Landolt-Börnstein Indexes of Organic Compounds

Subvolumes A-I

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Scidex Database online with graphical structure search on http://lb.chemie.uni-hamburg.de/

Or the easy to use html version on http://lb.chemie.uni-hamburg.de/static/

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Numerical Data and Functional Relationships in Science and Technology
New Series / Editor in Chief: W. Martienssen

Index of Organic Compounds

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Compounds with 8 to 12 Carbon Atoms

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Preface

This index is a guide to organic compounds which have material constants of general interest described in the Landolt-Börnstein / New Series. Compiled are volumes containing molecular constants, density, surface tension, dielectric constants, refractive index, vapor pressure, phase transition temperatures and transition enthalpies. In total in the subvolumes A, B and C, 16823 compounds with 33816 references to numerical data are recorded. All compounds are given with the drawing of the chemical structure, the molecular formula, chemical names, the Chemical Abstracts registration numbers (CAS-RN) and references to Landolt-Börnstein citations, including their occurence in binary mixtures.

This index ist the first step to a full electronisation of all Landolt-Börnstein volumes that have been published to date. The goals are, to create a material knowledge system, to provide a means of accessing all the data in electronic form and to be able to search effectively specific data. Parallel to the electronisation, the data will be indexed, similar to these volumes.

The referenced volumes contain only text descriptions of the chemical structures: name, CAS-RN and molecular formula. This data was assembled, analysed and matched with each other to yield a list of individual compounds without duplicates. This work becomes sometimes non-trivial because compounds can have multiple chemical names and even CAS-RN are sometimes not unique due to out-dated numbers (CAS-DR) and specialized CAS-RN (for trade names, partly defined stereo-chemistry, or individual characteristics more detailed than the drawing sketch). Furthermore, about 17000 structure drawings had to be prepared for all compounds, including the exact stereo information. All this data assembly has been performed with the new, object-oriented database technology SciDex.

The index is prepared in two different forms: a printed book in three subvolumes and an electronical database. Up to now, many users prefer printed books to electronical media. Books can show a large amount of information in high printing quality with one single glance. They are documents which survive all changes of computer systems and operating systems. Of course, the electronical version gives more functionality to the data, e.g. substructure search and structure comparison methods. Further, the electronical version contains additional links to third party references (Beilstein and LiqCryst registration numbers) as well as more alternative compound names.

Scientific data are not only numbers and words, but also rules, principles and complex data like molecular structures, spectra and reaction conditions, which have multiple relations between each other. Scientific information with the purpose of documentation can be handled with conventional relational databases. Scientific information with the function of a knowledge base with analysis and prediction methods require new methods, i.e. object oriented methods. ‘Objects’ are scientific data, connected with scientific rules and the relations to other data. A search for a particular information is an operator working on the documented knowledge: find, interpolate, deduce or calculate the requested data.

Some electronical media of chemical information are already established, e.g. Chemical Abstracts Service, Beilstein, SpecInfo, Brookhaven etc. The Landolt-Börnstein series contains numerical, evaluated data relevant for chemistry and physics, which is not limited by publication years, or restricted to single measurement spots. Thus, the electronical Landolt-Börnstein will yield a novel, powerful tool for quantitative structure/activity relationships (QSAR, QSPR) as well as reference, analysis and prediction instrument for physical chemistry.

Only evaluated data can be used as basis for a knowledge base. The critical work of the several, individual specialists as authors of the Landolt-Börnstein is here continued by the careful compilation and analysis of the full list of organic compounds. This could only be done by the decisive and competent help of Dipl. Chem. Gaja Peters, Sven Gerber and Oliver Konrad. We also thank Dr. Jürgen Vogt for his helpful comments. The Landolt-Börnstein team, and particular Dr. Rainer Poerschke and Dr. Hans Seemüller, jointly support this project.

Hamburg, November 1999

The Editor

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Subvolume D and following are to be supplements to subvolumes A through C

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Introduction

1 General remarks

1.1 Selection of data

1.1.1 Resources

The organic compounds compiled in this index have been extracted from the following volumes of the Landolt-Börnstein.

LB Volume	Data Description
II/4	Molecular constants from microwave spectroscopy
II/6	Molecular constants from microwave, molecular beam and ESR spectroscopy
II/14 a,b	Molecular constants mostly from microwave, molecular beam and ESR spectroscopy
II/19 a,b,c,d1,d2	Molecular constants mostly from microwave, molecular beam, ESR and sub-Doppler laser spectroscopy
III/38 a,b	Optical constants: refractive indices
IV/6	Dielectric constants
IV/7 a,b,c,d,e,f	Phase transitions of liquid crystals
IV/8 a,b,c,d,e,f	Thermodynamic properties: enthalpy of fusion, density
IV/16	Surface tension
IV/20 a	Vapor pressure of chemicals

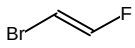
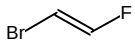
These volumes contain data of organic compounds which have multiple interests and applications. Further, the dependencies between these data can be used for QSPR. Volumes, which contain only specialized data or are not focused on organic molecules are not included here.
The six subvolumes of IV/7 (Phase transitions of liquid crystals) contain more than 40,000 compounds, whereas the other volumes combined contain about 17,000 compounds. The volume IV/7 is organised like an index itself and contains mainly data of specific interest. Therefore, and because it contains also more than two times as much as all the other volumes, only those compounds from IV/7 are recorded here, which are also referenced in other volumes.

1.1.2 Compounds

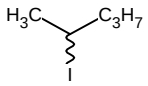
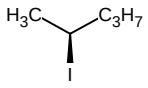
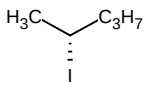
All compounds with at least one carbon atom are selected for this index. Also, binary mixtures including at least one organic compound are recorded. Mixtures which form molecular complexes with an exact relation (e.g. 1:1, 1:2) between the molecules are treated as one compound with an individual registration number. References to the single compounds will be given and marked with (S) behind the number. As well single compounds, which are part of such a defined mixture, will give a reference to it, denoted by (M) behind the number. These mixtures are mainly from the volumes with spectroscopic data (II/4, II/6, II/14 and II/19). Mixtures with variable concentrations are listed with the components, these are from volumes for material properties (III/38, IV/6 and IV/16).

Sometimes a compound is not identified uniquely in the primary literature, when the compound is described with partially defined stereo-chemistry. This is often the case when double bonds are involved that can be *trans* or *cis* configured, or when the compound contains asymmetric carbon atoms, or any combination of asymmetric carbon atoms and asymmetric substituted double bonds.

Two examples shall demonstrate this: The first shows an excerpt where a compound exists in unspecified configuration, and in *trans*-configuration or *cis*-configuration, therewith resulting in three entries in the table. The second example shows a compound that is three times clearly defined as R- or S- enantiomer and as racemate, and once is unspecified. Since nobody can know which configuration the unspecified compound corresponds to, it will get an entry of its own.

630	C_2H_2BrF 124.95 460-11-7		1-bromo-2-fluoro-ethene	**III/38b 2.1:1022**
631	C_2H_2BrF 124.95 2366-32-7		*trans*-1-bromo-2-fluoro-ethylene	**III/38b 2.1:1023**
632	C_2H_2BrF 124.95 2366-31-6		*cis*-1-bromo-2-fluoro-ethylene	**III/38b 2.1:1024**

Example 1: unspecified double bond, *trans* and *cis*-configuration, respectively

3556	$C_5H_{11}I$ 198.05 637-97-8		2-iodo-pentane	**III/38b 2.1:2648**
3557	$C_5H_{11}I$ 198.05 52152-72-4		(±)-2-iodo-pentane	**IV/16 2.1.7:828**
3558	$C_5H_{11}I$ 198.05 29882-59-5		(S)-2-iodo-pentane	**III/38b 2.1:2647**
3559	$C_5H_{11}I$ 198.05 29117-45-1		(R)-2-iodo-pentane	**III/38b 2.1:2646**

example 2: unspecified, racemate, R and S-enantiomer, respectively

As seen in the second example, unspecified stereo-bonds will usually be displayed with a wavy line in place of the wedge or dashed bond that specifies exact stereo-chemistry. Unspecified double bonds are usually drawn the same way as a *trans*-bond.

Since the data are excerpted from multiple volumes, sometimes inconsistencies in the data arose, for example occured in very few cases a mismatch between compound names, formula, and sometimes CAS-RN. The editor chose in most of these cases the CAS-RN, if a valid CAS-RN was given, and the compound name in all other cases as the most representative determination of the structure.

1.2 Drawing of structures

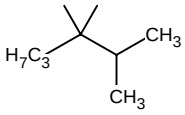
1.2.1 General remarks

The orientation of the structures has been optimised for space saving, to reduce the amount of total pages needed as much as possible. The bond-length of the structures was normalized where possible. In case of large structures, the bond-length was proportionally decreased, so that the compound would fit into the table cell.

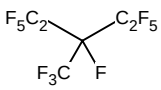
All structures are saved in the electronic version with their complete connectivity, but for display one can choose to abbreviate drawings, so as to make the structures easier readable. The printed version contains in all cases these abbreviated structures.

1.2.2 Methods of abbreviation of drawings

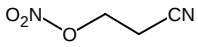
Alkyl chains: Alkyl chains of C_2 and longer are always abbreviated as a textstring, like C_3H_7 as in the example. Methyl groups are in most cases displayed as CH_3, except at quartary centers, to facilitate the reading of highly branched structures. The following example shows two CH_3-groups to the right, while the two groups in the middle are connected to a quartary center and only displayed as an "empty" line.

