

Landolt-Börnstein Indexes of Organic Compounds

Subvolumes A-I

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All printed index material has been used to build up the comprehensive

Scidex database index developed by LCI Publisher GmbH, Hamburg

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From this database a CD-ROM and two online versions were derived. The first is attached to each of the printed subvolumes and the latter are offered for free use at the following addresses:

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/>

Index of Organic Compounds

Subvolume D (Supplement to Subvolume A)
Compounds with 1 to 7 Carbon Atoms

Editor: V. Vill

Authors: C. Bauhofer, V. Vill, P. Weigner



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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. In total in the subvolumes D, E and F, **15160** compounds with **23642** references to numerical data are recorded. Compiled are volumes containing spectroscopic data, molecular constants, structure data, density, viscosity and vapor pressure data. All new 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. Compounds already contained in subvolumes A, B or C are listed without structure drawing.

This index is 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 electronization, the data will be indexed, similar to these volumes.

The referenced volumes contain either chemical names and CAS-RN or structure data. In each case missing information was supplemented, compared with the original reference if necessary. Afterwards this data was analyzed and matched with each other to yield a list of individual compounds without duplicates. This work became 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 15000 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 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 is 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 a 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 Maria Brehm, Dipl. Chem. Gaja Peters, Dr. Lenka Weignerová, Sven Gerber , Dipl. Chem. Götz Milkereit, Dr. Henry Sajus, Koen Veermans, Dipl. Chem. Matthias Wulf. The Landolt-Börnstein team, and particular Dr. Rainer Poerschke and Dr. Hans Seemüller, jointly support this project.

Hamburg, November 2001

The Editor

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Subvolume G and following are to be supplements to Subvolumes A through F

Table of contents of CD-ROM added to present subvolume D

readme.txt	General information about the electronic version
volume-d	PDF-version of subvolume D
program-d	SciDex database for all compounds presented in subvolumes A-C and D

Survey to the Index of Organic Compounds

Compounds with 1 to 7 Carbon Atoms	Subvolume A
Compounds with 8 to 12 Carbon Atoms	Subvolume B
Compounds with 13 to 100 Carbon Atoms	Subvolume C
Compounds with 1 to 7 Carbon Atoms (Supplement to Subvolume A)	Subvolume D
Compounds with 8 to 12 Carbon Atoms (Supplement to Subvolume B)	Subvolume E
Compounds with 13 to 100 Carbon Atoms (Supplement to Subvolume C)	Subvolume F

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/24 a,b	Spectroscopic data on diamagnetic and paramagnetic molecules
II/25 a,b,c	Structure Data of free polyatomic molecules
III/35 c1	¹ H-NMR data
IV/8 g,h	Thermodynamic properties: densities of organic compounds
IV/18 a,b	Viscosity of pure organic liquids and binary liquid mixtures
IV/20 b,c	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.

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.

1.2 Drawing of structures

1.2.1 General remarks

The orientation of the structures has been optimized 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.

To prevent loss of information the extra large structure drawings are displayed separately in the Appendix.

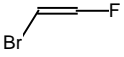
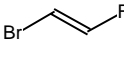
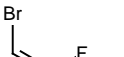
All structures are saved in the electronic version with their complete connectivity, but for display one can choose to abbreviate drawings, so as to make the structures easier readable. The printed version contains in all cases these abbreviated structures.

1.2.2 Stereo Chemistry


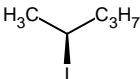
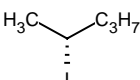
Sometimes a compound is not identified uniquely in the primary literature, when the compound is described with partially defined stereo-chemistry. This is often the case when double bonds are involved that can be *trans* or *cis* configured, or when the compound contains asymmetric carbon atoms, or any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

Not uniquely identified structures are treated as follows: The first example 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 clearly defined as racemate and as R- or S- enantiomer, respectively. In contrast to Index Subvolumes A-C all compounds with unspecified absolute configuration are displayed as racemates since it seems unlikely that materials with well-defined but unknown configuration should have been referenced.

630	C ₂ H ₂ BrF 124.95 460-11-7		1-bromo-2-fluoro-ethene (E/Z)-1-bromo-2-fluoro-ethene	III/38b 2.1:1022
631	C ₂ H ₂ BrF 124.95 2366-32-7		<i>trans</i> -1-bromo-2-fluoro-ethylene	III/38b 2.1:1023
632	C ₂ H ₂ BrF 124.95 2366-31-6		<i>cis</i> -1-bromo-2-fluoro-ethylene	III/38b 2.1:1024

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

3557	C ₅ H ₁₁ I 198.05 52152-72-4		(±)-2-iodo-pentane	IV/16 2.1.7:828
3558	C ₅ H ₁₁ I 198.05 29882-59-5		(S)-2-iodo-pentane	III/38b 2.1:2647
3559	C ₅ H ₁₁ I 198.05 29117-45-1		(R)-2-iodo-pentane	III/38b 2.1:2646

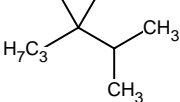
example 2: racemate, R and S-enantiomer, respectively

Compounds with more than one unspecified stereo-bonds will usually be displayed with a wavy line in place of the wedge or dashed bond that specifies exact stereo-chemistry.

