C ₁₁ -cyclo-paraffin	38.4	3	
C ₁₁ -iso-paraffin	38.4	3	
C ₁₁ -unidentified	86.8	3	
C ₁₂ -cyclo-paraffin	35.7	3	
C ₁₂ -iso-paraffin	35.7	3	
C ₁₃ -iso-paraffin	32.7	3	
C ₁₆ branched alkane	26.0	3	
cis-2-butene	114.6	1	Derwent et al., 1998
cis-2-pentene	112.1	1	Derwent et al., 1998
C ₆ H ₁₈ O ₃ Si ₃	0.0	3	
C ₇ isomers	72.2	3	
C ₇ -C ₁₆ paraffins	36.6	3	
C ₈ H ₂₄ O ₄ Si ₄	0.0	3	
C ₉	92.3	3	
C ₉ /C ₁₀	90.8	3	
C ₉ -cyclo-paraffin	41.4	3	
C ₉ -iso-paraffin	41.4	3	
camphor/fenchone	74.5	3	
carbon disulphide	0.0	3	
carbonyl sulphide	0.0	3	
carboxylic acids	15.2	3	
chlorobenzene	9.9	2	
chlorodifluoromethane	0.2	2	
chloroethane	10.4	2	
chloroethene	36.1	2	
chlorofluoromethane	1.9	2	
chloromethane	0.5	1	Derwent et al., 1998
chloroprene	43.7	2	
chloropropanes	12.4	3	
cis-2-butene	114.6	1	Derwent et al., 1998
cis-2-pentene	112.1	1	Derwent et al., 1998
coeluting-2-aromatics-1-iso-paraffin	0.0	3	
coelutingaromatic,cyclo-andiso-paraffin	62.8	3	
coelutingaromaticandiso-paraffin	62.8	3	
crotonaldehyde	70.0	2	
cycloheptane	53.4	2	

species	POCP	Method	reference (if 1)
cyclohexane	29.0	1	Derwent et al., 1998
cyclohexanol	51.8	1	Jenkin and Hayman 1999
cyclohexanone	29.9	1	Derwent et al., 1998
cyclo-paraffin	37.3	3	
cyclopentane	51.5	2	
decalin	44.4	2	
decalin(trans)	44.4	2	
decane	38.4	1	Derwent et al., 1998
decanes	38.4	3	
decenes	91.7	3	
diamonotoluene	51.3	3	
dichlorobenzene	12.0	3	
dichlorobenzenes	12.0	3	
dichlorobutenes	34.7	3	
dichlorodifluoromethane	0.0	1	By definition
dichlorofluoromethane	1.3	2	
dichloromethane	6.8	1	Derwent et al., 1998
diethyl disulphide	0.0	3	
diethyl ether	44.5	1	Jenkin and Hayman 1999
diethyl sulphate	0.0	3	
diethylbenzene	105.7	3	
difluoromethane	0.6	2	
diisopropyl ether	39.8	1	Jenkin and Hayman 1999
dimethyl disulphide	0.0	3	
dimethyl esters	17.1	3	
dimethyl ether	18.9	1	Jenkin and Hayman 1999
dimethyl furans	64.6	3	
dimethyl sulphate	0.0	3	
dimethyl sulphide	0.0	3	
dimethylamine	51.3	3	
dimethylcyclohexanes	48.2	3	
dimethylcyclopentanes	45.9	3	
dimethylformamide	51.3	3	
dimethylnonane	38.4	3	
dipentene	74.5	2	
dipropyl ethers	46.3	3	
dipropylene glycol ethers	42.6	3	
dodecane	35.7	1	Derwent et al., 1998
ethane	12.3	1	Derwent et al., 1998
ethanethiol	0.0	3	
ethanol	39.9	1	Jenkin and Hayman 1999
ethanolamine	51.3	3	
ethyl acetate	20.9	1	Jenkin and Hayman 1999
ethyl acrylate	41.4	2	
ethyl butanoate	30.1	2	
ethyl chloride	10.4	2	
ethyl chloroformate	10.1	2	
ethyl ether	44.5	1	Jenkin and Hayman 1999
ethyl hexanol	53.5	3	

species	POCP	Method	reference (if 1)
ethyl lactate	32.8	2	
ethyl pentanoate	32.4	2	
ethyl propionate	19.9	2	
ethylamine	51.3	3	
ethylbenzene	73.0	1	Derwent et al., 1998
ethylcyclohexane	48.3	2	
ethylcyclopentane	46.6	2	
ethyldimethylbenzene	132.0	3	
ethylene	100.0	1	Derwent et al., 1998
