

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

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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

Scidex database index developed by LCI Publisher GmbH, Hamburg

For further information please visit www.lci-publisher.com

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/>

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.

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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)	Subvolume I
C13 – C25 printed	
C13 – C162 in electronic version	

Landolt-Börnstein
GROUP Index of Organic Compounds
VOLUME
Compound with 1 to 7 Carbon AtomsSUBVOLUME G

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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
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.

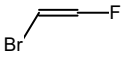
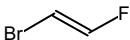
To prevent loss of information the extra large structure drawings are displayed separately in the Appendix.

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.

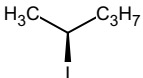
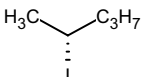
1.2.2 Stereo Chemistry

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 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 198.05 637-97-8		(±)-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

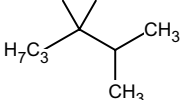
Example 2: racemate, R and S-enantiomer, respectively

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

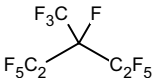
Since the data are excerpted from multiple volumes, sometimes inconsistencies in the data arose, i.e. mismatches between compound name, formula, and/or structure drawing occurred. The editor chose in most of these cases the chemical structure drawing as the most representative information. Often, even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

1.2.3 Methods of abbreviation of drawings

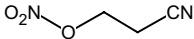
Alkyl chains: Alkyl chains of C₂ and longer are always abbreviated as a textstring, like C₃H₇ as in the example. Methyl groups are in most cases displayed as CH₃, except at quaternary centers, to facilitate the reading of highly branched structures. The following example shows two CH₃-groups to the right, 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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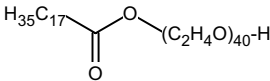
Persubstituted chains: Alkyl chains that are persubstituted with a particular element, like Fluorine, or Deuterium are shortened just like in the above example. CF_3 or CD_3 will for obvious reasons never be omitted like CH_3 .

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

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. Dudgeck; G. Toth; A. Simon

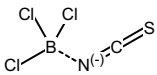
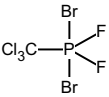
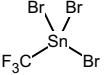
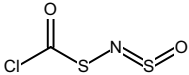
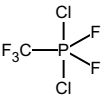
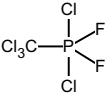
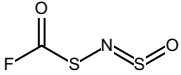
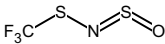
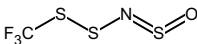
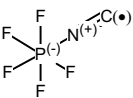
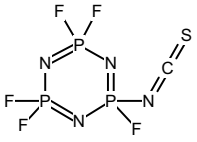
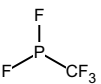
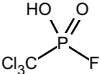
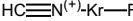
2002, VII; 320 pages. ISBN 3-540-42501-2

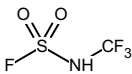
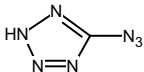
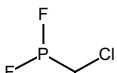
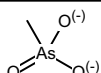
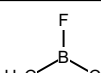
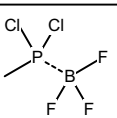
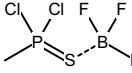
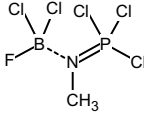
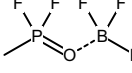
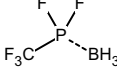
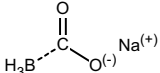
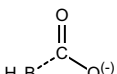
Data

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Compounds with 1 to 7 carbon atoms

2.1 New Compounds

26673	CBCl ₃ NS 175.25		[BCl ₃ NCS] ⁻	III/35a 2.2:153
26674	CBr ₂ Cl ₃ F ₂ P 347.15		Dibromo-difluoro-(trichloromethyl)- phosphorane; Phosphorane, dibromodifluoro(trichloromethyl)-	III/35a 3.2:8
26675	CBr ₃ F ₃ Sn 427.41		Tribromo-(trifluoro-methyl)-stannane	III/35b 2.2:1
26676	CCINO ₂ S ₂ 157.6		CCINO ₂ S ₂	III/35e 2.2.5:3904
26677	CCl ₂ F ₅ P 208.88		Dibromo-difluoro(trifluoromethyl)- phosphorane; Phosphorane, dibromodifluoro(trifluoromethyl)-	III/35a 3.2:9
26678	CCl ₅ F ₂ P 258.25 1667-44-3		Phosphorane, dichlorodifluoro(trichloromethyl)-	III/35a 3.2:11
26679	CFNO ₂ S ₂ 141.15		CFNO ₂ S ₂	III/35e 2.2.5:3905
26680	CF ₃ NOS ₂ 163.14		CF ₃ NOS ₂	III/35e 2.2.5:3906
26681	CF ₃ NOS ₃ 195.21		CF ₃ NOS ₃	III/35e 2.2.5:3907
26682	CF ₅ NP 151.98		CF ₅ NP	III/35a 3.2:14
26683	CF ₅ N ₄ P ₃ S 288.02 28650-12-6		2,2,4,4,6-Pentafluoro-6-isothiocyanato- 2λ ⁵ ,4λ ⁵ ,6λ 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 ₅ P 137.98		CF ₅ P	III/35a 3.2:16
26685	CHCl ₃ FO ₂ P 201.35		CHCl ₃ FO ₂ P	III/35a 3.2:18
26686	CHFKrN 129.82		[HC::N-Kr-F] ⁺	III/35b 3.2:5