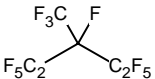
Since the data are excerpted from multiple volumes, sometimes inconsistencies in the data arose, for example occurred in very few cases a mismatch between compound names, formula, and sometimes CAS-RN. The editor chose in most of these cases the CAS-RN, if a valid CAS-RN was given, and the compound name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

1.2.3 Methods of abbreviation of drawings

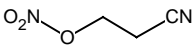
Alkyl chains: Alkyl chains of C₂ and longer are always abbreviated as a textstring, like C₃H₇ as in the example. Methyl groups are in most cases displayed as CH₃, except at quaternary centers, to facilitate the reading of highly branched structures. The following example shows two CH₃-groups to the right, while the two groups in the middle are connected to a quaternary center and only displayed as an "empty" line.

8124	C ₉ H 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
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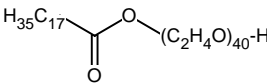
Persubstituted chains: Alkyl chains that are persubstituted with a particular element, like Fluor, or Deuterium are shortened just like in the above example. CF_3 or CD_3 will for obvious reasons never be omitted as CH_3 .

3772	C_6F_{14} 338.04 865-71-4		perfluoro-3-methylpentane; undecafluoro-3-(trifluoromethyl)pentane	IV/20a 4.4:1039
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Special groups: For example cyano groups, nitro groups as well as carbonic acids will be abbreviated in the drawing.

1379	$\text{C}_3\text{H}_4\text{N}_2\text{O}_3$ 116.08 50434-02-1		nitric acid 2-cyano-ethyl ester	III/38b 2.1:1286
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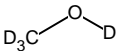
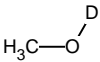
Poly-ethoxy chains: will be identified and shortened as well.

16821	$\text{C}_{98}\text{H}_{196}\text{O}_{42}$ 2046.63 9004-99-3		myrj 52	IV/16 2.1.7:2704
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1.2.4 Cross-references

In some cases, the third column will show cross-references to other entries in the index-file. This applies for structures which have a deuterated and a "normal" form in the database. The cross-reference contains always the running number plus an identifier for the relationship. The relationships H and D, are defined as follows:

- H The cross-reference shows the same compound non-deuterated
D The cross-reference shows the same compound (possibly partly) deuterated

71	CD_4O 36.07 811-98-3	 see also: 263(D) , 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	$\text{H}_3\text{C}-\text{OH}$ see also: 71(D) , 263(D)	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.

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. Molecular 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 marked 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.

1.5 Table structure

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.

1.5.1 Index by new 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
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.

1.5.2 Index of already registered compounds

The table is organized in four columns as follows:

Column	Contents
1	Running number of the previously registered compound
2	Molecular formula; CAS-RN
3	Compound name(s)
4	Landolt-Börnstein references Single compound references are written out in full, mixtures are preceded with the word 'Mixtures:' and written in a concatenated format.

1.5.3 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-RN *
2	Volume and running number

Out-dated, deleted CAS-RN (= CAS-DR) are displayed with a star *.

1.5.4 Appendix

To prevent loss of data the large structures were drawn in the Appendix. The index of new chemical formula and chemical structure includes instead drawing only a reference to the Appendix. Chemical structure is identified according to its running number.

1.6 Exact volume titles and references

Volume II/24: Molecular Constants mostly from Microwave, Molecular Beam, and Sub-Doppler Laser Spectroscopy

(Supplement to volumes II/4, II/6, II/14, and II/19)

Editor: W. Hüttner

Subvolume a: Rotational, *l*-type, Centrifugal Distortion and Related Constants of Diamagnetic Diatomic, Linear, and Symmetric Top Molecules

Authors: J. Demaison; H. Hübner; G. Włodarczak

1998. VIII, 286 pages. ISBN 3-540-63267-0

Volume II/24: Molecular Constants mostly from Microwave, Molecular Beam, and Sub-Doppler Laser Spectroscopy

(Supplement to volumes II/4, II/6, II/14, and II/19)

Editor: W. Hüttner

Subvolume b: Rotational, Centrifugal Distortion and Related Constants of Diamagnetic Asymmetric Top Molecules

