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

Bearbeitet von
C Bauhofer, G Peters, P Weigner

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Landolt-Börnstein Indexes of Organic Compounds

Subvolumes A-I

By V. Vill, C. Bauhofer, G. Peters, H. Sajus, P. Weigner,
LCI-Publisher and Chemistry Department of the University of Hamburg

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

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

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

Index of Organic Compounds

Subvolume G
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Editor: V. Vill

Authors: C. Bauhofer, G. Peters, 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 G, H and I, **15775** compounds with **16123** references to numerical data are recorded. Compiled are volumes containing nuclear magnetic resonance (NMR) data for different isotopes (chemical shifts and coupling constants). All new compounds are given with the drawing of the chemical structure, the molecular formula, chemical names, the Chemical Abstracts registration numbers (CAS-RN) where known and references to Landolt-Börnstein citations. Compounds already contained in subvolumes A to F 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 electronisation, the data will be indexed, similar to these volumes.

The referenced volumes contain in most cases only structure data, in some cases even nothing beyond the simple molecular formula. Missing information, such as chemical names, or CAS-numbers, was supplemented, and compared with the original reference if necessary. Afterwards this data was analysed and matched with each other and with the index-volumes A through F, to yield a list of individual compounds without duplicates. This work is non-trivial especially in cases where no, or no exact chemical structure was supplied in the indexed volumes. Furthermore, about 17,000 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 electronic database. Up to now, many users prefer printed books to electronic 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 electronic version gives more functionality to the data, e.g. substructure search and structure comparison methods. Further, the database is a comprehensive compilation of ALL compounds listed in the sub-volumes A through I, containing by now over 42,000 compounds, and more than 75,000 LB-references, all of which lead directly by hyperlink to the full texts of the original LB-volumes.

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 electronic 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 electronic 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 Dr. Lenka Weignerová and Dr. Hermann Langen. The Landolt-Börnstein team, and in particular Dr. Rainer Poerschke, supports this project.

Hamburg, March 2005 The Editor

Editor

V. Vill
Institut für Organische Chemie
Universität Hamburg
D-20146 Hamburg, Germany
&
LCI Publisher GmbH
Bundesstr. 8
D-20146 Hamburg, Germany

Authors

C. Bauhofer
LCI Publisher GmbH
Bundesstr. 8
D-20146 Hamburg, Germany

G. Peters
Institut für Organische Chemie
Universität Hamburg
D-20146 Hamburg, Germany
&
LCI Publisher GmbH
Bundesstr. 8
D-20146 Hamburg, Germany

P. Weigner
LCI Publisher GmbH
Bundesstr. 8
D-20146 Hamburg, Germany

Landolt-Börnstein

Editorial Office
Gagernstr. 8, D-64283 Darmstadt, Germany
fax: +49 (6151) 171760
e-mail: lb@springer-sbm.com

Internet
http://www.landolt-boernstein.com

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
Compounds with 1 to 7 Carbon Atoms (Supplement to Subvolume A and D)	**Subvolume G**
Compounds with 8 to 12 Carbon Atoms (Supplement to Subvolume B and E)	Subvolume H
Compounds with 13 to 162 Carbon Atoms (Supplement to Subvolume C and F) C13 – C25 printed C13 – C162 in electronic version	Subvolume I

Landolt-Börnstein
GROUP Index of Organic Compounds

VOLUME
Compound with 1 to 7 Carbon AtomsSUBVOLUME G

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
III/35 A	Nuclear Magnetic Resonance (NMR) Data for Boron-11 and Phosphorus-31
III/35 B	Nuclear Magnetic Resonance (NMR) Data for Fluorine-19 and Nitrogen-15
III/35 C2	Nuclear Magnetic Resonance (NMR) Data for Hydrogen-1: Heterocycles
III/35 C4	Nuclear Magnetic Resonance (NMR) Data for Hydrogen-1: Inorganic and Organometallic compounds
III/35 E	Nuclear Magnetic Resonance (NMR) Data for Oxygen-17

1.1.2 Compounds

All compounds with at least one carbon atom are selected for this index. The database in the electronic version contains additionally the purely inorganic compounds from the volumes listed above.

1.2 Drawing of structures

1.2.1 General remarks

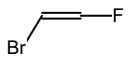
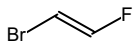
The orientation of the structures has been optimized for space saving, to reduce the amount of total pages needed as much as possible. The bond-length of the structures was normalized where possible. In case of large structures, the bond-length was proportionally decreased, so that the compound would fit into the table cell.
To prevent loss of information the extra large structure drawings are displayed separately in the Appendix.