ethylene glycol	37.3	1	Jenkin and Hayman 1999
ethylene oxide	2.4	2	
ethylisopropylbenzene	105.7	3	
ethyltoluenes	94.1	3	
ethyne	8.5	1	Derwent et al., 1998
formaldehyde	51.9	1	Derwent et al., 1998
formanilide	0.0	3	
formic acid	3.2	1	Derwent et al., 1998
fumaric acid	17.1	2	
glycerol	39.2	2	
glycol acetates unspecified	15.2	3	
glycol ethers unspecified	38.6	3	
glycols unspecified	42.0	3	
glyoxal	58.0	2	
heptadecane	12.2	2	
heptadienes	100.6	3	
heptane	49.4	1	Derwent et al., 1998
heptane other isomers	42.3	3	
heptene	103.5	3	
hexadecane	26.0	2	
hexamethyldisilane	0.0	3	
hexamethyldisiloxane	0.0	3	
hexamethylenediamine	51.3	3	
hexanal	100.0	2	
hexane	48.2	1	Derwent et al., 1998
hexane isomers	43.3	3	
hexane other isomers	43.3	3	
hexene	100.5	3	
hexylcyclohexane	36.7	2	
hydrocarbons C13	80.3	3	
indan	79.7	2	
indane	79.7	2	
iodomethane	0.7	2	
isobutane	30.7	1	Derwent et al., 1998
isomers of dodecane	35.7	3	
isomers of hexane	43.3	3	
isomers of pentadecane	28.4	3	
isomers of pentane	32.4	3	
isomers of pentene	91.7	3	
isomers of tetradecane	30.7	3	

species	POCP	Method	reference (if 1)
isopentane	40.5	1	Derwent et al., 1998
isopentylbenzene	67.3	2	
isophorone	77.6	2	
isoprene	109.2	1	Derwent et al., 1998
isopropanolamine	51.3	3	
isopropylbenzene	50.0	1	Derwent et al., 1998
kerosene	62.8	3	
ketones	42.0	3	
limonene	74.5	2	
maleic anhydride	26.8	2	
menthene	89.9	3	
methacrylic acid	50.2	2	
methanethiol	0.0	3	
methanol	14.0	1	Jenkin and Hayman 1999
methoxy propanol	35.5	3	
methyl acetate	5.9	1	Jenkin and Hayman 1999
methyl acrylate	39.1	2	
methyl butanoate	29.6	2	
methyl ethyl ether	25.3	2	
methyl formate	2.7	1	Jenkin and Hayman 1999
methyl furans	40.2	3	
Methyl glyoxal	72.0	2	
methyl methacrylate	46.7	2	
methyl naphthalenes	125.2	3	
methyl pentanoate	31.9	2	
methyl styrene	14.2	3	
methylamine	0.0	3	
methylcyclodecane	39.3	2	
methylcyclohexane	51.0	2	
methylcyclopentane	48.1	2	
methylethylbenzene	94.1	3	
methylheptanes	45.3	3	
methylhexane	38.8	3	
methylindane	80.0	2	
methylnonanes	38.4	3	
methyloctanes	41.4	3	
methylpropene	62.7	1	Derwent et al., 1998
methylpropylbenzene	105.7	3	
methyltetralin	114.0	3	
m-xylene	110.8	1	Derwent et al., 1998
m-xylene & p-xylene	105.9	3	
N-(hydroxymethyl) acrylamide	51.3	3	
N,N-dimethylformamide	51.3	3	
naphthalene	97.7	2	
nitrobenzene	0.0	3	
nitromethane	0.0	3	
nitropropane	0.0	3	
N-methyl pyrrolidone	51.3	3	
nonadienes	93.6	3	

species	POCP	Method	reference (if 1)
nonane	41.4	1	Derwent et al., 1998
nonanes	41.4	3	
nonenes	95.6	3	
octahydroindan	44.5	2	
octahydro-indan	44.5	2	
octane	45.3	1	Derwent et al., 1998
octane isomers	45.3	3	
octane other isomers	45.3	3	
octanes	45.3	3	
octene	99.6	3	
octenes	99.6	3	
octylamine	51.3	3	
olefins other	97.5	3	
organic amines	51.3	3	
other terpenes	74.5	3	