8124	C_9H_{20} 128.26 16747-28-7		2,3,3-trimethylhexane	**III/38b 2.1:5323;** **IV/8b 2.3:67;** **IV/16 2.1.7:1745;** **IV/20a 2.2:534**

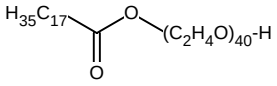
Persubstituted chains: Alkyl chains that are persubstituted with a particular element, like Fluor, or Deuterium are shortened just like in the above example. CF_3 or CD_3 will for obvious reasons never be omitted as CH_3.

3772	C_6F_{14} 338.04 865-71-4		perfluoro-3-methylpentane; undecafluoro-3- (trifluoromethyl)pentane	**IV/20a 4.4:1039**

Special groups: For example cyano groups, nitro groups as well as carbonic acids will be abbreviated in the drawing.

1379	$C_3H_4N_2O_3$ 116.08 50434-02-1		nitric acid 2-cyano-ethyl ester	**III/38b 2.1:1286**

Poly-ethoxy chains: will be identified and shortened as well.

16821	$C_{98}H_{196}O_{42}$ 2046.63 9004-99-3		myrj 52	**IV/16 2.1.7:2704**

1.3 Sort criteria

1.3.1 Sort criteria for index by molecular formula and chemical structures

The compounds are sorted according to the following criteria, in descending precedence.

1. Molecula formula
2. Ring count
3. Ring size
    a) Ring size of smallest ring
    b) Size of other rings
4. Number of branches in a compound (linearity)
5. Number of substituents on rings
6. Substituent count at highest substituted atom
7. Stereochemistry

1.3.2 Sort criteria for index by Chemical Abstracts registration numbers (CAS-RN)

This index is simply sorted by the numerical value of the CAS-RN and points for each CAS-RN to the running number in the index by molecular formula. Out-dated, deleted CAS-RN (= CAS-DR) have been included in this index, and are displayed in the CAS index in *italics* and marked additionally with a star *.

1.4 Reference description

The reference shortcut can be used to directly localize the compounds in the LB volumes. Because every volume contains an individual way of naming subvolumes, chapters and tables, slightly differing ways of descriptions were applied. In general, an entry will look like <group>/<volume><subvolume> <chapter>.<section>:<compound>, e.g. IV/20a 3.1:53 → the compound can be found in volume IV/20a in chapter 3, section 1, and has the running number 53 in that chapter or volume. The only exception is the volume IV/8a, which has no running numbers, so that the page-number in that volume is recorded instead. For a detailed description of the references in the various volumes, see the following table.

LB Vol. Citation	Description
II/4 2.b:c	chapter 2; section ‘b’; compound ‘c’
II/6 a.b:c (or) 2.b.bb:c	chapter ‘a’; section ‘b’ or ‘b.bb’; compound ‘c’
II/14x a.b.bb:c	subvolume ‘x’ (a or b); chapter ‘a’; section ‘b.bb’ (sometimes ‘b.bb.bbb’); compound ‘c’
II/19x 2.b.bb:c	subvolume ‘x’ (a to c, d1, d2); section ‘b.bb’ (sometimes ‘b.bb.bbb’); compound ‘c’
III/38a a.1:c	chapter ‘a’ (2 = pure liquids, 3 = binary mixtures); section 1; compound ‘c’
III/38b 2.1:c	chapter 2; section 1; compound ‘c’ (only single compounds)
IV/6 a.1:c (or) a.1.bb:c	chapter ‘a’ (2 = pure liquids, 3 = binary mixtures); section 1 or ‘1.bb’; compound ‘c’
IV/7x a.b:c	subvolume ‘x’ (a to f); chapter ‘a’; section ‘b’; compound ‘c’
IV/8a 3.5.bb, p. d	section ‘bb’; page ‘d’ (no running numbers for this subvolume)
IV/8x a.b:c	subvolume ‘x’ (b to f); chapter ‘a’; section ‘b’; compound ‘c’
IV/16 a.1.bb:c	chapter ‘a’ (2 = pure liquids, 3 = binary mixtures); section ‘1.bb’; compound ‘c’
IV/20x a.b:c	subvolume ‘x’ (always a); chapter ‘a’; section ‘b’; compound ‘c’

1.5 Table structure

1.5.1 Index by molecular formula and chemical structures

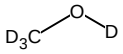
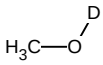
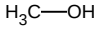
The table is organized in five columns as follows:

Column	Contents
1	Running number of the compound
2	Molecular formula; Molecular mass [g/mol]; CAS-RN
3	Chemical structure drawing If applicable also references to isotopes, molecular mixtures, single compounds
4	Compound name(s)
5	Landolt-Börnstein references Single compound references are written out in full, mixtures are preceded with the word ‘Mixtures:’ and written in a concatenated format.

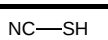
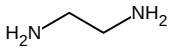
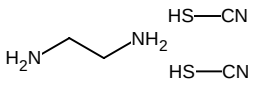
In order to facilitate the search for a particular compound in the large amount of data, the carbon count of the first molecule in the current page will be displayed at the top of each page, and the table will show a dividing horizontal bar between two compounds with differing carbon count.

In some cases, the third column will show crossreferences to other entries in the index-file. This applies for structures which have a deuterated and a "normal" form in the database, and for structures which are either part of a binary defined micture, or are a defined mixture themselves. The crossreference contains always the running number plus an identifier for the relationship. The relationships H, D, M and S are defined as follows:

- H The crossreference shows the same compound non-deuterated
- D The crossreference shows the same compound (possibly partly) deuterated
- M This compound is also part of a defined binary mixture
- S Crossreference to the single compounds of a defined mixture.

71	CD_4O 36.07 811-98-3	 see also: **263**(H), **327**(H)	tetradeuterio-methanol	**III/38b 2.1:918**
263	CH_3DO 33.05 1455-13-6	 see also: **71**(D), **327**(H)	O-deuterio-methanol; methanol-D_1; methyl alcohol-d	**III/38b 2.1:952;** **IV/6 2.1.3:115;** **IV/8a 3.5.1,p.36**
327	CH_4O 32.04 67-56-1	 see also: **71**(D), **263**(D), **311**(M), **341**(M), **368**(M), **1022**(M)	methanol; methyl alcohol	**II/4 2.5:38;** **II/4 2.6:110;** **[...]** **Mixtures:** **[...]**

Explanation: Compound 71 has two references to compounds with "less Deuterium"
Compound 263 has one reference to 71 which is deuterated, and one to 327, which is "normal"
Compound 327 has two references to the deuterated forms, as well as references to defined binary mixtures.

167	CHNS 59.09 463-56-9	 see also: **2680**(M), **3604**(M), **3618**(M)	hydrogen thiocyanate; thiocyanic acid	**IV/20a 3.1:65**
1037	$C_2H_8N_2$ 60.10 107-15-3	 see also: **2680**(M)	1,2-diaminoethane; dimethylenediamine; ethane-1,2-diamine; 1,2-ethanediamine; ethylenediamine	**II/14a 2.5.2:176;** **II/14a 2.6.3.2:88;** **III/38b 2.1:1171;** **IV/6 2.1.3:198;** **IV/8a 3.5.1,p.52;** **IV/16 2.1.7:495;** **Mixtures:** **III/38a 3.1:22;** **IV/6 3.1:233, 238**
2680	$C_4H_{10}N_4S_2$ 178.28 22205-63-6	 see also: **167**(S), **1037**(S)	ethylenediamine dihydrothiocyanate; thiocyanic acid, compd. with ethylenediamine (2:1)	**IV/8a 3.5.2,p.87**

Explanation: The defined mixture 2680 has two crossreferences to the single compounds
The compounds 1037 and 167 point to their mixture
Compound 167 appears in other defined mixtures with other compounds as well.
Noteworthy is also that compound 1037 has in the LB-references "Mixtures" entries as well, these are mixtures which are not an exact relation, and therefore not taken into the database as a separate entry.

1.5.2 Index sorted by Chemical Abstracts registry numbers

This index combines both entries of actual (current) CAS-RN and deleted (old) Registry Numbers that have been removed from the Chemical Abstracts System, but remain visible as CAS-DR numbers. The CAS-DR numbers will not be shown in the compound index, since in some cases there are very many deleted numbers for one compound.

The table is organized in two columns as follows:

Column	Contents
1	CAS-RN or *CAS-DR**
2	Volume and running number

Out-dated, deleted CAS-RN (= CAS-DR) are displayed in the CAS index in *italics* and marked additionally with a star *.