All structures are stored in the electronic version with their complete connectivity suitable for substructure-search, 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. In cases where there was ambiguity about the identity of compounds, NO structure drawing has been made, and instead the „descriptive line-formula“ as cited in the LB-sources has been used.

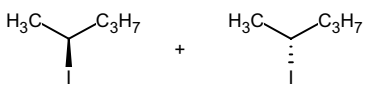
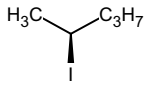
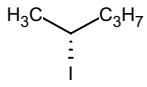
1.2.2 Stereo Chemistry

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_2H_2BrF 124.95 460-11-7		1-bromo-2-fluoro-ethene (E/Z)-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

3557	$C_5H_{11}I$ 198.05 637-97-8		(±)-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**

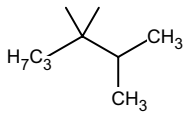
Example 2: racemate, R and S-enantiomer, respectively

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

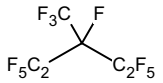
Since the data are excerpted from multiple volumes, sometimes inconsistencies in the data arose, i.e. mismatches between compound name, formula, and/or structure drawing occurred. The editor chose in most of these cases the chemical structure drawing as the most representative information. Often, even the original source (occasionally down to the primary literature) has been consulted.

1.2.3 Methods of abbreviation of drawings

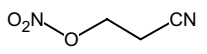
Alkyl chains: Alkyl chains of C_2 and longer are always abbreviated as a textstring, like C_3H_7 as in the example. Methyl groups are in most cases displayed as CH_3, except at quartary centers, to facilitate the reading of highly branched structures. The following example shows two CH_3-groups to the 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**

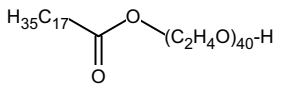
Persubstituted chains: Alkyl chains that are persubstituted with a particular element, like Fluorine, or Deuterium are shortened just like in the above example. CF_3 or CD_3 will for obvious reasons never be omitted like CH_3.

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. 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 of new compounds by molecular formula and chemical structures

"New compounds" in this context are compounds which have not already appeared in Subvolumes A through F.
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
4	Compound name(s)
5	Landolt-Börnstein references

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 and subvolume of first appearance
2	Molecular formula; CAS-RN
3	Compound name
4	Landolt-Börnstein references

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 and enhance legibility the large structures were drawn in the Appendix. For these cases, the main index by chemical formula and structure includes only a reference to the Appendix instead of a drawing. Chemical structure drawings are identified according to their running number.

1.6 Exact volume titles and references

Volume III/35: Nuclear Magnetic Resonance (NMR) Data
Editor: R.R. Gupta and M.D. Lechner
Subvolume a: Chemical Shifts and Coupling Constants for Boron-11 and Phosphorus-31
Authors: R.R. Gupta; M. Jain; P. Pardasani; R.T. Pardasani; A. Pelter
1997. VIII, 242 pages. ISBN 3-540-60366-2

Volume III/35: Nuclear Magnetic Resonance (NMR) Data
Editor: R.R. Gupta and M.D. Lechner
Subvolume b: Chemical Shifts and Coupling Constants for Fluorine-19 and Nitrogen-15
Authors: M. Balasubramanian; R.R. Gupta; M. Jain; S. Perumal
1998. VII, 242 pages. ISBN 3-540-63275-1

Volume III/35: Nuclear Magnetic Resonance (NMR) Data
Editor: R.R. Gupta and M.D. Lechner
Subvolume c: Chemical Shifts and Coupling Constants for Hydrogen-1, Part 2: Heterocycles
Authors: R.R. Gupta; M. Jain
2003. VIII; 310 pages. ISBN 3-540-41057-0

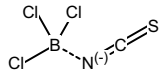
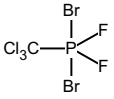
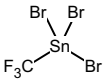
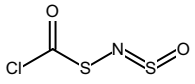
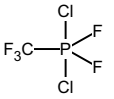
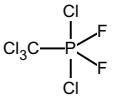
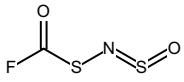
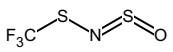
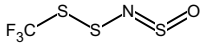
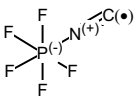
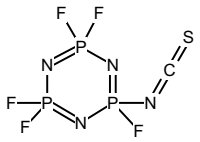
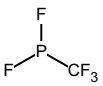
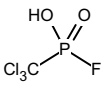
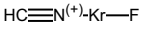
Volume III/35: Nuclear Magnetic Resonance (NMR) Data
Editor: R.R. Gupta and M.D. Lechner
Subvolume c: Chemical Shifts and Coupling Constants for Hydrogen-1, Part 4: Inorganic and Organometallic Compounds
Authors: R.R. Gupta; N. Platzer
2001. VII; 299 pages. ISBN 3-540-41059-7

