

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/>

Landolt-Börnstein

Numerical Data and Functional Relationships in Science and Technology

New Series / Editor in Chief: W. Martienssen

Index of Organic Compounds

Subvolume I (Supplement to Subvolumes C and F)

Compounds with 13 to 162 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. 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 Subvolume D
(Supplement to Subvolume A)

Compounds with 8 to 12 Carbon Atoms Subvolume E
(Supplement to Subvolume B)

Compounds with 13 to 100 Carbon Atoms Subvolume F
(Supplement to Subvolume C)

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

Compounds with 8 to 12 Carbon Atoms Subvolume H
(Supplement to Subvolumes B and E)

Compounds with 13 to 162 Carbon Atoms Subvolume I
(Supplement to Subvolumes C and F)

C13 – C25 printed

C13 – C162 in electronic version

Landolt-Börnstein
GROUP Index of Organic Compounds
SUBVOLUME I
Compounds with 13 to 162 Carbon Atoms

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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.

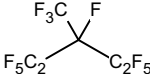
Since the data are excerpted from multiple volumes, sometimes inconsistencies in the data arose, i.e. mismatches between compound name, formula, and/or structure drawing occurred. The editor chose in most of these cases the chemical structure drawing as the most representative information. Often, even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

1.2.3 Methods of abbreviation of drawings

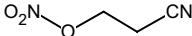
Alkyl chains: Alkyl chains of C₂ and longer are always abbreviated as a textstring, like C₃H₇ as in the example. Methyl groups are in most cases displayed as CH₃, except at quaternary centers, to facilitate the reading of highly branched structures. The following example shows two CH₃-groups to the right,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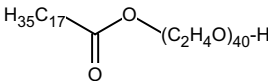
Persubstituted chains: Alkyl chains that are persubstituted with a particular element, like Fluorine, or Deuterium are shortened just like in the above example. CF_3 or CD_3 will for obvious reasons never be omitted like CH_3 .

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-13 978-3-540-60366-5

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-13 978-3-540-63275-7

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-13 978-3-540-41057-7

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-13 978-3-540-41059-1

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. Dudgeon; G. Toth; A. Simon

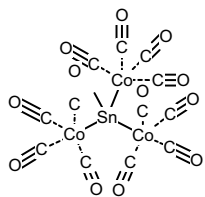
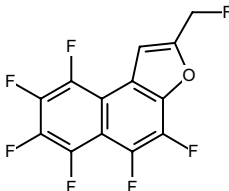
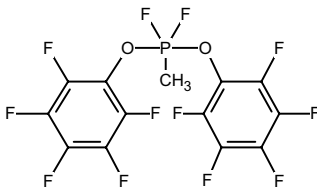
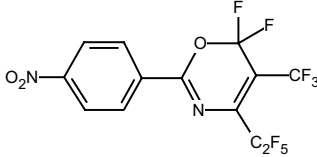
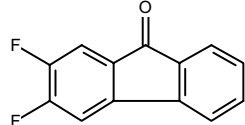
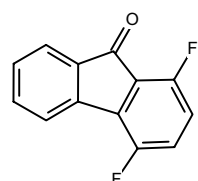
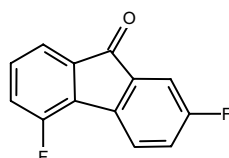
2002, VII, 320 pages. ISBN-13 978-3-540-42501-4