1.6 Exact volume titles and references

Volume II/4: Molecular Constants from Microwave Spectroscopy
Editors: K.-H. Hellwege, A.M. Hellwege
Author: B. Starck
1967. 67 figs., X, 225 pages. ISBN 3-540-03896-5

Volume II/6: Molecular Constants from Microwave, Molecular Beam, and Electron Spin Resonance Spectroscopy
(Supplement and extension to volume II/4)
Editors: K.-H. Hellwege, A.M. Hellwege
Authors: J. Demaison, W. Hüttner, B. Starck, I. Buck, R. Tischer, M. Winnewisser
1974. 153 figs., XIII, 688 pages. ISBN 3-540-05977-6

Volume II/14: Molecular Constants Mostly from Microwave, Molecular Beam and Electron Resonance Spectroscopy
(Supplement to volumes II/4 and II/6)
Editors: K.-H. Hellwege, A.M. Hellwege
Subvolume a: Diamagnetic Molecules
Authors: J. Demaison, A. Dubrulle, W. Hüttner, E. Tiemann
1982. 196 figs., XI, 788 pages. ISBN 3-540-11365-7

Volume II/14: Molecular Constants Mostly from Microwave, Molecular Beam and Electron Resonance Spectroscopy
(Supplement to volumes II/4 and II/6)
Editors: K.-H. Hellwege, A.M. Hellwege
Subvolume b: Radicals, Diatomic Molecules and Substance Index
Authors: J.M. Brown, J. Demaison, A. Dubrulle, W. Hüttner, E. Tiemann
1983. 196 figs., IX, 373 pages. ISBN 3-540-11857-8

Volume II/19: Molecular Constants Mostly from Microwave, Molecular Beam, and Sub-Doppler Laser Spectroscopy
(Supplement to volumes II/4, II/6 and II/14)
Editor: W. Hüttner
Subvolume a: Rotational, l-type, Centrifugal Distortion and Related Constants of Diamagnetic Diatomic, Linear, and Symmetric Top Molecules
Authors: J. Demaison, W. Hüttner, E. Tiemann, G. Wlodarczak
1992. XI, 143 pages. ISBN 3-540-54409-7

Volume II/19: Molecular Constants Mostly from Microwave, Molecular Beam, and Sub-Doppler Laser Spectroscopy
(Supplement to volumes II/4, II/6 and II/14)
Editor: W. Hüttner
Subvolume b: Rotational, Centrifugal Distortion and Related Constants of Diamagnetic Asymmetric Top Molecules
Authors: J. Demaison, W. Hüttner, J. Vogt, G. Wlodarczak,
1992. XI, 488 pages. ISBN 3-540-54578-6

Volume II/19: Molecular Constants Mostly from Microwave, Molecular Beam, and Sub-Doppler Laser Spectroscopy

(Supplement to volumes II/4, II/6 and II/14)
Editor: W. Hüttner
Subvolume c: Dipole Moments, Quadrupole Coupling Constants, Hindered Rotation and Magnetic Constants of Diamagnetic Molecules
Authors: J. Demaison, W. Hüttner, E. Tiemann, J. Vogt, G. Wlodarczak
1992. 8 figs., XI, 295 pages. ISBN 3-540-54893-9

Volume II/19: Molecular Constants Mostly from Microwave, Molecular Beam, and Sub-Doppler Laser Spectroscopy

(Supplement to volumes II/4, II/6 and II/14)
Editor: W. Hüttner
Subvolume d1: Diatomic Radicals and Ions
Author: E. Tiemann
1995.VIII, 208 pages. ISBN 3-540-55462-9

Volume II/19: Molecular Constants Mostly from Microwave, Molecular Beam, and Sub-Doppler Laser Spectroscopy

(Supplement to volumes II/4, II/6, and II/14)
Editor: W. Hüttner
Subvolume d2: Polyatomic Radicals and Ions
Author: J.M. Brown
1995. VIII, 355 pages. ISBN 3-540-58210-X

Volume III/38: Optical Constants

Editors: M.D. Lechner
Subvolume a: Refractive Indices of Inorganic, Organometallic, and Organononmetallic Liquids and Binary Liquid Mixtures
Authors: Ch. Wohlfarth, B. Wohlfarth
1996. VII, 400 pages. ISBN 3-540-60539-8

Volume III/38: Optical Constants

Editors: M.D. Lechner
Subvolume b: Refractive Indices of Organic Liquids
Authors: Ch. Wohlfarth, B. Wohlfarth
1996. VII, 421 pages. ISBN 3-540-60596-7

Volume IV/6: Static Dielectric Constants of Pure Liquids and Binary Liquid Mixtures

Editor: O. Madelung
Author: Ch. Wohlfarth
1991. VIII, 521 pages. ISBN 3-540-54417-8

Volume IV/7: Liquid Crystals

Editor: J. Thiem
Subvolume a: Transition Temperatures and Related Properties of One-Ring Systems and Two-Ring Systems without Bridging Groups
Author: V. Vill
1992. 10 figs., VIII, 268 pages. ISBN 3-540-55503-X

Volume IV/7: Liquid Crystals
Editor: J. Thiem
Subvolume b: Transition Temperatures and Related Properties of Two-Ring Systems with Bridging Group
Author: V. Vill
1992. 10 figs., VIII, 653 pages. ISBN 3-540-55504-8

Volume IV/7: Liquid Crystals
Editor: J. Thiem
Subvolume c: Transition Temperatures and Related Properties of Three-Ring Systems without Bridging Groups
Author: V. Vill
1993. 10 figs., VIII, 228 pages. ISBN 3-540-56136-6

Volume IV/7: Liquid Crystals
Editor: J. Thiem
Subvolume d: Transition Temperatures and Related Properties of Three Ring Systems with One Bridging Group
Author: V. Vill
1994. VIII, 527 pages. ISBN 3-540-56757-7

Volume IV/7: Liquid Crystals
Editor: J. Thiem
Subvolume e: Transition Temperatures and Related Properties of Three Ring Systems with Two Bridging Groups
Author: V. Vill
1995. VIII, 612 pages. ISBN 3-540-56758-5

Volume IV/7: Liquid Crystals
Editor: J. Thiem
Subvolume f: Transition Temperatures and Related Properties of Four Ring Systems, Five Ring Systems, and More than Five Rings
Author: V. Vill
1995. VIII, 589 pages. ISBN 3-540-58853-1

Volume IV/8: Thermodynamic Properties of Organic Compounds and their Mixtures
Editor: K.N. Marsh
Subvolume a: Enthalpies of Fusion and Transition of Organic Compounds
Authors: Z.-Y- Zhang, M- Frenkel, K.N. March, R.C. Wilhoit
1995. VIII, 588 pages. ISBN 3-540-58854-X

Volume IV/8: Thermodynamic Properties of Organic Compounds and their Mixtures
Editor: K.N. Marsh
Subvolume b: Densities of Aliphatic Hydrocarbons: Alkanes
Authors: R.C. Wilhoit, K.N. Marsh, X. Hong, N. Gadalla, M. Frenkel
1996. 119 figs., X, 410 pages. ISBN 3-540-61029-4

Volume IV/8: Thermodynamic Properties of Organic Compounds and their Mixtures
Editor: K.N. March
Subvolume c: Densities of Aliphatic Hydrocarbons: Alkenes, Alkadienes, Alkynes, and Miscellaneous Compounds
Authors: R.C. Wilhoit, K.N. Marsh, X. Hong, N. Gadalla, M. Frenkel
1996. 78 figs., X, 381 pages. ISBN 3-540-61554-7

Volume IV/8: Thermodynamic Properties of Organic Compounds and their Mixtures

Editor: K.R. Hall, K.N.Marsh
Subvolume d: Densities of Monocyclic Hydrocarbons
Authors: R.C. Wilhoit, X. Hong, M. Frenkel, K.R. Hall
1997. 117 figs., XIV, 466 pages. ISBN 3-540-62509-7

Volume IV/8: Thermodynamic Properties of Organic Compounds and their Mixtures

Editor: K.R. Hall, K.N.Marsh
Subvolume e: Densities of Aromatic Hydrocarbons
Authors: R.C. Wilhoit, X. Hong, M. Frenkel, K.R. Hall
1998. X, 373 pages. ISBN 3-540-62510-0

Volume IV/8: Thermodynamic Properties of Organic Compounds and their Mixtures

Editor: K.R. Hall, K.N.Marsh
Subvolume f: Densities of Polycyclic Hydrocarbons
Authors: R.C. Wilhoit, X. Hong, M. Frenkel, K.R. Hall
1999. XI, 538 pages, ISBN 3-540-65162-4

Volume IV/16: Surface tension of pure liquids and binary mixtures

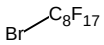
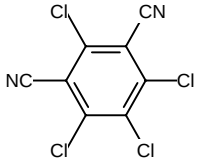
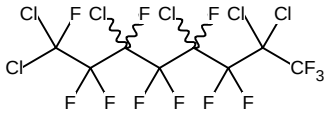
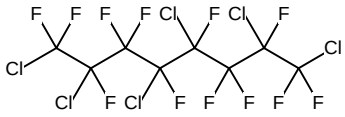
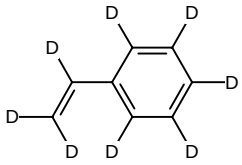
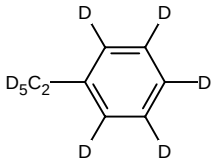
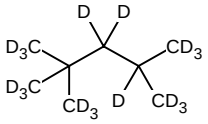
Editor: M.D. Lechner
Authors: Ch. Wohlfarth, B. Wohlfarth
1997. VII, 439 pages. ISBN 3-540-63276-X

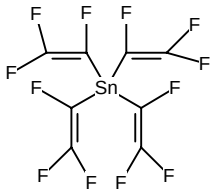
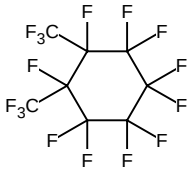
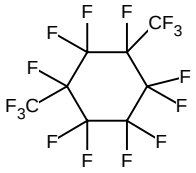
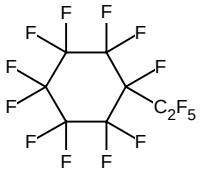
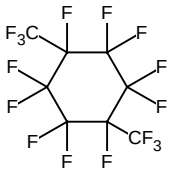
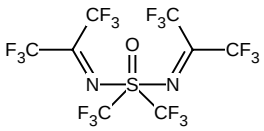
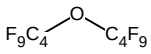
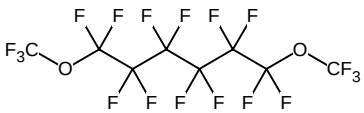
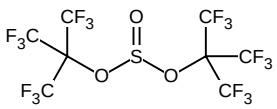
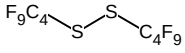
Volume IV/20: Vapor Pressure of Chemicals