Authors: J. Demaison; J. Vogt; G. Włodarczak

2000. VIII, 525 pages. ISBN 3-540-65345-7

Volume II/25: Structure Data of Free Polyatomic Molecules

(Supplements to volumes II/7 (1976), II/15 (1987), II/21 (1992) and II/23 (1995))

Editor: K. Kuchitsu

Subvolume a: Inorganic Molecules

Authors: G. Graner; E. Hirota; T. Iijima; K. Kuchitsu; D.A. Ramsay; J. Vogt, N. Vogt

1997. 67 figs., X; 359 pages. ISBN 3-540-61713-2

Volume II/25: Structure Data of Free Polyatomic Molecules

(Supplements to volumes II/7 (1976), II/15 (1987), II/21 (1992) and II/23 (1995))

Editor: K. Kuchitsu

Subvolume b: Molecules containing One or Two Carbon Atoms

Authors: G. Graner; E. Hirota; T. Iijima; K. Kuchitsu; D.A. Ramsay; J. Vogt, N. Vogt

1999. X, 512 pages. ISBN 3-540-63645-5

Volume II/25: Structure Data of Free Polyatomic Molecules

(Supplements to volumes II/7 (1976), II/15 (1987), II/21 (1992) and II/23 (1995))

Editor: K. Kuchitsu

Subvolume c: Molecules containing Three or Four Carbon Atoms

Authors: G. Graner; E. Hirota; T. Iijima; K. Kuchitsu; D.A. Ramsay; J. Vogt, N. Vogt

1999. X, 481 pages. ISBN 3-540-66774-1

Volume III/35: Nuclear Magnetic Resonance, (NMR) Data

Editors: R.R. Gupta, M.D. Lechner

Subvolume c: Chemical Shifts and Coupling Constants for Hydrogen-1

Part 1: Aliphatic and Aromatic Hydrocarbons, Steroids, Carbohydrates

Authors: R.R. Gupta; M. Jain

1999. VIII, 310 pages, ISBN 3-540-66780-6

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

Editor: K.R. Hall and K.N. Marsh

Subvolume g: Densities of Alcohols

Authors: M. Frenkel; X. Hong; R.C. Wilhoit; K.R. Hall

1999, 105 figs, XI, 413 pages, ISBN 3-540-66233-2

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

Editor: K.R. Hall and K.N. Marsh

Subvolume h: Densities of Esters and Ethers

Authors: M. Frenkel; X. Hong; R.C. Wilhoit; K.R. Hall

2000, 105 figs, XI, 485 pages, ISBN 3-540-41035-X

Volume IV/18: Viscosity of Pure Organic Liquids and Binary Liquid Mixtures

Editor: M.D. Lechner

Subvolume a: Pure Organometallic and Organononmetallic Liquids, Binary Liquid Mixtures

Authors: Ch. Wohlfarth, B. Wohlfarth

2001. VII, 409 pages, ISBN 3-540-64584-5

Volume IV/18: Viscosity of Pure Organic Liquids and Binary Liquid Mixtures

Editor: M.D. Lechner

Subvolume b: Pure Organic Liquids

Authors: Ch. Wohlfarth, B. Wohlfarth

2002. VII, 389 pages, ISBN 3-540-66234-0

Volume IV/20: Vapor Pressure of Chemicals

Editor: K.R. Hall

Subvolume b: Vapor Pressure and Antoine Constants for Oxygen Containing Organic Compounds

Authors: J. Dykyj, J. Svoboda, R.C. Wilhoit, M. Frenkel, K.R. Hall

2000. VII, 320 pages, ISBN 3-540-64968-9

Volume IV/20: Vapor Pressure of Chemicals

Editor: K.R. Hall

Subvolume c: Vapor Pressure and Antoine Constants for Nitrogen Containing Organic Compounds

Authors: J. Dykyj, J. Svoboda, R.C. Wilhoit, M. Frenkel, K.R. Hall

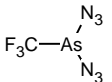



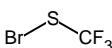
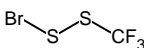