26687	CHFNXe 177.32	$\text{HC}\equiv\text{N}^{(+)}\text{Xe}-\text{F}$	$[\text{HC}::\text{N}-\text{Xe}-\text{F}]^+$	III/35b 3.2:6
26688	$\text{CHF}_4\text{NO}_2\text{S}$ 167.08		(Trifluoro-methyl)sulfamoyl fluoride	III/35c4 2.2:34
26689	CHN_2O_4 105.03	$\text{O}_2\text{N}-\text{CH}^{(-)}-\text{NO}_2$	$[\text{CH}-(\text{NO}_2)_2]^-$	III/35e 2.2.3:3204
26690	CHN_7 111.07		5-Azido-2H-tetrazole	III/35b 3.2:9
26691	$\text{CH}_2\text{ClF}_2\text{P}$ 118.45 1113-28-6		Chloromethyl difluorophosphine	III/35a 3.2:20
26692	$\text{CH}_2\text{F}_3\text{N}$ 85.03	$\text{F}_3\text{C}-\text{NH}_2$	C-Trifluoro-methylamine	III/35b 2.2:5
26693	CH_2NO_2 60.03	$\text{O}_2\text{N}-\text{CH}_2^{(-)}$	$[\text{CH}_2\text{NO}_2]^-$	III/35e 2.2.3:3207
26694	CH_3AsO_3 137.95		$[\text{CH}_3\text{AsO}_3]^{2-}$	III/35e 2.2.6:4411
26695	CH_3BClF 80.3		CH_3BClF	III/35a 2.2:154
26696	$\text{CH}_3\text{BCl}_2\text{F}_3\text{P}$ 184.72		$\text{CH}_3\text{BCl}_2\text{F}_3\text{P}$	III/35c4 2.2:35
26697	$\text{CH}_3\text{BCl}_2\text{F}_3\text{PS}$ 216.78		Dichloro-methyl-thiophosphonic acid trifluoro-borane	III/35c4 2.2:36
26698	$\text{CH}_3\text{BCl}_5\text{FNP}$ 267.09		$\text{CH}_3\text{BCl}_5\text{FNP}$	III/35a 2.2:157
26699	$\text{CH}_3\text{BF}_5\text{OP}$ 167.81		Difluoro-methyl-phosphonic acid trifluoro-borane	III/35c4 2.2:37
26700	$\text{CH}_3\text{BF}_5\text{P}$ 151.81 6153-93-1		Phosphonous difluoride, (trifluoromethyl)-, compound with borane (1:1)	III/35c4 2.2:38
26701	CH_3BN 39.85	$\text{H}_3\text{B}---\text{C}^{(-)}\equiv\text{N}$	BH_3CN^-	III/35a 2.2:158
26702	CH_3BNNa 62.84	$\text{H}_3\text{B}---\text{C}^{(-)}\equiv\text{N} \quad \text{Na}^{(+)}$	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 ₃ BrO ₂ S 159. 41138-92-5		Methanesulfonyl bromide	III/35e 2.2:5:3908
26706	CH ₃ Br ₂ OP 221.82 19430-64-9		Phosphonic dibromide, methyl-	III/35a 3.2:23
26707	CH ₃ Br ₃ Ge 327.39 6558-57-2		Tribromo(methyl)germane	II/25b 3:252
26708	CH ₃ Br ₃ Sn 373.44 993-15-7		Stannane, tribromomethyl-	III/35c4 2.4:3310
26709	CH ₃ ClFO ₃ P 148.46		((R,S)-Chloro-fluoro-methyl)-phosphonic acid	III/35a 3.2:24
26710	CH ₃ ClFPS ₂ 164.59		S-Methyl-fluoro-chloro-dithiophosphate	III/35c4 2.2:40
26711	CH ₃ ClFPSe 179.42		CH ₃ ClFPSe	III/35a 3.2:25
26712	CH ₃ ClF ₃ NOP ₂ S 231.5		CH ₃ ClF ₃ NOP ₂ S	III/35a 3.2:26
26713	CH ₃ ClHgO ₄ 315.07 16522-09-1		Methylperchlorato-mercury	III/35c4 2.2:42
26714	CH ₃ Cl ₂ F ₂ NOP ₂ S 247.96		CH ₃ Cl ₂ F ₂ NOP ₂ S	III/35a 3.2:27
26715	CH ₃ Cl ₂ F ₂ NOP ₂ S 247.96		CH ₃ Cl ₂ F ₂ NOP ₂ S	III/35a 3.2:28
26716	CH ₃ Cl ₂ P 116.91 125750-80-3		Dichloro-phosphanyl-methane; Dichloromethyl-phosphane	III/35a 3.2:29
26717	CH ₃ Cl ₃ FNOP ₂ S 264.41		CH ₃ Cl ₃ FNOP ₂ S	III/35a 3.2:30
26718	CH ₃ Cl ₄ NOP ₂ S 280.87		CH ₃ Cl ₄ NOP ₂ S	III/35a 3.2:31
26719	CH ₃ Cl ₄ NO ₂ P ₂ 264.8		CH ₃ Cl ₄ NO ₂ P ₂	III/35b 3.2:12
26720	CH ₃ Cl ₄ NP ₂ 232.8 17648-16-7		Bis(dichlorophosphino)methylamine	III/35a 3.2:32