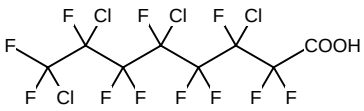
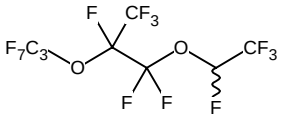
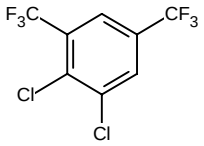
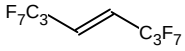
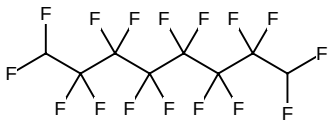
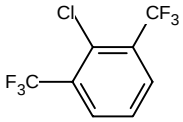
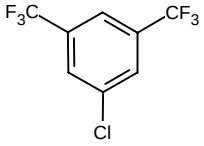
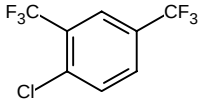
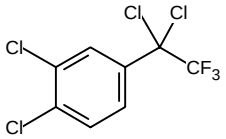
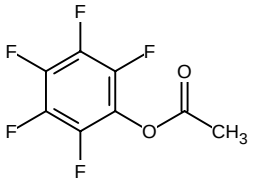
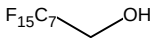
Editor: K.R. Hall
Subvolume a: Vapor Pressure and Antoine Constants for Hydrocarbons and Sulfur -, Selenium -, Tellurium -, and Halogen – Containing Organic Compounds
Authors: J. Dykyj, J. Svoboda, R. C. Wilhoit, M. Frenkel, K. R. Hall
1999. VIII, 373 pages. ISBN 3-540-64735-X

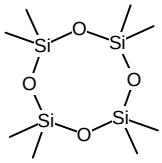
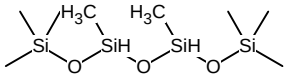
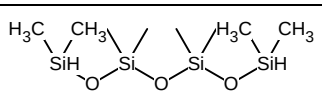
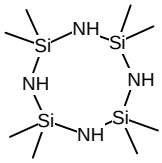
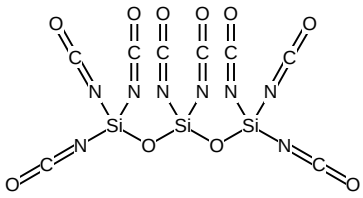
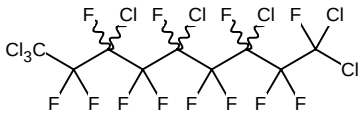
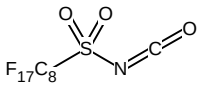
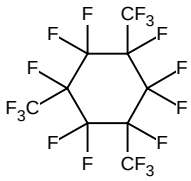
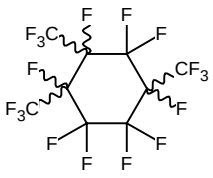
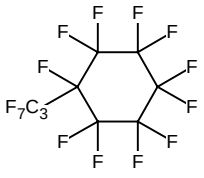
Data

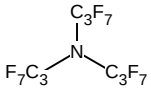
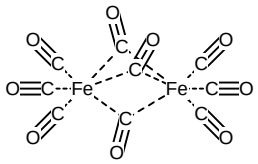
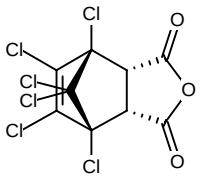
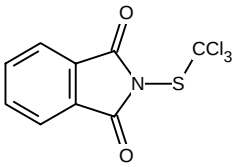
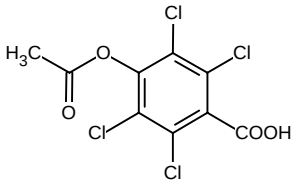
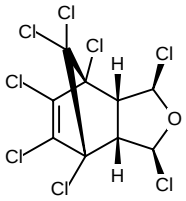
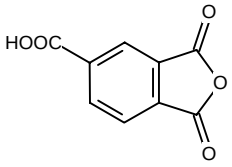
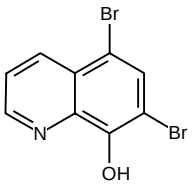
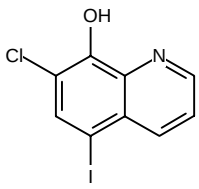
2 Tabulated index sorted by molecular formula and chemical structures

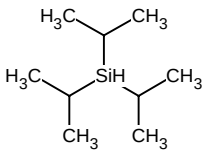
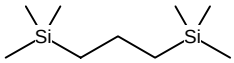
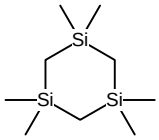
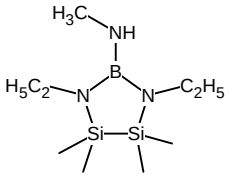
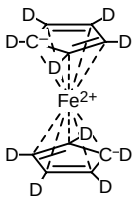
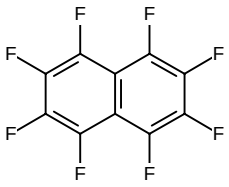
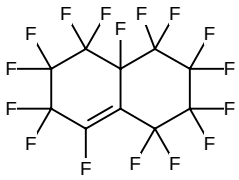
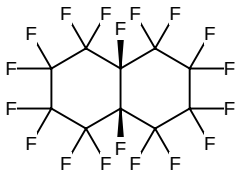
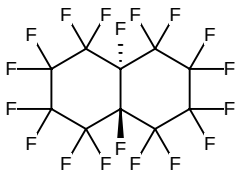
5953	C_8BrF_{17} 498.97 423-55-2		1-bromo-heptadecafluoro-octane	**IV/16 2.1.7:1325**
5954	$C_8Cl_4N_2$ 265.92 1897-45-6		chlorophthalonil; 2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile; 2,4,5,6-tetrachloro-1,3-isophthalonitrile; tetrachlorobenzene-1,3-dicarbonitrile	**IV/8a 3.5.4,p.184;** **IV/20b 4.5:1281**
5955	$C_8Cl_6F_{12}$ 536.79 57504-37-7		1,1,3,5,7,7-hexachloro-1,2,2,3,4,4,5,6,6,8,8,8-dodecafluoro-octane	**IV/16 2.1.7:1326**
5956	$C_8Cl_6F_{12}$ 536.79 647-20-1		hexachloro-1,1,2,3,3,4,5,5,6,7,7,8-dodecafluorooctane; 1,2,4,5,7,8-hexachloro-dodecafluoro-octane	**III/38b 2.1:4162;** **IV/6 2.1.3:1027**
5957	C_8D_8 112.20 19361-62-7	 see also: **6098**(H)	styrene-d8	**IV/8a 3.5.4,p.188**
5958	C_8D_{10} 116.23 25837-05-2	 see also: **6242**(H)	decadeutero-ethylbenzene	**IV/16 2.1.7:1327**
5959	C_8D_{18} 132.34	 see also: **7001**(H)	octadecadeuterio-2,2,4-trimethyl-pentane	**III/38b 2.1:4163**
5960	C_8D_{18} 132.34 17252-77-6	C_8D_{18} see also: **6985**(H)	octadecadeuterio-octane; octadecadeutero-octane	**III/38b 2.1:4164;** **IV/16 2.1.7:1328**

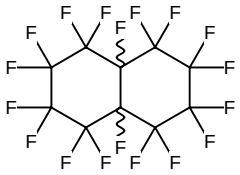
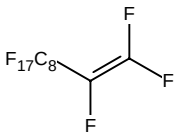
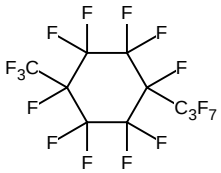
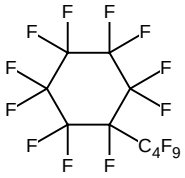
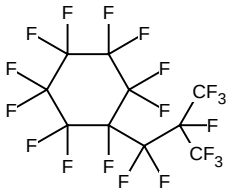
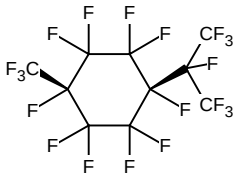
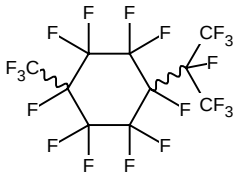
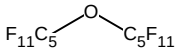
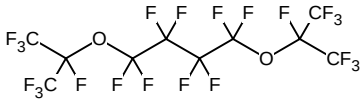
5961	$C_8F_{12}Sn$ 442.76 756-25-2		tetrakis-(trifluoro-ethenyl)-stannane	**III/38a 2.1.2:102**
5962	C_8F_{16} 400.06 306-98-9		decafluoro-1,2-bis-trifluoromethyl-cyclohexane; perfluoro-1,2-dimethyl-cyclohexane	**III/38b 2.1:4165;** **IV/16 2.1.7:1329**
5963	C_8F_{16} 400.06 335-27-3		cyclohexane, 1,1,2,2,3,3,4,5,5,6-decafluoro-4,6-bis(trifluoromethyl)-; decafluoro-1,3-bis(trifluoromethyl)cyclohexane; perfluoro-1,3-dimethylcyclohexane	**III/38b 2.1:4166;** **IV/6 2.1.3:1028;** **IV/20b 4.5:1282**
5964	C_8F_{16} 400.06 335-21-7		hexadecafluoroethylcyclohexane; pentafluoroethylundecafluorocyclohexane; perfluoroethyl-cyclohexane	**IV/20b 4.5:1283**
5965	C_8F_{16} 400.06 374-77-6		perfluoro-1,4-dimethyl-cyclohexane	**IV/16 2.1.7:1330**
5966	C_8F_{18} 438.06 307-34-6	C_8F_{18}	octadecafluorooctane; perfluorooctane	**III/38b 2.1:4167;** **IV/8a 3.5.4,p.184;** **IV/16 2.1.7:1331;** **IV/20b 4.5:1284**
5967	$C_8F_{18}N_2OS$ 514.14		oxobis(trifluoro-methyl)bis[[2,2,2-trifluoro-1-(trifluoro-methyl)ethylidene]-amino]sulfur	**IV/20b 3.2:404;** **IV/20b 4.5:1285**
5968	$C_8F_{18}O$ 454.06 308-48-5		bis(nonafluorobutyl)ether; perfluoro-1-butoxybutane; perfluorodibutyl ether	**IV/16 2.1.7:1332;** **IV/20b 4.5:1286**
5969	$C_8F_{18}O_2$ 470.06		dodecafluoro-1,6-bis(trifluoromethoxy)hexane	**IV/20b 4.5:1287**
5970	$C_8F_{18}O_3S$ 518.12 53517-90-1		sulfuric acid, bis[2,2,2-trifluoro-1,1-bis(trifluoromethyl)ethyl] ester	**IV/20b 3.2:405**
5971	$C_8F_{18}S_2$ 502.19 42060-69-5		bis(nonafluorobutyl) disulfide	**IV/20b 3.2:406**