o-xylene	105.3	1	Derwent et al., 1998
paraffin	36.8	3	
paraffins other	36.8	3	
pentadecane	28.4	2	
pentadienes	107.0	3	
pentafluoroethane	0.1	2	
pentanal	76.5	1	Derwent et al., 1998
pentane	39.5	1	Derwent et al., 1998
pentane other isomers	32.4	3	
pentanes	32.4	3	
pentanethiols	0.0	3	
pentenes	91.7	3	
pentyl benzenes	67.3	3	
pentylbenzene	67.3	2	
pentylcyclohexane	39.6	2	
phenol	63.3	2	
phenoxyacetic acid (phenoxy acid)	15.2	3	
phenylacetic acid	15.2	3	
phenylacetonitrile	51.3	3	
phorate	0.0	3	
phthalic anhydride	105.3	3	
pine oil	74.5	3	
potassium phenylacetate	51.3	3	
propanal	79.8	1	Derwent et al., 1998
propane	17.6	1	Derwent et al., 1998
propanoic acid	15.0	1	Derwent et al., 1998
propionitrile	0.0	3	
propyl acetate	28.2	1	Jenkin and Hayman 1999
propyl butanoate	31.9	2	
propylamine	51.3	3	
propylbenzene	63.6	1	Derwent et al., 1998
propylcyclohexane	45.4	2	
propylcyclohexanes	45.4	3	
propylcyclopentane	44.5	2	

species	POCP	Method	reference (if 1)
propylene	112.3	1	Derwent et al., 1998
propylene oxide	13.4	2	
propyl propionate	28.5	2	
p-xylene	101.0	1	Derwent et al., 1998
pyridene	51.3	3	
Sat C ₇ 's	42.3	3	
Saturated C ₆	43.3	3	
Saturated C ₈ 's	45.3	3	
sodium 2-ethylhexanoate	51.3	3	
sodium phenylacetate	51.3	3	
styrene	14.2	1	Derwent et al., 1998
trans-2-butene	113.2	1	Derwent et al., 1998
trans-2-pentene	111.7	1	Derwent et al., 1998
tert-butylamine	51.3	3	
tertbutylcyclopropane	11.5	2	
tertpentylbenzene	67.3	2	
tetrachloroethene	2.9	1	Derwent et al., 1998
tetradecane	30.7	2	
tetrafluoroethene	9.4	2	
tetrahydrofuran	57.0	2	
tetramethylcyclohexane	38.5	3	
texanol	27.5	3	
toluene	63.7	1	Derwent et al., 1998
trichloroethene	32.5	1	Derwent et al., 1998
trichlorofluoromethane	0.0	1	By definition
trichloromethane	2.3	1	Derwent et al., 1998
tridecane	32.7	2	
triethylamine	51.3	3	
trifluoroethene	54.7	2	
trifluoromethane	0.0	3	
trimethylamine	51.3	3	
trimethylcyclohexanes	45.4	3	
trimethylcyclopentanes	43.6	3	
trimethylfluorosilane	0.0	3	
undecane	38.4	1	Derwent et al., 1998
undecanes	38.4	3	
undecenes	38.4	3	
unidentified iso-paraffin	37.3	3	
unidentified C ₈ -paraffin	45.3	3	
unidentified iso-paraffin	36.8	3	
Unsat C ₆ 's	100.5	3	
unspeciated	51.3	3	
unspeciated hydrocarbons	71.9	3	
vinyl acetate	48.5	2	
vinyl chloride	36.1	2	
vinylidene chloride	52.6	2	
xylenes	105.7	3	

Appendix 5

Speciation of Kerosene

Species	POCP	%w/w	Notes
n-dodecane		6.99	In existing speciation as dodecane
n-tridecane		6.1	In existing speciation as tridecane
n-tetradecane		4.51	In existing speciation as tetradecane
n-undecane		4.27	In existing speciation as undecane
decahydro-methyl-naphthalene	41.4	2.07	assume as 2-methyldecalin
2-methyl-dodecane	32.4	1.93	
C13 iso-paraffin	32.4	1.92	assume as 2-methyldodecane
C13 iso-paraffin	32.4	1.85	assume as 2-methyldodecane