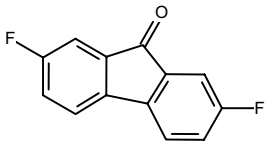
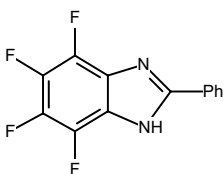
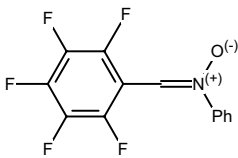
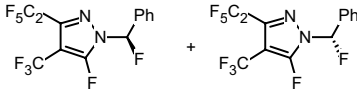
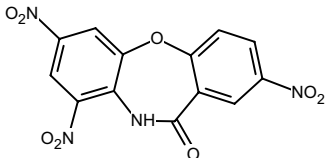
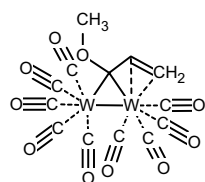
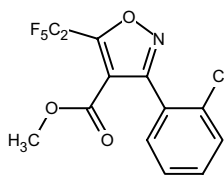
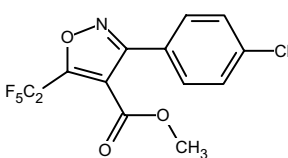
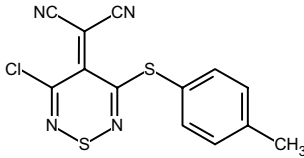
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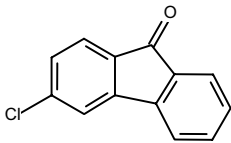
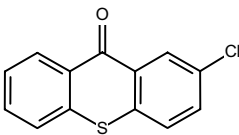
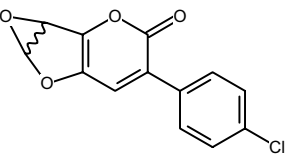
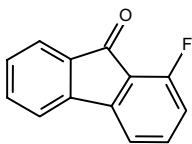
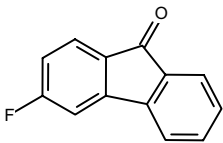
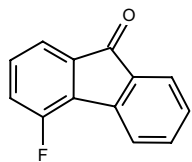
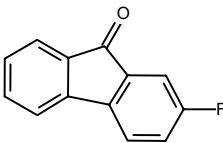
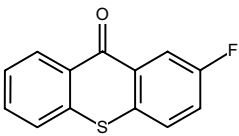
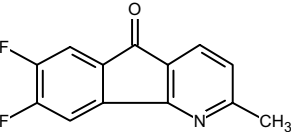
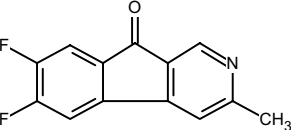
2 Index sorted by molecular formula and chemical structures

Compounds with 13 to 25 carbon atoms

2.1 New Compounds

36307	C ₁₃ H ₃ Co ₃ O ₁₂ Sn 646.64		C ₁₃ H ₃ Co ₃ O ₁₂ Sn	III/35e 2.2.7:4582
36308	C ₁₃ H ₃ F ₇ O 308.15		4,5,6,7,8,9-Hexafluoro-2-fluoromethyl-naphtho[2,1- <i>b</i>]furan	III/35c2 2.2:1537
36309	C ₁₃ H ₃ F ₁₂ O ₂ P 450.12		C ₁₃ H ₃ F ₁₂ O ₂ P	III/35a 3.2:1099
36310	C ₁₃ H ₄ F ₁₀ N ₂ O ₃ 426.17		6,6-Difluoro-2-(4-nitro-phenyl)-4-pentafluoroethyl-5-trifluoromethyl-6H-[1,3]oxazine	III/35b 2.2:1325
36311	C ₁₃ H ₆ F ₂ O 216.18		2,3-Difluoro-fluoren-9-one	III/35b 2.2:1326
36312	C ₁₃ H ₆ F ₂ O 216.18		1,4-Difluoro-fluoren-9-one	III/35e 2.2.1:1525
36313	C ₁₃ H ₆ F ₂ O 216.18		2,5-Difluoro-fluoren-9-one	III/35e 2.2.1:1526