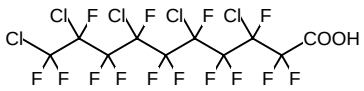
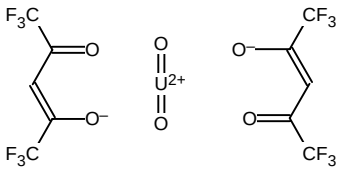
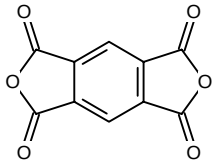
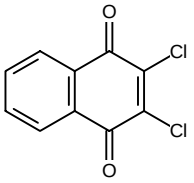
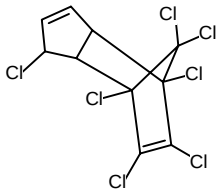
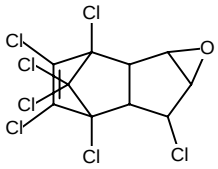
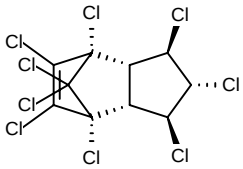
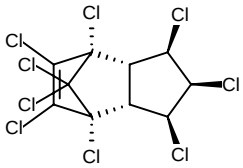
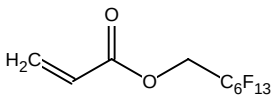
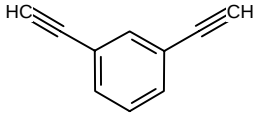
5972	$C_8HCl_4F_{11}O_2$ 479.89 2923-68-4		3,5,7,8-tetrachloro-undecafluoro-octanoic acid	**IV/16 2.1.7:1333;** **IV/20b 4.5:1288**
5973	$C_8HF_{17}O_2$ 452.07 3330-14-1		1,1,1,2,3,3-hexafluoro-2-(1,1,2,2,3,3,3-heptafluoro-propoxy)-3-(1,2,2,2-tetrafluoro-ethoxy)-propane	**IV/16 2.1.7:1334**
5974	$C_8H_2Cl_2F_6$ 283.00 327-73-1		1,2-dichloro-3,5-bis(trifluoromethyl)benzene	**III/38b 2.1:4168;** **IV/6 2.1.3:1029**
5975	$C_8H_2F_{14}$ 364.08 3910-82-5		1,1,1,2,2,3,3,6,6,7,7,8,8,8-tetradecafluoro-4-octene	**IV/20b 4.5:1289**
5976	$C_8H_2F_{16}$ 402.08 307-99-3		1,8-dihydrohexadecafluorooctane; 1H,8H-hexadecafluorooctane; octane, 1,8-dihydrohexadecafluoro-	**IV/20b 4.5:1290**
5977	$C_8H_3ClF_6$ 248.56 63430-02-4		2-chloro-1,3-bis(trifluoromethyl)benzene	**IV/6 2.1.3:1030**
5978	$C_8H_3ClF_6$ 248.56 328-72-3		benzene, 5-chloro-1,3-bis(trifluoromethyl)-; 5-chloro-1,3-bis(trifluoromethyl)-benzene; 5-chloro-1,3-bis(trifluoromethyl)benzene	**IV/20b 4.5:1292**
5979	$C_8H_3ClF_6$ 248.56 327-76-4		4-chloro-1,3-bis(trifluoromethyl)benzene; 1-chloro-2,4-bis-trifluoromethyl-benzene	**III/38b 2.1:4169;** **IV/6 2.1.3:1031;** **IV/20b 4.5:1291**
5980	$C_8H_3Cl_4F_3$ 297.92 328-82-5		1,1-dichloro-1-(3,4-dichlorophenyl)-2,2,2-trifluoroethane; 1,2-dichloro-4-(1,1-dichloro-2,2,2-trifluoroethyl)benzene	**IV/20b 4.5:1293**
5981	$C_8H_3F_5O_2$ 226.10 19220-93-0		pentafluorophenyl acetate	**IV/20b 4.5:1294**
5982	$C_8H_3F_{15}O$ 400.09 307-30-2		1,1-dihydroperfluorooctanol; (pentadecafluoroheptyl)methanol; (perfluoroheptyl)methanol	**IV/20b 4.5:1295**

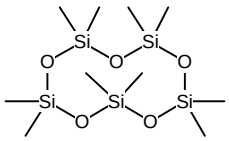
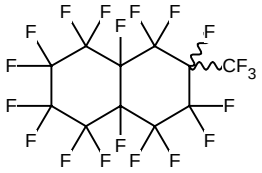
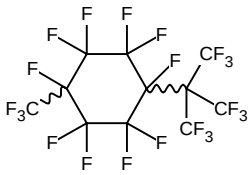
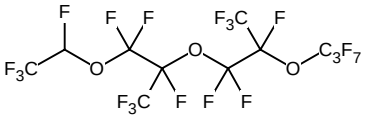
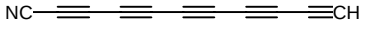
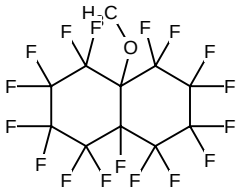
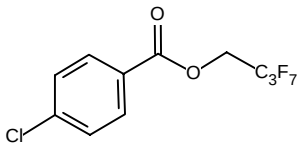
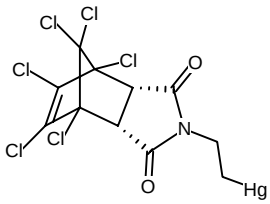
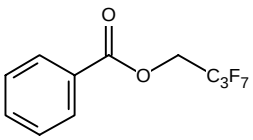
7210	$C_8H_{24}O_4Si_4$ 296.62 556-67-2		octamethylcyclotetrasiloxane; tetracyclosiloxane, octamethyl-	**III/38a 2.1.5:477;** **IV/6 2.1.3:1236;** **IV/8a 3.5.4,p.209;** **IV/16 2.1.5:219;** **Mixtures:** **IV/16 3.1.4:128, 721**
7211	$C_8H_{26}O_3Si_4$ 282.64 16066-09-4		1,1,1,3,5,7,7,7-octamethyl-tetrasiloxane	**III/38a 2.1.5:478**
7212	$C_8H_{26}O_3Si_4$ 282.64 1000-05-1		1,1,3,3,5,5,7,7-octamethyl-tetrasiloxane	**III/38a 2.1.5:479**
7213	$C_8H_{28}N_4Si_4$ 292.68 1020-84-4		2,2,4,4,6,6,8,8- octamethylcyclotetrasilazane	**IV/8a 3.5.4,p.209**
7214	$C_8N_8O_{10}Si_3$ 452.39 17883-45-3		octaisocyanato-trisiloxane	**III/38a 2.1.5:480**
7215	$C_9Cl_8F_{12}$ 619.71 53281-03-1		1,1,1,3,5,7,9,9-octachloro 2,2,3,4,4, 5,6,6,7,8,8,9-dodecafluoro-nonane	**IV/16 2.1.7:1564**
7216	$C_9F_{17}NO_3S$ 525.14 34834-20-3		heptadecafluorooctanesulfonyl isocyanate; octanesulfonyl isocyanate, 1,1,2,2,3,3,4,4, 5,5,6,6,7,7,8,8,8-heptadecafluoro-	**IV/20b 3.2:434;** **IV/20b 4.5:1388**
7217	C_9F_{18} 450.07 374-76-5		perfluoro-1,3,5-trimethyl-cyclohexane	**IV/16 2.1.7:1567**
7218	C_9F_{18} 450.07 423-05-2		perfluoro-1,2,4-trimethyl-cyclohexane	**IV/16 2.1.7:1566**
7219	C_9F_{18} 450.07 374-59-4		perfluoro(propyl-cyclohexane); perfluoro-propylcyclohexane	**IV/16 2.1.7:1565;** **IV/20b 4.5:1389**
7220	C_9F_{20} 488.07 375-96-2	C_9F_{20}	eicosafluorononane; perfluorononane	**III/38b 2.1:4864;** **IV/16 2.1.7:1568;** **IV/20b 4.5:1390**