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50-06-6	H 35643	89-91-8	G 28454	103-20-8	G 23509	122-04-3	G 29831	254-86-4	G 29927
51-20-7	G 27552	89-63-4	G 28798	103-53-7	G 24389	123-24-0	G 24559	261-67-6	H 33205
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77-24-7	G 23454	94-62-2	G 24438	109-98-8	G 27261	131-53-3	G 23169	302-84-1	G 27317
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82-28-0	G 23595	98-10-2	G 29006	115-71-9	G 23821	140-04-5	G 25746	336-67-4	G 23147
82-39-3	G 23580	98-97-5	G 28128	115-88-8	G 25075	141-19-5	G 25516	336-37-8	G 23145
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376-86-3	G 24001	459-56-3	G 30052	542-63-2	G 27840	607-34-1	H 32224	626-64-2	G 28185
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381-08-8	G 25406	464-33-5	G 25367	552-37-4	G 29987	609-41-6	G 28996	629-80-1	G 24266
381-26-0	G 25230	464-32-4	G 25229	553-82-2	G 29953	609-36-9	G 28364	634-36-6	H 32733
383-09-5	G 24044	464-37-9	G 25046	553-97-9	G 30022	610-15-1	G 30001	635-93-8	G 29882
383-79-9	G 24221	464-30-2	G 25641	554-68-7	G 29627	610-43-5	G 24069	637-53-6	H 31298
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384-22-5	G 29850	470-74-6	G 26249	556-53-6	G 27445	610-99-1	H 32537	638-66-4	G 24801
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429-20-9	G 24580	516-06-3	G 28490	593-03-3	G 24299	619-44-3	H 31071	688-61-9	H 32861
429-95-8	G 25819	519-87-9	G 23177	594-19-4	G 27799	619-84-1	H 32616	693-98-1	G 27649
429-74-3	G 25921	520-03-6	I 37100	595-50-6	G 29557	619-65-8	H 30912	694-24-6	G 27709
429-39-0	G 25013	523-31-9	G 25379	595-86-8	G 26902	619-72-7	G 29862	694-82-6	G 29119
429-78-7	G 25818	525-82-6	I 37829	595-90-4	I 40832	619-57-8	G 30084	695-30-7	G 29391
431-44-7	G 27178	525-06-4	I 37137	596-30-5	G 26527	619-80-7	G 29999	695-35-2	G 30640
439-14-5	I 38438	525-41-7	H 35625	597-79-5	G 26251	619-73-8	G 30088	695-15-8	G 30637
451-40-1	G 23158	526-86-3	H 31206	598-52-7	G 27020	619-24-9	G 29863	696-18-4	H 31254
451-85-4	G 29797	527-17-3	H 33696	598-41-4	G 27017	619-56-7	G 29948	696-63-9	G 30168
455-16-3	G 30057	527-61-7	H 31207	599-69-9	H 32790	620-63-3	G 24769	698-70-4	H 31364
455-24-3	H 30898	527-85-5	H 31263	599-66-6	I 37363	620-81-5	I 37218	698-69-1	H 31333
455-68-5	H 31045	530-44-9	I 38029	602-37-9	H 33184	620-32-6	I 37362	698-67-9	G 29944
456-71-3	H 30970	531-59-9	H 33364	602-60-8	I 37102	621-59-0	H 31211	699-98-9	G 29812
456-22-4	G 29898	531-81-7	H 33213	603-71-4	H 32615	621-07-8	I 37390	701-53-1	H 31046
456-21-3	G 29827	532-55-8	H 30909	605-61-8	H 33185	621-10-3	G 23647	701-56-4	H 32767
456-55-3	G 29909	533-37-9	H 31257	605-32-3	G 23107	622-87-7	G 24095	701-49-5	H 31148
458-65-1	G 24577	540-09-0	G 25621	605-45-8	G 23306	622-34-4	G 29989	703-07-1	H 31350