36314	$C_{13}H_6F_2O$ 216.18		2,7-Difluoro-fluoren-9-one	III/35e 2.2.1:1527
36315	$C_{13}H_6F_4N_2$ 266.19		4,5,6,7-Tetrafluoro-2-phenyl-1H-benzimidazole	III/35b 2.2:1327
36316	$C_{13}H_6F_5NO$ 287.19		$C_{13}H_6F_5NO$	III/35e 2.2.3:3634
36317	$C_{13}H_6F_{10}N_2$ 380.18		5-Fluoro-1-((R,S)-fluoro-phenyl-methyl)-3-pentafluoroethyl-4-trifluoromethyl-1H-pyrazole	III/35b 2.2:1328; III/35c2 2.2:1538
36318	$C_{13}H_6N_4O_8$ 346.21		2,7,9-Trinitro-10H-dibenzo[b,f][1,4]oxazepin-11-one	III/35c2 2.2:1539
36319	$C_{13}H_6O_{10}W_2$ 689.86		$C_{13}H_6O_{10}W_2$	III/35c4 2.2:1410
36320	$C_{13}H_7ClF_5NO_3$ 355.64		3-(2-Chloro-phenyl)-5-pentafluoroethyl-isoxazole-4-carboxylic acid methyl ester	III/35b 2.2:1329
36321	$C_{13}H_7ClF_5NO_3$ 355.64		3-(4-Chloro-phenyl)-5-pentafluoroethyl-isoxazole-4-carboxylic acid methyl ester	III/35b 2.2:1330
36322	$C_{13}H_7ClN_4S_2$ 318.8		2-(3-Chloro-5-p-tolylsulfanyl-[1,2,6]thiadiazin-4-ylidene)-malononitrile	III/35c2 2.2:1540

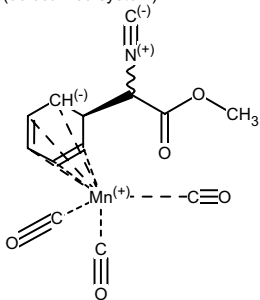
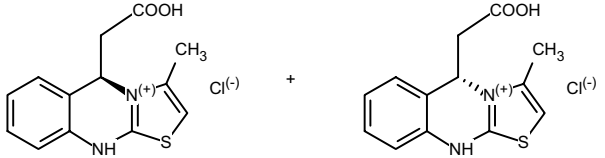
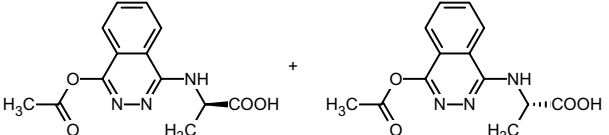
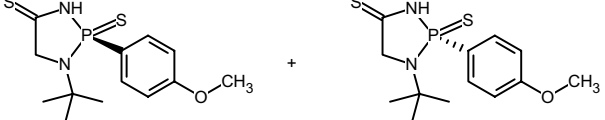