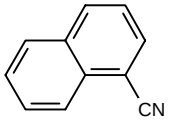
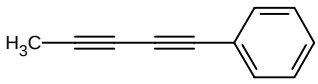
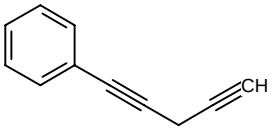
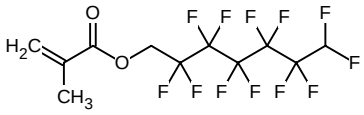
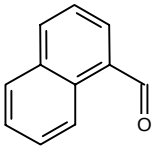
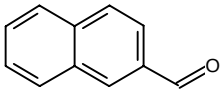
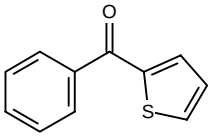
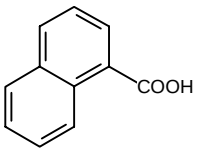
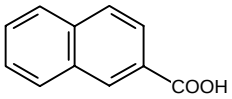
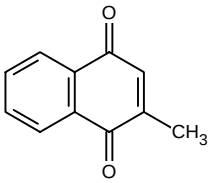
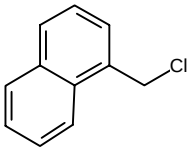
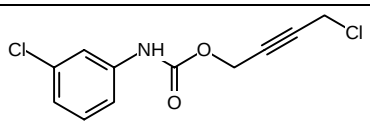
7221	$C_9F_{21}N$ 521.07 338-83-0		tris-heptafluoropropyl-amine	**III/38b 2.1:4865;** **IV/16 2.1.7:1569**
7222	$C_9Fe_2O_9$ 363.79 15321-51-4		nonacarbonyldiiron	**IV/20b 4.5:1391**
7223	$C_9H_2Cl_6O_3$ 370.83 7365-74-4		3aα,4β,7β,7aα-hexachloro-3a,4,7,7a-tetrahydro-4,7-methanoisobenzofuran-1,2-dione; 5-norbornene-2,3-dicarboxylic anhydride, 1,4,5,6,7,7-hexachloro-, *endo*-	**IV/8a 3.5.5,p.213**
7224	$C_9H_4Cl_3NO_2S$ 296.56 133-07-3		folpet; 2-[(trichloromethyl)thio]-1H-isoindole-1,3(2H)-dione	**IV/8a 3.5.5,p.213**
7225	$C_9H_4Cl_4O_4$ 317.94 887-54-7		4-acetoxy-2,3,5,6-tetrachlorobenzoic acid; dacthal monoacid; methyltetrachloroterephthalic acid ester	**IV/8a 3.5.5,p.213**
7226	$C_9H_4Cl_8O$ 411.76 297-78-9		isobenzan; 1,3,4,5,6,7,8,8-octachloro-1,3,3a,4,7,7a-hexahydro-4,7-methanoisobenzofuran	**IV/8a 3.5.5,p.213**
7227	$C_9H_4O_5$ 192.13 552-30-7		1,2,4-benzenetricarboxylic acid 1,2-anhydride; 4-carboxyphthalic anhydride; 5-isobenzofurancarboxylic acid, 1,3-dihydro-1,3-dioxo-; trimellic acid anhydride	**IV/8a 3.5.5,p.214**
7228	$C_9H_5Br_2NO$ 302.96 521-74-4		5,7-dibromo-8-hydroxyquinoline; 5,7-dibromo-8-quinolinol; quinoline, 5,7-dibromo-8-hydroxy-	**IV/20b 4.5:1392**
7229	C_9H_5ClINO 305.50 35048-13-6		chloro-5-iodo-8-quinolinol; 7-chloro-5-iodo-8-quinolinol	**IV/20b 4.5:1393**

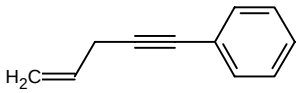
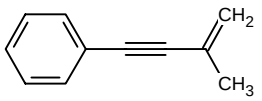
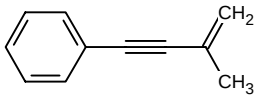
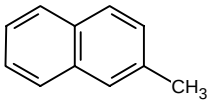
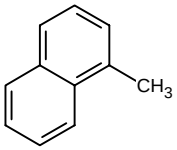
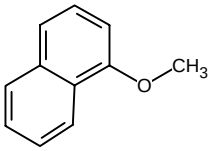
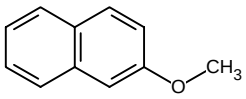
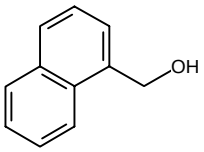
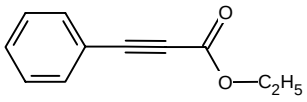
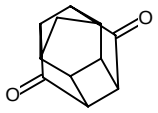
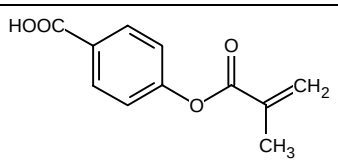
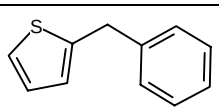
8232	$C_9H_{22}Si$ 158.36 6485-79-6		triisopropyl-silane	**III/38a 2.1.5:513**
8233	$C_9H_{24}Si_2$ 188.46 2295-05-8		1,3-bis(trimethylsilyl)propane; propane, 1,3-bis(trimethylsilyl)-; silane, 1,3-propanediylbis(trimethyl)-	**IV/8a 3.5.5,p.232**
8234	$C_9H_{24}Si_3$ 216.55 1627-99-2		1,1,3,3,5,5-hexamethyl-1,3,5-trisilacyclohexane	**IV/8a 3.5.5,p.232**
8235	$C_9H_{26}BN_3Si_2$ 243.31 112848-89-2		1-methylamino-3,3,4,4-tetramethyl-2,5-diethyl-cyclo-1-bor-3,4-disil-2,5-diazane	**III/38a 2.1.4:232**
8236	$C_{10}D_{10}Fe$ 196.10 12082-87-0	 see also: **8366**(H)	Di(cyclopentadienyl-d5)iron; ferrocene-d10; iron, di(cyclopentadienyl-d5)-	**IV/8a 3.5.5,p.241**
8237	$C_{10}F_8$ 272.10 313-72-4		octafluoronaphthalene; 1,2,3,4,5,6,7,8-octafluoronaphthalene; perfluoronaphthalene	**IV/20b 4.5:1429**
8238	$C_{10}F_{16}$ 424.09 54939-04-7		naphthalene, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-hexadecafluoro-1,2,3,4,5,6,7,8-octahydro-	**IV/8a 3.5.5,p.232**
8239	$C_{10}F_{18}$ 462.08 60433-11-6		*cis*-perfluorodecahydronaphthalene; *cis*-perfluorodecalin	**IV/8a 3.5.5,p.233;** **IV/20b 4.5:1430**
8240	$C_{10}F_{18}$ 462.08 60433-12-7		*trans*-perfluorodecahydronaphthalene; *trans*-perfluorodecalin	**IV/8a 3.5.5,p.233;** **IV/20b 4.5:1431**

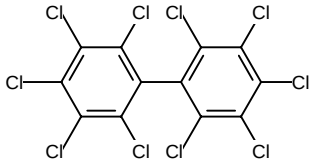
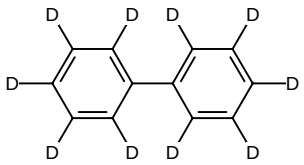
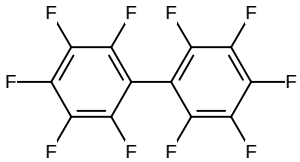
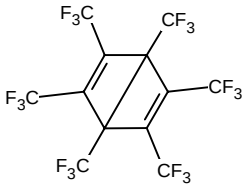
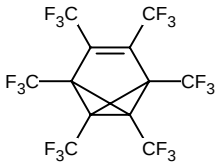
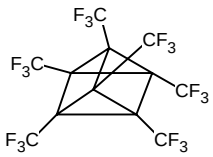
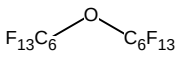
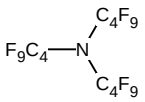
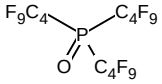
8241	$C_{10}F_{18}$ 462.08 306-94-5		octadecafluoro-decahydro-naphthalene; octadecafluoro-naphthalene	**III/38b 2.1:5360;** **IV/16 2.1.7:1765**
8242	$C_{10}F_{20}$ 500.08 35328-43-9		eicosafluoro-1-decene; eicosofluoro-1-decene; perfluoro-1-decene	**IV/20b 4.5:1432**
8243	$C_{10}F_{20}$ 500.08 80274-98-2		perfluoro-(2-methylpropyl)-cyclohexane	**IV/16 2.1.7:1768**
8244	$C_{10}F_{20}$ 500.08 374-60-7		perfluoro-butyl-cyclohexane	**IV/16 2.1.7:1766**
8245	$C_{10}F_{20}$ 500.08 132868-02-1		perfluoro(isobutylcyclohexane)	**IV/20b 4.5:1434**
8246	$C_{10}F_{20}$ 500.08 116667-53-9		perfluoro-(1-methyl-4-isopropylcyclohexane), *cis*-	**IV/20b 4.5:1433**
8247	$C_{10}F_{20}$ 500.08 423-03-0		perfluoro-1-methyl-4-(1-methylethyl)-cyclohexane; perfluoro-*p*-menthane	**IV/16 2.1.7:1767**
8248	$C_{10}F_{22}$ 538.08 307-45-9	$C_{10}F_{22}$	docosafluorodecane; perfluorodecane	**III/38b 2.1:5361;** **IV/16 2.1.7:1769;** **IV/20b 4.5:1435**
8249	$C_{10}F_{22}O$ 554.08 464-36-8		bis(undecafluoropentyl)ether	**IV/16 2.1.7:1770;** **IV/20b 4.5:1436**
8250	$C_{10}F_{22}O_2$ 570.08 23228-90-2		octafluoro-1,4-bis(heptafluoroisopropoxy)-butane	**IV/16 2.1.7:1771**