n-pentadecane		1.78	In existing speciation as pentadecane
methyl-decahydronaphthalen	41.4	1.72	assume as 2-methyldecalin
N.I		1.62	unspeciated
hexyl-cyclohexane		1.52	In existing speciation as hexylcyclohexane
C15 iso-paraffin	27.1	1.43	assume as 2-methyltetradecane
C12 naphthen	38.4	1.32	assume as 2,3-dimethyldecalin
N.I		1.29	unspeciated
1,2-di-methyl-decahydronaphthalene	38.4	1.28	
2-methyl-undecane		1.24	In existing speciation as 2-methylundecane
N.I		1.23	unspeciated
6-methyl-undecane		1.21	In existing speciation as 6-methylundecane
tran-decahydro-naphthalen		1.16	In existing speciation as decalin(trans)
C13 iso-paraffin	32.4	1.13	assume as 2-methyldodecane
C12 naphthen	38.4	1.12	assume as 2,3-dimethyldecalin
C13 iso-paraffin	32.4	1.1	assume as 2-methyldodecane
4-methyl-undecane	35.1	1.09	
3-methyl-undecane		1.06	In existing speciation as 3-methylundecane
4-methyl-dodecane	32.5	1.05	
bicyclo-hexyl	38.2	1.05	
2-methyl-tridecane	29.8	0.94	
N.I		0.93	unspeciated
4-methyl-tridecane	29.9	0.92	
N.I		0.92	unspeciated
C13 iso-paraffin	32.4	0.86	assume as 2-methyldodecane
ethyl-decahydro-naphthalene	38.5	0.85	assume 2-ethyldecalin
C13 naphthen	35.5	0.85	assume as 2-ethyl-3-methyldecalin
1,6-di-methyl-decahydronaphthalene	38.4	0.84	
C14 naphtene	32.5	0.83	assume as 2,3-diethyldecalin
C11 naphthen	41.4	0.78	assume as 2-methyldecalin
N.I		0.78	unspeciated
C13 naphthen+C13 iso-paraffin	34	0.76	assume mean of 2-methyldodecane and 2-ethyl-3-methyldecalin

Species	POCP	%w/w	Notes
5-methyl-undecane+C12 naphthen	36.8	0.75	assume mean of 5-methylundecane and 2,3-dimethyldecalin
1-ethyl-2-propyl-cyclohexane		0.74	In existing speciation as 1-ethyl-2-propylcyclohexane
C14 naphtene	32.5	0.7	assume as 2,3-diethyldecalin
n-decane		0.67	In existing speciation as decane
C13 iso-paraffin	32.4	0.65	assume as 2-methyldodecane
di-methyl-decahydro-naphtalene	38.4	0.61	assume as 2,3-dimethyldecalin
2-methyl-decane		0.59	In existing speciation as 2-methyldecane
5-methyl-undecane		0.59	In existing speciation as 5-methylundecane
N.I		0.59	unspeciated
di-methyl-decahydro-naphtalene	38.4	0.55	assume as 2,3-dimethyldecalin
1,6-di-methyl-decahydro-naphtalen		0.54	duplicate of A40
3-methyl-tridecane	29.9	0.54	
C13 naphthen	35.5	0.53	assume as 2-ethyl-3-methyldecalin
1-methyl-4-(1-methyl-butyl)-cyclohexane	37	0.51	
C13 naphthen	35.5	0.49	assume as 2-ethyl-3-methyldecalin
C13 naphthen	35.5	0.46	assume as 2-ethyl-3-methyldecalin
1-undecene	72	0.45	
C12 naphthen	38.4	0.44	assume as 2,3-dimethyldecalin
C13 naphthen + di-methyl-decahydro-naphtalene	37	0.44	assume mean of 2-ethyl-3-methyldecalin and 2,3-dimethyldecalin
C13 iso-paraffin+C13 naphthen	34	0.44	assume mean of 2-ethyl-3-methyldecalin and 2-methyldodecane
C14 iso-paraffin	29.8	0.44	assume as 2-methyltridecane