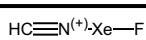
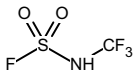
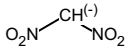
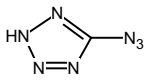
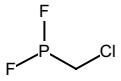
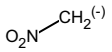
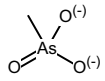
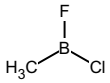
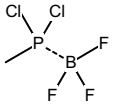
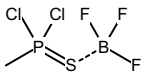
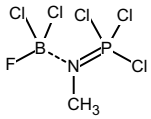
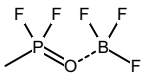
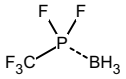
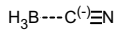
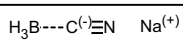
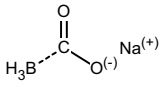
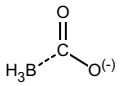
Volume III/35: Nuclear Magnetic Resonance (NMR) Data
Editor: R.R. Gupta and M.D. Lechner
Subvolume e: Chemical Shifts for Oxygen-17
Authors: H. Duddeck; G. Toth; A. Simon
2002, VII; 320 pages. ISBN 3-540-42501-2

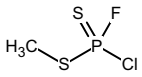
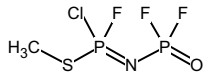
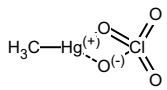
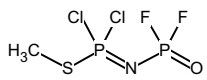
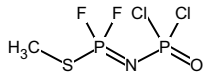
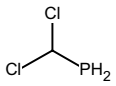
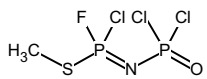
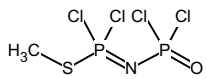
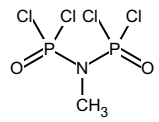
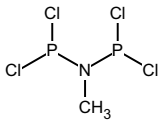
Data

2 Index sorted by molecular formula and chemical structures Compounds with 1 to 7 carbon atoms

2.1 New Compounds

26673	$CBCl_3NS$ 175.25		$[BCl_3NCS]^-$	**III/35a 2.2:153**
26674	$CBr_2Cl_3F_2P$ 347.15		Dibromo-difluoro-(trichloromethyl)-phosphorane; Phosphorane, dibromodifluoro(trichloromethyl)-	**III/35a 3.2:8**
26675	CBr_3F_3Sn 427.41		Tribromo-(trifluoro-methyl)-stannane	**III/35b 2.2:1**
26676	$CClNO_2S_2$ 157.6		$CClNO_2S_2$	**III/35e 2.2.5:3904**
26677	CCl_2F_5P 208.88		Dibromo-difluoro(trifluoromethyl)-phosphorane; Phosphorane, dibromodifluoro(trifluoromethyl)-	**III/35a 3.2:9**
26678	CCl_5F_2P 258.25 1667-44-3		Phosphorane, dichlorodifluoro(trichloromethyl)-	**III/35a 3.2:11**
26679	$CFNO_2S_2$ 141.15		$CFNO_2S_2$	**III/35e 2.2.5:3905**
26680	CF_3NOS_2 163.14		CF_3NOS_2	**III/35e 2.2.5:3906**
26681	CF_3NOS_3 195.21		CF_3NOS_3	**III/35e 2.2.5:3907**
26682	CF_5NP 151.98		CF_5NP	**III/35a 3.2:14**
26683	$CF_5N_4P_3S$ 288.02 28650-12-6		2,2,4,4,6-Pentafluoro-6-isothiocyanato-$2\lambda^5,4\lambda^5,6\lambda^5$-[1,3,5,2,4,6]triazatriphosphinine; 1,3,5,2,4,6-Triazatriphosphorine, 2,2,4,4,6-pentafluoro-2,2,4,4,6,6-hexahydro-6-isothiocyanato-	**III/35a 3.2:15**
26684	CF_5P 137.98		CF_5P	**III/35a 3.2:16**
26685	$CHCl_3FO_2P$ 201.35		$CHCl_3FO_2P$	**III/35a 3.2:18**
26686	CHFKrN 129.82		$[HC:::N\text{-}Kr\text{-}F]^+$	**III/35b 3.2:5**