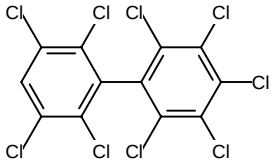
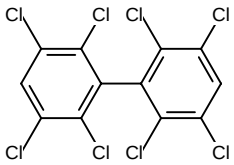
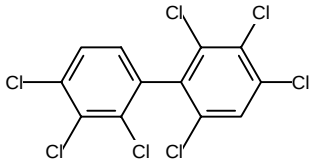
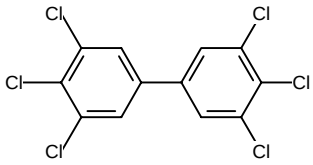
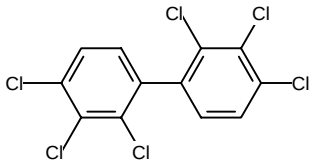
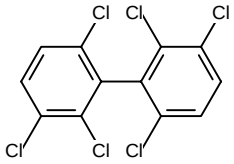
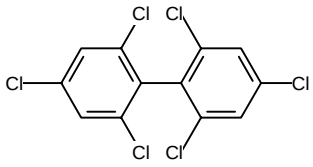
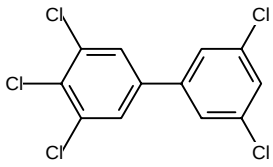
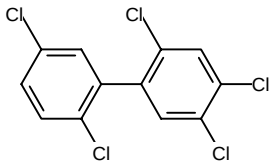
8251	$C_{10}HCl_5F_{14}O_2$ 596.36 335-74-0		3,5,7,9,10-pentachloro-tetradecafluoro-decanoic acid	**IV/16 2.1.7:1772; IV/20b 4.5:1437**
8252	$C_{10}H_2F_{12}O_6U$ 684.14 67316-66-9		bis(1,1,1,5,5,5-hexafluoro(2,4-pentandione)dioxouranium	**IV/20b 4.5:1438**
8253	$C_{10}H_2O_6$ 218.12 89-32-7		1,2,4,5-benzenetetracarboxylic 1,2:4,5-dianhydride; 1H,3H-benzo[1,2-c:4,5-c']difuran-1,3,5,7-tetrone; pyromellitic anhydride	**IV/8a 3.5.5,p.233**
8254	$C_{10}H_4Cl_2O_2$ 227.05 117-80-6		dichlone; 2,3-dichloro-1,4-naphthalenedione; 2,3-dichloro-1,4-naphthoquinone	**IV/8a 3.5.5,p.233**
8255	$C_{10}H_5Cl_7$ 373.32 76-44-8		1H-1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-4-methanoindene; velsicol 104	**IV/8a 3.5.5,p.233**
8256	$C_{10}H_5Cl_7O$ 389.32 1024-57-3		(1aα,1bβ,2α,5α,5aα,6aα)-2,3,4,5,6,7,7-heptachloro-1a,1b,2,5,5a,6,6a-hexahydro-2,5-methano-2H-indeno[1,2-b]oxirene	**IV/8a 3.5.5,p.234**
8257	$C_{10}H_5Cl_9$ 444.23 39765-80-5		*trans*-nonachlordane; (1α,2β,3α,3aα,4β,7β,7aα)-1,2,3,4,5,6,7,8,8-nonachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H-indene	**IV/8a 3.5.5,p.234**
8258	$C_{10}H_5Cl_9$ 444.23 5103-73-1		(1α,2α,3α,4β,7β,7aβ)-1,2,3,4,5,6,7,8,8-nonachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H-indene; *cis*-nonachlordane	**IV/8a 3.5.5,p.234**
8259	$C_{10}H_5F_{13}O_2$ 404.13 559-11-5		acrylic acid 1H,1H-tridecafluoro-heptyl ester	**IV/16 2.1.7:1773**
8260	$C_{10}H_6$ 126.16		1,3-diethynylbenzene	**IV/8e 6:670**

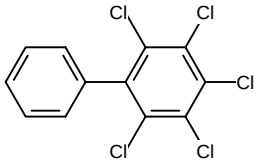
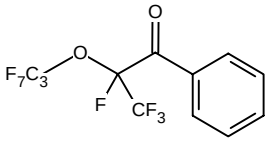
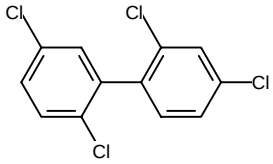
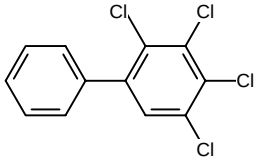
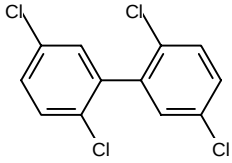
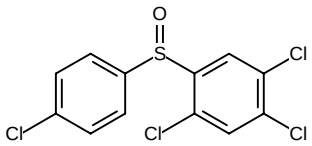
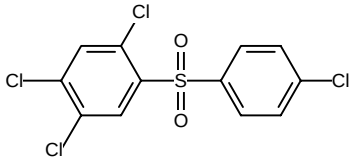
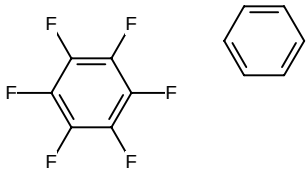
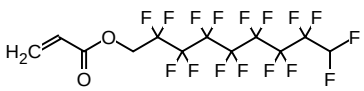
9573	$C_{10}H_{30}O_5Si_5$ 370.78 541-02-6		decamethyl cyclopentasiloxane	**III/38a 2.1.5:550;** **IV/6 2.1.3:1488;** **IV/16 2.1.5:223**
9574	$C_{11}F_{20}$ 512.09 306-92-3		perfluoro-1-methyldecalin; perfluoro-2-methyl-decahydronaphthalene	**III/38b 2.1:6053;** **IV/6 2.1.3:1489;** **IV/16 2.1.7:1962**
9575	$C_{11}F_{22}$ 550.09 75169-50-5		perfluoro(1-methyl-4-tert-butylcyclohexane), (mix *cis*+*trans*)	**IV/16 2.1.7:1963;** **IV/20b 4.6:1474**
9576	$C_{11}F_{24}$ 588.08 307-49-3	$C_{11}F_{24}$	perfluoro-undecane	**IV/16 2.1.7:1964**
9577	$C_{11}F_{24}O_2$ 620.08		octadecafluoro-1,9-bis(trifluoromethoxy)nonane	**IV/20b 4.6:1475**
9578	$C_{11}HF_{23}O_3$ 618.09 3330-16-3		1,1,1,2,3,3-hexafluoro-2-(1,1,2,2,3,3,3-heptafluoro-propoxy)-3-[1,2,2-trifluoro-2-(1,2,2,2-tetrafluoro-ethoxy)-1-trifluoromethyl-ethoxy]-propane	**IV/16 2.1.7:1965**
9579	$C_{11}HN$ 147.14 78950-25-1		cyanodecapentayne	**II/19a 2.3.2:60**
9580	$C_{11}H_3F_{17}O$ 474.12 110085-12-6		1,1,2,2,3,3,4,4,4a,5,5,6,6,7,7,8,8-heptadecafluoro-8a-methoxy-decahydro-naphthalene	**IV/16 2.1.7:1966**
9581	$C_{11}H_6ClF_7O_2$ 338.61 67103-76-8		4-chlorobenzoic acid heptafluoro-butyl ester; heptafluorobutyl 4-chlorobenzoate	**III/38b 2.1:6054;** **IV/6 2.1.3:1490**
9582	$C_{11}H_6Cl_6HgNO_2$ 597.48 2597-93-5		emmi; hexachlorophthalimide; ethylmercurichlorendimide	**IV/8a 3.5.6,p.263**
9583	$C_{11}H_7F_7O_2$ 304.17 67103-72-4		benzoic acid heptafluoro-butyl ester; heptafluorobutyl benzoate	**III/38b 2.1:6055;** **IV/6 2.1.3:1491**

9584	$C_{11}H_7N$ 153.18 86-53-3		naphthalene-1-carbonitrile	**IV/16 2.1.7:1967**
9585	$C_{11}H_8$ 140.19 4009-22-7		norcapillene; 1,3-pentadiynylbenzene; 1-phenyl-1,3-pentadiyne	**IV/8e 6:671**
9586	$C_{11}H_8$ 140.19 6088-96-6		1,4-pentadiynylbenzene; 1-phenyl-1,4-pentadiyne	**IV/8e 6:672**
9587	$C_{11}H_8F_{12}O_2$ 400.17 2261-99-6		2-methyl-acrylic acid 2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro-heptyl ester	**IV/16 2.1.7:1968**
9588	$C_{11}H_8O$ 156.19 66-77-3		naphthalene-1-carbaldehyde	**III/38b 2.1:6056**
9589	$C_{11}H_8O$ 156.19 66-99-9		naphthalene-2-carbaldehyde	**III/38b 2.1:6057**
9590	$C_{11}H_8OS$ 188.25 135-00-2		2-benzoylthiophene	**III/38b 2.1:6058**
9591	$C_{11}H_8O_2$ 172.18 86-55-5		1-naphthalenecarboxylic acid; 1-naphthoic acid	**IV/8a 3.5.6,p.263**
9592	$C_{11}H_8O_2$ 172.18 93-09-4		2-naphthalenecarboxylic acid; 2-naphthoic acid; β-naphthoic acid	**IV/8a 3.5.6,p.263**
9593	$C_{11}H_8O_2$ 172.18 58-27-5		menadione; menaquinone; 2-methyl-1,4-naphthalenedione; 2-methyl-1,4-naphthoquinone	**IV/8a 3.5.6,p.263**
9594	$C_{11}H_9Cl$ 176.65 86-52-2		1-(chloromethyl)naphthalene; naphthalene, 1-(chloromethyl)-; 1-naphthylmethyl chloride	**IV/16 2.1.7:1969;** **IV/20b 4.6:1476**
9595	$C_{11}H_9Cl_2NO_2$ 258.11 101-27-9		barban; carbanilic acid, *m*-chloro-, 4-chloro-2-butynyl ester; carbyne; 4-chloro-2-butynyl 3-chlorocarbanilate; 4-chloro-2-butynyl N-(3-chlorophenyl)carbamate	**IV/8a 3.5.6,p.263**