N.I		0.44	unspeciated
C14	31.2	0.43	assume mean of 2-methyltridecane and 2,3-diethyldecalin
C14 naphtene	32.5	0.43	assume as 2,3-diethyldecalin
pentyl-cyclohexane		0.41	In existing speciation as pentylcyclohexane
C11 naphthen	41.4	0.4	assume as 2-methyldecalin
C11 naphthen	41.4	0.4	assume as 2-methyldecalin
C13 naphthen	35.5	0.4	assume as 2-ethyl-3-methyldecalin
3-methyl-decane		0.39	In existing speciation as 3-methyldecane
C12 naphthen	38.4	0.39	assume as 2,3-dimethyldecalin
C14 iso-paraffin	29.8	0.39	assume as 2-methyltridecane
N.I		0.38	unspeciated
methyl-decahydronaphtalene	41.4	0.37	assume as 2-methyldecalin
N.I		0.35	unspeciated
C13 naphthen	35.5	0.34	assume as 2-ethyl-3-methyldecalin
C12 naphthen + C12 iso-paraffin	36.7	0.33	assume mean of 2-methylundecane and 2,3-dimethyldecalin
N.I		0.33	unspeciated
5-methyl-undecane+N.I	35.1	0.32	assume as 5-methylundecane
N.I		0.31	unspeciated
C14 iso-paraffin	29.8	0.3	assume as 2-methyltridecane
C14 naphtene	32.5	0.3	assume as 2,3-diethyldecalin
5-methyl-decane		0.29	In existing speciation as 5-methyldecane
C12 naphthen	38.4	0.29	assume as 2,3-dimethyldecalin
C12 naphthen	38.4	0.29	assume as 2,3-dimethyldecalin
N.I		0.28	unspeciated
C11 naphthen	41.4	0.27	assume as 2-methyldecalin
C14	31.2	0.27	assume mean of 2-methyltridecane and 2,3-diethyldecalin
C15 iso-paraffin	27.1	0.26	assume as 2-methyltetradecane
N.I		0.25	unspeciated

Species	POCP	%w/w	Notes
methyl-decahydronaphtalene	41.4	0.25	assume as 2-methyldecalin
4-methyl-decane		0.24	In existing speciation as 4-methyldecane
4-methyl-decane		0.24	Duplicate - see previous entry
C13 naphthen	35.5	0.24	assume as 2-ethyl-3-methyldecalin
somme des > n-hexadecane	20.5	0.24	assume mean of heptadecane and octadecane
C14 iso-paraffin	29.8	0.23	assume as 2-methyltridecane
C14	31.2	0.23	assume mean of 2-methyltridecane and 2,3-diethyldecalin
N.I		0.23	unspeciated
N.I		0.22	unspeciated
C12 naphthen	38.4	0.22	assume as 2,3-dimethyldecalin
N.I		0.22	unspeciated
1-methyl-3-propyl-cyclohexane	42.7	0.21	
C11 naphthen	41.4	0.21	assume as 2-methyldecalin
N.I		0.21	unspeciated
C14 iso-paraffin	29.8	0.21	assume as 2-methyltridecane
C12 naphthen	38.4	0.2	assume as 2,3-dimethyldecalin
C14	31.2	0.2	assume mean of 2-methyltridecane and 2,3-diethyldecalin
C14	31.2	0.2	assume mean of 2-methyltridecane and 2,3-diethyldecalin
N.I		0.2	unspeciated
n-hexadecane		0.2	In existing speciation as HEXADECANE
C10 naphthen+1-methyl-4-isopropyl-cyclohexane	43.5	0.19	assume mean of decalin and 1-methyl-4-isopropylcyclohexane
C12 naphthen	38.4	0.19	assume as 2,3-dimethyldecalin
1-ethyl-2-propyl-cyclohexane		0.19	In existing speciation as 1-ethyl-2-propylcyclohexane
C13 naphthen	35.5	0.19	assume as 2-ethyl-3-methyldecalin
N.I		0.18	unspeciated