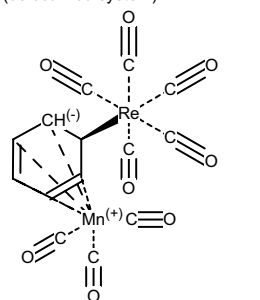
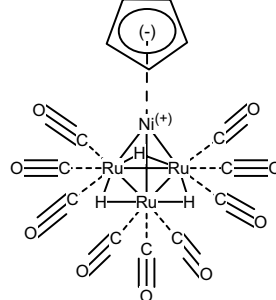
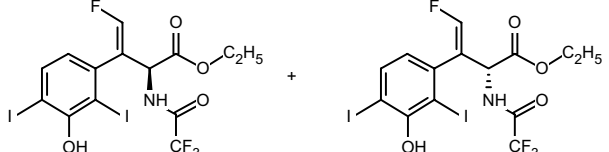
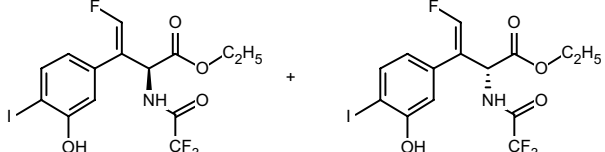
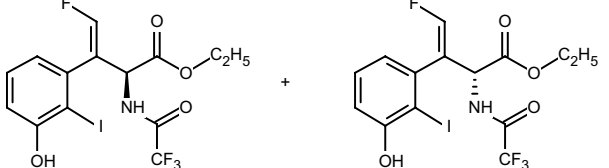
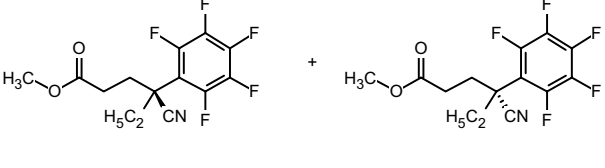
36323	C ₁₃ H ₇ ClO 214.65 7254-06-0		3-Chloro-fluoren-9-one	III/35e 2.2.1:1528
36324	C ₁₃ H ₇ ClOS 246.71 86-39-5		2-Chloro-thioxanthen-9-one; 2-Chlorothioxanthone; Thioxanthen-9-one, 2-chloro-; 9H-Thioxanthen-9-one, 2-chloro-	III/35e 2.2.1:1529
36325	C ₁₃ H ₇ ClO ₄ 262.64		4-(4-Chloro-phenyl)-1a,6a-dihydro-1,2,6-trioxa-cyclopropa[a]inden-3-one	III/35c2 2.2:1541
36326	C ₁₃ H ₇ FO 198.19 1514-16-5		1-Fluoro-9-fluorenone; 1-Fluoro-fluoren-9-one	III/35e 2.2.1:1530
36327	C ₁₃ H ₇ FO 198.19 1514-15-4		3-Fluoro-9-fluorenone; 3-Fluoro-fluoren-9-one	III/35e 2.2.1:1532
36328	C ₁₃ H ₇ FO 198.19 1514-18-7		4-Fluoro-9-fluorenone; 4-Fluoro-fluoren-9-one	III/35e 2.2.1:1533
36329	C ₁₃ H ₇ FO 198.19 343-01-1		2-Fluoro-fluoren-9-one	III/35e 2.2.1:1531
36330	C ₁₃ H ₇ FOS 230.26 60086-39-7		2-Fluoro-thioxanthen-9-one	III/35e 2.2.1:1534
36331	C ₁₃ H ₇ F ₂ NO 231.2		7,8-Difluoro-2-methyl-indeno[1,2-b]pyridin-5-one	III/35b 2.2:1331
36332	C ₁₃ H ₇ F ₂ NO 231.2		6,7-Difluoro-3-methyl-indeno[2,1-c]pyridin-9-one	III/35b 2.2:1332