9596	$C_{11}H_{10}$ 142.20		4-penten-1-ynylbenzene	**IV/8e 5:655**
9597	$C_{11}H_{10}$ 142.20		(3-methyl-3-buten-1-ynyl)benzene (I)	**IV/8e 5:659**
9598	$C_{11}H_{10}$ 142.20		(3-methyl-1-butyn-3-enyl)benzene; (3-methyl-3-buten-1-ynyl)benzene (II)	**IV/8e 5:654**
9599	$C_{11}H_{10}$ 142.20 91-57-6		2-methylnaphthalene	**III/38b 2.1:6060;** **IV/6 2.1.3:1493;** **IV/8a 3.5.6,p.263;** **IV/8f 5.3.1:1093;** **IV/20a 2.3:717**
9600	$C_{11}H_{10}$ 142.20 90-12-0	 see also: **14159**(M), **14421**(M)	1-methylnaphthalene	**III/38b 2.1:6059;** **IV/6 2.1.3:1492;** **IV/8a 3.5.6,p.263;** **IV/8f 5.3.1:1092;** **IV/16 2.1.7:1970;** **IV/20a 2.3:716**
9601	$C_{11}H_{10}O$ 158.20 2216-69-5		1-methoxynaphthalene	**III/38b 2.1:6061;** **IV/6 2.1.3:1494;** **IV/16 2.1.7:1971**
9602	$C_{11}H_{10}O$ 158.20 93-04-9		2-methoxynaphthalene	**IV/6 2.1.3:1495**
9603	$C_{11}H_{10}O$ 158.20 4780-79-4		1-naphthalenemethanol	**IV/16 2.1.7:1972**
9604	$C_{11}H_{10}O_2$ 174.20 2216-94-6		3-phenyl-prop-2-ynoic acid ethyl ester	**IV/16 2.1.7:1973**
9605	$C_{11}H_{10}O_2$ 174.20 2958-72-7		hexahydro-1,2,4-ethanylidene-1H-cyclobuta[cd]pentalene-5,7[1aH]-dione	**IV/8a 3.5.6,p.264**
9606	$C_{11}H_{10}O_4$ 206.20 15721-10-5		*p*-methacryloyloxybenzoic acid; 4-[(2-methyl-1-oxo-2-propenyl)oxy]benzoic acid	**IV/8a 3.5.6,p.264**
9607	$C_{11}H_{10}S$ 174.27 13132-15-5		2-benzyl-thiophene	**IV/16 2.1.7:1974**

10420	$C_{12}Cl_{10}$ 498.66 2051-24-3		decachlorobiphenyl; 2,2',3,3',4,4', 5,5',6,6'-decachlorobiphenyl; perchlorobiphenyl	**IV/8a 3.5.6,p.273;** **IV/20b 4.6:1492**
10421	$C_{12}D_{10}$ 164.27 1486-01-7	 see also: **10510**(H)	biphenyl-d10; 1,1'-biphenyl-d10	**IV/8a 3.5.6,p.281**
10422	$C_{12}F_{10}$ 334.12 434-90-2		1,1'-biphenyl, 2,2' ,3,3' ,4,4' ,5,5' ,6,6'-decafluoro; decafluorobiphenyl; perfluorobiphenyl	**IV/16 2.1.7:2057;** **IV/20b 4.6:1493**
10423	$C_{12}F_{18}$ 486.11 23174-55-2		hexakis(trifluoromethyl)bicyclo[2.2.0]hexa-2,5-diene	**IV/20b 4.6:1494**
10424	$C_{12}F_{18}$ 486.11 22186-64-7		hexakis(trifluoromethyl)tricyclo[3.1.0.0^{2,6}hex-3-ene	**IV/20b 4.6:1495**
10425	$C_{12}F_{18}$ 486.11 22736-20-5		hexakis(trifluoro-methyl)tetracyclo-[2.2.0.0^{2,6}.0^{3,5}-hexane	**IV/20b 4.6:1496**
10426	$C_{12}F_{26}$ 638.09 307-59-5	$C_{12}F_{26}$	hexacosafluorododecane; perfluorododecane	**IV/8a 3.5.6,p.273;** **IV/16 2.1.7:2058**
10427	$C_{12}F_{26}O$ 654.09 424-20-4		bis-(tridecafluorohexyl) ether	**IV/16 2.1.7:2059**
10428	$C_{12}F_{27}N$ 671.10 311-89-7		N,N,-bis(nonafluorobutyl)-nonafluoro-1-butanamine; 1-butanamine, nonafluoro, N,N-bis(nonafluorobutyl)-; heptacosafluorotributylamine; perfluorotributylamine; tris(nonafluorobutyl)amine; tris(perfluorobutyl)amine	**III/38b 2.1:6385;** **IV/6 2.1.3:1534;** **IV/16 2.1.7:2060;** **IV/20b 4.6:1497**
10429	$C_{12}F_{27}OP$ 704.06 58431-34-8		tri-(perfluorobutyl)-phosphine oxide; tris(perfluorobutyl)phosphine oxide	**IV/6 2.1.3:1533**

10430	$C_{12}HCl_9$ 464.22 5121-88-0		2,2',3,3',4,5,5',6,6'-nonochloro-1,1'-biphenyl	**IV/8a 3.5.6,p.274**
10431	$C_{12}H_2Cl_8$ 429.77 2136-99-4		2,2',3,3',5,5',6,6'-octachloro-1,1'-biphenyl; 2,2',3,3',5,5',6,6'-octachlorobiphenyl	**IV/8a 3.5.6,p.274;** **IV/20b 4.6:1498**
10432	$C_{12}H_3Cl_7$ 395.33 52663-71-5		2,3,4,2',3',4',6'-heptachlorobiphenyl; 2,3,4,6,2',3',4'-heptachlorobiphenyl	**IV/8a 3.5.6,p.274**
10433	$C_{12}H_4Cl_6$ 360.88 26601-64-9		hexachlorodiphenyl	**IV/6 2.1.3:1535**
10434	$C_{12}H_4Cl_6$ 360.88 38380-07-3		2,2',3,3',4,4'-hexachloro-1,1'-biphenyl; 2,2',3,3',4,4'-hexachlorobiphenyl; 2,3,4,2',3',4'-hexachlorobiphenyl	**IV/8a 3.5.6,p.274**
10435	$C_{12}H_4Cl_6$ 360.88 38411-22-2		2,2',3,3',6,6'-hexachloro-1,1'-biphenyl; 2,2',3,3',6,6'-hexachlorobiphenyl; 2,3,6,2',3',6'-hexachlorobiphenyl	**IV/8a 3.5.6,p.274**
10436	$C_{12}H_4Cl_6$ 360.88 33979-03-2		2,2',4,4',6,6'-hexachloro-1,1'-biphenyl; 2,2',4,4',6,6'-hexachlorobiphenyl; 2,4,6,2',4',6'-hexachlorobiphenyl	**IV/8a 3.5.6,p.274**
10437	$C_{12}H_5Cl_5$ 326.44 25429-29-2		pentachlorodiphenyl	**IV/6 2.1.3:1536**
10438	$C_{12}H_5Cl_5$ 326.44 37680-73-2		2,2',4,5,5'-pentachlorobiphenyl; 2,2',4',5,5'-pentachlorobiphenyl	**IV/8a 3.5.6,p.274;** **IV/20b 4.6:1499**

10439	$C_{12}H_5Cl_5$ 326.44 18259-05-7		biphenyl, 2,3,4,5,6-pentachloro-; 2,3,4,5,6-pentachloro-1,1'-biphenyl; 2,3,4,5,6-pentachlorobiphenyl	**IV/8a 3.5.6,p.274**
10440	$C_{12}H_5F_{11}O_2$ 390.15 67727-67-7		2,3,3,3-tetrafluoro-2-(1,1,2,2,3,3,3-heptafluoro-propoxy)-1-phenyl-propan-1-one	**IV/16 2.1.7:2061**
10441	$C_{12}H_6Cl_4$ 291.99 41464-40-8		2,2',4,5'-tetrachloro-1,1'-biphenyl; 2,2',4,5'-tetrachlorobiphenyl; 2,2',4',5-tetrachlorobiphenyl	**IV/8a 3.5.6,p.275**
10442	$C_{12}H_6Cl_4$ 291.99 33284-53-6		biphenyl, 2,3,4,5-tetrachloro-; 2,3,4,5-tetrachloro-1,1'-biphenyl; 2,3,4,5-tetrachlorobiphenyl	**IV/8a 3.5.6,p.275**
10443	$C_{12}H_6Cl_4$ 291.99 35693-99-3		tetrachloro-1,1'-biphenyl; tetrachlorobiphenyl; 2,2',5,5'-tetrachlorobiphenyl	**IV/20b 4.6:1500**
10444	$C_{12}H_6Cl_4OS$ 340.06 35850-29-4		sulfoxide, *p*-chlorophenyl 2,4,5-trichlorophenyl; tetrasul sulfoxide; 1,2,4-trichloro-5-[(4-chlorophenyl)sulfinyl]benzene	**IV/8a 3.5.6,p.275**
10445	$C_{12}H_6Cl_4O_2S$ 356.06 116-29-0		2,4,4',5-tetrachlorodiphenyl sulfone	**IV/8a 3.5.6,p.275**
10446	$C_{12}H_6F_6$ 264.17 783-33-5	 see also: **3757**(S), **3991**(S)	benzene, hexafluoro-, compd. with benzene (1:1); benzene-hexafluorobenzene complex	**IV/8a 3.5.6,p.275**
10447	$C_{12}H_6F_{16}O_2$ 486.15 4180-26-1		acrylic acid 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9-hexadecafluoro-nonyl ester	**IV/16 2.1.7:2062**