C11 naphthen	41.4	0.18	assume as 2-methyldecalin
C12 naphthen	38.4	0.18	assume as 2,3-dimethyldecalin
N.I		0.18	unspeciated
N.I		0.18	unspeciated
N.I		0.18	unspeciated
C14	31.2	0.17	assume mean of 2-methyltridecane and 2,3-diethyldecalin
N.I		0.17	unspeciated
C12 naphthen	38.4	0.16	assume as 2,3-dimethyldecalin
C14 iso-paraffin	29.8	0.16	assume as 2-methyltridecane
N.I		0.16	unspeciated
C11 naphthen	41.4	0.15	assume as 2-methyldecalin
C11 N.I	39.5	0.15	assume mean of 2-methyldecane and 2-methyldecalin
N.I		0.15	unspeciated
N.I		0.14	unspeciated
C10+autre	41.4	0.13	assume mean of decalin and decane
C11 iso-paraffin	37.5	0.13	assume as 2-methyldecane
C11 naphthen	41.4	0.13	assume as 2-methyldecalin
C11 naphthen	41.4	0.13	assume as 2-methyldecalin
C11 naphthen	41.4	0.13	assume as 2-methyldecalin
N.I		0.13	unspeciated
N.I		0.13	unspeciated
C11 naphthen	41.4	0.12	assume as 2-methyldecalin
C11 naphthen	41.4	0.12	assume as 2-methyldecalin
N.I		0.12	unspeciated
N.I		0.12	unspeciated
1,2,3,5-tetra-methyl-cyclohexane		0.11	In existing speciation as 1,2,3,5-

Species	POCP	%w/w	Notes
			tetramethylcyclohexane
N.I		0.11	unspeciated
C12 iso-paraffin	34.9	0.11	assume as 2-methylundecane
1-methyl-2-propyl-cyclohexane	42.7	0.1	
C11 naphthen	41.4	0.1	assume as 2-methyldecalin
N.I		0.1	unspeciated
C14	31.2	0.1	assume mean of 2-methyltridecane and 2,3-diethyldecalin
C14	31.2	0.1	assume mean of 2-methyltridecane and 2,3-diethyldecalin
N.I		0.1	unspeciated
N.I		0.1	unspeciated
n-nonane		0.09	In existing speciation as nonane
propyl-cyclohexane		0.09	In existing speciation as propylcyclohexane
1-ethyl-1,3-di-methyl-cyclohexane	38.7	0.09	
N.I		0.09	unspeciated
C14	31.2	0.09	assume mean of 2-methyltridecane and 2,3-diethyldecalin
N.I		0.09	unspeciated
1-methyl-4-isopropyl-cyclohexane		0.08	In existing speciation as 1-methyl-4-isopropylcyclohexane
N.I		0.08	unspeciated
1-methyl-2-propyl-cyclohexane		0.08	duplicate of entry A147
N.I		0.08	unspeciated
2-methyl-nonane		0.07	In existing speciation as 2-methylnonane
C10 naphthen	44.4	0.07	assume as decalin
cis-decahydro-naphthalene	44.4	0.07	
C11 paraffin	37.5	0.07	assume as 2-methyldecane
C11 naphthen	41.4	0.07	assume as 2-methyldecalin
C12 naphthen	38.4	0.07	assume as 2,3-dimethyldecalin
C12 naphthen	38.4	0.07	assume as 2,3-dimethyldecalin
C13 naphthen	35.5	0.07	assume as 2-ethyl-3-methyldecalin
N.I		0.07	unspeciated
N.I		0.07	unspeciated
N.I		0.07	unspeciated
cis-1-ethyl-3-methyl-cyclohexane	45.6	0.06	
C9 naphthen	42.7	0.06	assume as 1,2,3,5-tetramethylcyclohexane
1-ethyl-2,3-di-methyl-cyclohexane		0.06	In existing speciation as 1-ethyl-2,3-dimethylcyclohexane
1,2,3,5-tetra-methylcyclohexane		0.06	duplicate of A144
1,1,2,3-tetra-methyl-cyclohexane	40.5	0.06	
1-ethyl-2,4-di-methyl-cyclohexane	42.3	0.06	