26687	$CHFNXe$ 177.32		$[HC:::N\text{-}Xe\text{-}F]^{+}$	**III/35b 3.2:6**
26688	CHF_4NO_2S 167.08		(Trifluoro-methyl)sulfamoyl fluoride	**III/35c4 2.2:34**
26689	CHN_2O_4 105.03		$[CH\text{-}(NO_2)_2]^{-}$	**III/35e 2.2.3:3204**
26690	CHN_7 111.07		5-Azido-2*H*-tetrazole	**III/35b 3.2:9**
26691	CH_2ClF_2P 118.45 1113-28-6		Chloromethyl difluorophosphine	**III/35a 3.2:20**
26692	CH_2F_3N 85.03		*C*-Trifluoro-methylamine	**III/35b 2.2:5**
26693	CH_2NO_2 60.03		$[CH_2NO_2]^{-}$	**III/35e 2.2.3:3207**
26694	CH_3AsO_3 137.95		$[CH_3AsO_3]^{2-}$	**III/35e 2.2.6:4411**
26695	CH_3BClF 80.3		CH_3BClF	**III/35a 2.2:154**
26696	$CH_3BCl_2F_3P$ 184.72		$CH_3BCl_2F_3P$	**III/35c4 2.2:35**
26697	$CH_3BCl_2F_3PS$ 216.78		Dichloro-methyl-thiophosphonic acid trifluoro-borane	**III/35c4 2.2:36**
26698	CH_3BCl_5FNP 267.09		CH_3BCl_5FNP	**III/35a 2.2:157**
26699	CH_3BF_5OP 167.81		Difluro-methyl-phosphonic acid trifluoro-borane	**III/35c4 2.2:37**
26700	CH_3BF_5P 151.81 6153-93-1		Phosphonous difluoride, (trifluoromethyl)-, compound with borane (1:1)	**III/35c4 2.2:38**
26701	CH_3BN 39.85		BH_3CN^{-}	**III/35a 2.2:158**
26702	CH_3BNNa 62.84		BH_3CNNa	**III/35a 2.2:158**
26703	CH_3BNaO_2 80.83		BH_3COONa	**III/35a 2.2:160**
26704	CH_3BO_2 57.84		BH_3COO^{-}	**III/35a 2.2:160**

26705	CH_3BrO_2S 159. 41138-92-5		Methanesulfonyl bromide	**III/35e 2.2.5:3908**
26706	CH_3Br_2OP 221.82 19430-64-9		Phosphonic dibromide, methyl-	**III/35a 3.2:23**
26707	CH_3Br_3Ge 327.39 6558-57-2		Tribromo(methyl)germane	**II/25b 3:252**
26708	CH_3Br_3Sn 373.44 993-15-7		Stannane, tribromomethyl-	**III/35c4 2.4:3310**
26709	CH_3ClFO_3P 148.46		((R,S)-Chloro-fluoro-methyl)-phosphonic acid	**III/35a 3.2:24**
26710	CH_3ClFPS_2 164.59		*S*-Methyl-fluoro-chloro-dithiophosphate	**III/35c4 2.2:40**
26711	$CH_3ClFPSe$ 179.42		$CH_3ClFPSe$	**III/35a 3.2:25**
26712	$CH_3ClF_3NOP_2S$ 231.5		$CH_3ClF_3NOP_2S$	**III/35a 3.2:26**
26713	CH_3ClHgO_4 315.07 16522-09-1		Methylperchlorato-mercury	**III/35c4 2.2:42**
26714	$CH_3Cl_2F_2NOP_2S$ 247.96		$CH_3Cl_2F_2NOP_2S$	**III/35a 3.2:27**
26715	$CH_3Cl_2F_2NOP_2S$ 247.96		$CH_3Cl_2F_2NOP_2S$	**III/35a 3.2:28**
26716	CH_3Cl_2P 116.91 125750-80-3		Dichloro-phosphanyl-methane; Dichloromethyl-phosphane	**III/35a 3.2:29**
26717	$CH_3Cl_3FNOP_2S$ 264.41		$CH_3Cl_3FNOP_2S$	**III/35a 3.2:30**
26718	$CH_3Cl_4NOP_2S$ 280.87		$CH_3Cl_4NOP_2S$	**III/35a 3.2:31**
26719	$CH_3Cl_4NO_2P_2$ 264.8		$CH_3Cl_4NO_2P_2$	**III/35b 3.2:12**
26720	$CH_3Cl_4NP_2$ 232.8 17648-16-7		Bis(dichlorophosphino)methylamine	**III/35a 3.2:32**

3 Index sorted by Chemical Abstracts registry numbers