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Data

2 Index sorted by molecular formula and chemical structures

Compounds with 1 to 7 Carbon-Atoms

2.1 New Compounds

16824	C Ar O 67.96	$\text{C}\equiv\text{O}-\text{Ar}$	Carbon monoxide - argon (1/1)	II/24b 2.5.2:22; II/25b 3:3
16825	C Ar ₂ O S 139.97	$\text{O}=\text{C}=\text{S}-\text{Ar}\cdots\text{Ar}$	Carbon oxysulfide - diargon (1/1)	II/25b 3:6
16826	C Ar ₂ O S 139.97	$\text{O}=\text{C}=\text{S}$ Ar Ar	Carbonoxidesulfide - Argon (1/2)	II/24b 2.5.2:25
16827	C Ar ₂ O ₂ 123.91	$\text{O}=\text{C}=\text{O}$ Ar Ar	Carbondioxide - Argon (1/2)	II/24b 2.5.2:26
16828	C Ar ₂ O ₂ 123.91	$\text{O}=\text{C}=\text{O}-\text{Ar}\cdots\text{Ar}$	Carbon dioxide - diargon (1/1)	II/25b 3:7
16829	C As F ₃ N ₆ 227.97		Diazido(trifluoromethyl)arsane	II/25b 3:8
16830	C B F ₃ O 95.82	$\text{C}\equiv\text{O}$ 	Carbon monoxide - boron trifluoride (1/1)	II/25b 3:9
16831	C B F ₃ O ₂ 111.82	$\text{O}=\text{C}=\text{O}$ 	Carbon dioxide - boron trifluoride (1/1)	II/25b 3:10
16832	C Br Cl O 143.37	$\text{O}\equiv\text{C}-\text{Br}-\text{Cl}$	Carbon monoxide - bromine chloride (1/1)	II/24a 2.3.2:7; II/25b 3:12
16833	C Br F 110.92 13590-47-1		Bromofluoromethylene	II/25b 3:14
16834	C Br F ₃ S 180.98		Bromo(trifluoromethyl)sulfur	II/25b 3:17
16835	C Br F ₃ S ₂ 213.04		Bromo(trifluoromethyl)disulfane	II/25b 3:18
16836	C Br N 105.93	$\text{Br}-\text{C}\equiv\text{N}^{(+)}$	Cyanogen bromide cation	II/25b 3:20
16837	C Br N O 121.93	$\text{Br}-\text{C}\equiv\text{N}^{(+)}-\text{O}^{(-)}$	Bromcyanid-N-oxide	II/24b 2.5.2:28
16838	C Br ₂ 171.83 4371-77-1		Dibromomethylene radical	II/25b 3:24
16839	C Br ₂ F ₃ N 242.83		N,N-Dibromo-1,1,1-trifluoromethanamine	II/25b 3:25
16840	C Br ₂ S 203.89		Thiocarbonyl dibromide	II/25b 3:27

16841	C Br ₃ 251.74		Tribromomethyl radical	II/25b 3:28
16842	C Cl F 66.46		Chlorofluoromethylene	II/25b 3:31
16843	C Cl F O 82.46	O≡C Cl—F	Carbonmonooxide - Chlorofluoride (1/1)	II/24a 2.3.2:9
16844	C Cl F O S 114.53 16829-32-6		(Fluorocarbonyl)sulphenyl chloride	II/25b 3:33
16845	C Cl F ₃ O ₂ S 168.52 421-83-0		Trifluoromethanesulfonyl chloride	II/25b 3:39
16846	C Cl F ₃ S ₂ 168.59 53268-50-1		Chloro(trifluoromethyl)disulfane	II/25b 3:41
16847	C Cl F ₄ N O ₁₂ S ₄ 457.71 53684-03-0		Fluorosulfuric acid bis[(fluorosulfonyl)oxy]amino chloro- methylene ester	IV/20c 2.1:37
16848	C Cl N 61.47	Cl—≡N ⁽⁺⁾	Cyanogen chloride cation	II/25b 3:44
16849	C Cl N O ₃ S 141.53 1189-71-5		Sulfonyl chloride isocyanate	II/24b 2.5.2:30; II/25b 3:46
16850	C Cl P 78.44	Cl—≡P	(Chloromethyldiyne)phosphine	II/24a 2.3.2:11; II/25b 3:49
16851	C Cl ₂ F ₂ S 152.98		Chlorodifluoromethanesulphenyl chloride	II/25b 3:52
16852	C Cl ₂ F ₆ Si ₂ 253.08		Dichlorobis(trifluorosilyl)methane	II/25b 3:54
16853	C Cl ₂ N O ₂ P 159.90		Dichloroisocyanatophosphine oxide	II/25b 3:55
16854	C Cl ₂ O 98.92	O≡C Cl—Cl	Carbon monoxide - dichlorine (1/1)	II/24a 2.3.2:12; II/25b 3:58
16855	C Cl ₂ O S 130.98		Carbonyl chloride thiohypochlorite	II/25b 3:59
16856	C Cl ₂ O S 130.98		Thiocarbonyl dichloride S-oxide	II/25b 3:60
16857	C Cl ₃ F S 169.43		Dichlorodifluoromethanesulphenyl chloride	II/25b 3:63

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