2-ethyl-1,3-di-methyl-cyclohexane	42.3	0.06	
1,3-dimethyl-2-(methylethenyl)-cyclopentane	67.3	0.06	
di-ethyl-cyclohexane	43	0.06	assume as 1,2-diethylcyclohexane
1-methyl-4-iso-propyl-cyclohexane		0.06	duplicate of A160
decahydro-naphthalene		0.06	In existing speciation as decalin
1,2-di-ethyl-3-methyl-cyclohexane	40.2	0.06	
decahydro-methyl-naphthalene	41.4	0.06	assume as 2-methyldecalin
N.I		0.06	unspeciated
1-ethyl-3-methyl-cyclohexane (cis)		0.05	duplicate of A175
4-methyl-nonane		0.05	In existing speciation as 4-methylnonane
1-ethyl-2,3-di-methyl-cyclohexane		0.05	duplicate of A177
undecene + C11 naphthen	56.7	0.05	assume mean of 1-undecene and 2-methyldecalin
N.I		0.05	unspeciated

Species	POCP	%w/w	Notes
N.I		0.05	unspeciated
2,6-di-methyl-octene	91.7	0.04	assume internal alkene
3-ethyl-2-methyl-heptane		0.04	In existing speciation as 3-ethyl-2-methylheptane
1-ethyl-2,4-di-methyl-cyclohexane		0.04	duplicate of A180
3-ethyl-octane		0.04	In existing speciation as 3-ethyloctane
1,2,3,5-tetra-methyl-cyclohexane		0.04	duplicate of A144
C11 naphthen	41.4	0.04	assume as 2-methyldecalin
C11 naphthen	41.4	0.04	assume as 2-methyldecalin
N.I		0.04	unspeciated
N.I		0.04	unspeciated
N.I		0.04	unspeciated
N.I		0.04	unspeciated
N.I		0.04	unspeciated
N.I		0.04	unspeciated
N.I		0.04	unspeciated
(cis,trans,trans)1,2,4-trimethyl-cyclohexane	45.4	0.03	
1-ethyl-3-methyl-cyclohexane (cis,trans)	45.6	0.03	
C9 naphthen	42.7	0.03	assume as 1,2,3,5-tetramethylcyclohexane
C10 naphthen	44.4	0.03	assume as decalin
1,1,3,5-tetra-methyl-cyclohexane	40.5	0.03	
2-ethyl-1,3-di-methyl-cyclohexane		0.03	duplicate of A181
C11 naphthen	41.4	0.03	assume as 2-methyldecalin
N.I		0.03	unspeciated
N.I		0.03	unspeciated
N.I		0.03	unspeciated
N.I		0.03	unspeciated
N.I		0.03	unspeciated
cis,cis,cis-1,3,5-tri-methyl-cyclohexane+ethyl-cyclohexane	46.9	0.02	assume mean of 1,3,5-cyclohexane and ethylcyclohexane
3-methyl-octane		0.02	In existing speciation as 3-methyloctane
cis,trans,cis-1,2,4-tri-methyl-cyclohexane	45.4	0.02	
1,2,4-trimethylcyclohexane(trans,cis,trans)	45.4	0.02	
1,1,2-tri-methyl-cyclohexane		0.02	In existing speciation as 1,1,2-trimethylcyclohexane
1,1,3,5-tetra-methyl-cyclohexane		0.02	duplicate of A213
1-ethyl-4-methyl-cyclohexane		0.02	In existing speciation as 1-ethyl-4-methylcyclohexane
cis-octahydro-1-H-indene	44.5	0.02	
C9 naphthen	42.7	0.02	assume as 1,2,3,5-tetramethylcyclohexane
butyl-cyclopentane	42.2	0.02	
tetra-methyl-cyclohexane	42.7	0.02	assume as 1,2,3,5-tetramethylcyclohexane
3,3,5-tri-methyl-heptane		0.02	In existing speciation as 3,3,5-trimethylheptane
1,2,3,5-tetra-methyl-cyclohexane		0.02	duplicate of A144
2,6-di-methyl-3-octene	91.7	0.02	
penta-methyl-cyclohexane	40	0.02	
C10 olefin	91.7	0.02	assume internal alkene
C11 iso-paraffin	37.5	0.02	assume as 2-methyldecane
N.I		0.02	unspeciated
N.I		0.02	unspeciated
N.I		0.02	unspeciated
N.I		0.02	unspeciated
N.I		0.02	unspeciated
1,3,5-tri-methyl-cyclohexane	45.4	0.01	
C6 naphthen+1,2,3-tri-methyl-cyclohexane	37.2	0.01	assume mean of cyclohexane and 1,2,3-trimethylcyclohexane

Species	POCP	%w/w	Notes
2,4,6-trimethyl-heptane	40.2	0.01	
C9 naphthen	42.7	0.01	assume as 1,2,3,5-tetramethylcyclohexane
diethyl-cyclohexane	43	0.01	assume as 1,2-diethylcyclohexane
1,2,3,5-tetra-methyl-cyclohexane		0.01	duplicate of A144
N.I		0.01	unspeciated
N.I		0.01	unspeciated
N.I		0.01	unspeciated
N.I		0.01	unspeciated
N.I		0.01	unspeciated
N.I		0.01	unspeciated
N.I		0.01	unspeciated
N.I		0.01	unspeciated
N.I		0.01	unspeciated
2-methyl-octane		<0.01	In existing speciation as 2-methyloctane
1,1,3-tri-methyl-cyclohexane		<0.01	In existing speciation as 1,1,3-trimethylcyclohexane
N.I		<0.01	unspeciated
methyl-cyclohexane		<0.005	In existing speciation as methylcyclohexane
2-methyl-heptane		<0.005	In existing speciation as 2-methylheptane
cis-1,3-di-methyl-cyclohexane + 3-methyl heptane	46.6	<0.005	assume mean of 1,3-dimethylcyclohexane and 3-methylheptane
trans-1,4-di-methyl-cyclohexane	48.2	<0.005	
N.I		<0.005	unspeciated
cis-1-ethyl-2-methyl-cyclopentane	44.2	<0.005	
C8 iso-olefin	99.6	<0.005	assume internal alkene
trans-1,2-di-methyl-cyclohexane	48.2	<0.005	
n-octane		<0.005	In existing speciation as octane
cis-1,4-di-methyl-cyclohexane	48.2	<0.005	
C9 N.I	42.1	<0.005	assume mean of 1,2,3,5-tetramethylcyclohexane & nonane
2,4-di-methyl-heptane		<0.005	In existing speciation as 2,4-dimethylheptane
cis-1,2-dimethyl-cyclohexane	48.2	<0.005	
1,1,3-tri-methyl-cyclohexane		<0.005	duplicate of A259
1,1,4-tri-methyl-cyclohexane	41.2	<0.005	
C9 naphthen	42.7	<0.005	assume as 1,2,3,5-tetramethylcyclohexane
C9 naphthen	42.7	<0.005	assume as 1,2,3,5-tetramethylcyclohexane
C9 naphthen	42.7	<0.005	assume as 1,2,3,5-tetramethylcyclohexane
C9 naphthen	42.7	<0.005	assume as 1,2,3,5-tetramethylcyclohexane
C9 naphthen	42.7	<0.005	assume as 1,2,3,5-tetramethylcyclohexane
2,3-di-methyl-heptane		<0.005	In existing speciation as 2,3-dimethylheptane
octahydro-pentalene	51.3	<0.005	??? Unknown ??? Use average
4-methyl-octane		<0.005	In existing speciation as 4-methyloctane
C9 naphthen	42.7	<0.005	assume as 1,2,3,5-tetramethylcyclohexane
1,2,4-tri-methyl-cyclohexane		<0.005	In existing speciation as 1,2,4-trimethylcyclohexane
iso-butyl-cyclopentane	42.3	<0.005	
N.I		<0.005	unspeciated
2,2-di-methyl-octane	36.2	<0.005	
N.I		<0.005	unspeciated
N.I		<0.005	unspeciated
N.I		<0.005	unspeciated
N.I		<0.005	unspeciated
N.I		<0.005	unspeciated
N.I		<0.005	unspeciated
N.I		<0.005	unspeciated
N.I		<0.005	unspeciated
Total		99.99	