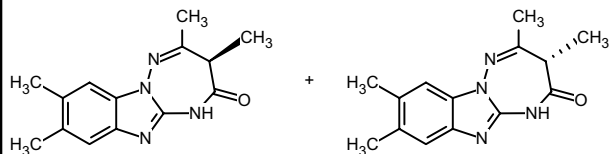
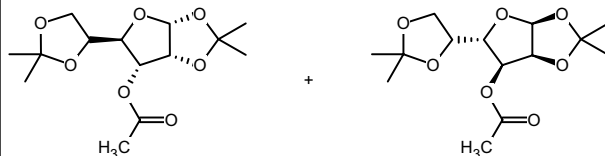
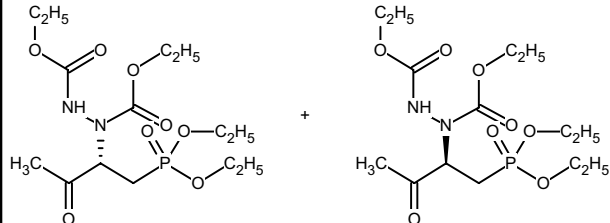
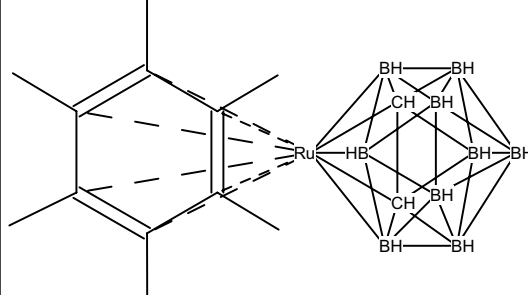
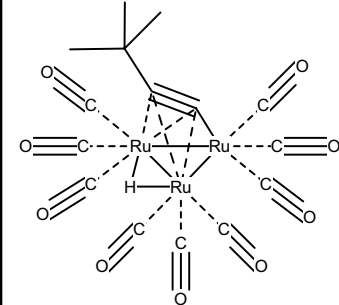
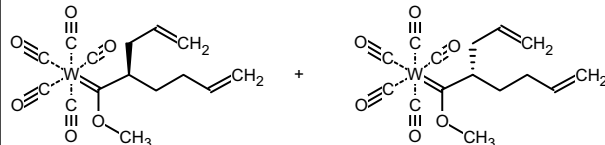
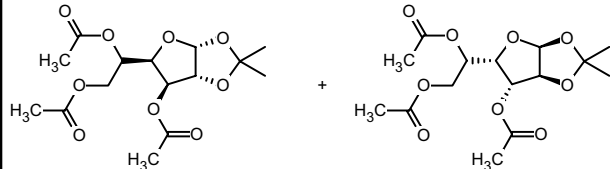
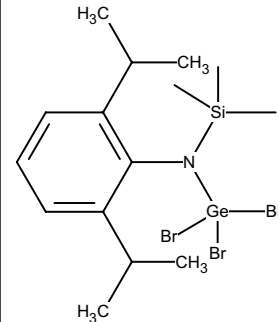
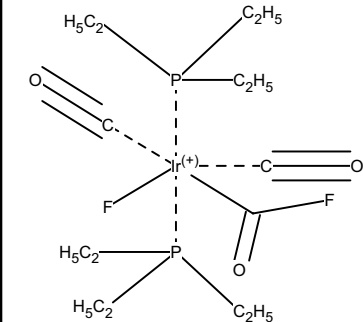
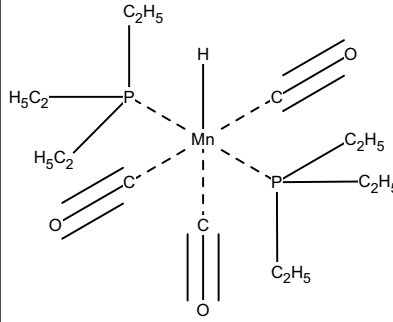
2.2 Compounds registered in Subvolumes C or F

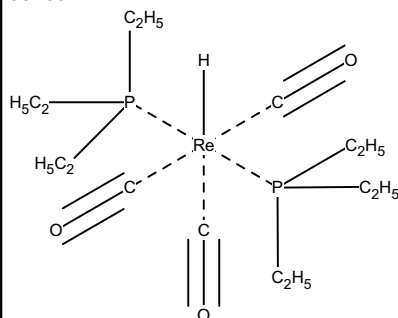
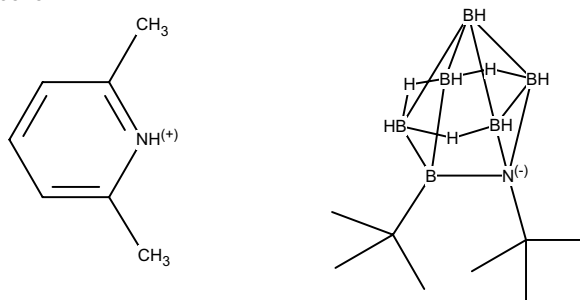
22697 Vol. F	C ₁₃ H ₁₀ F ₅ NO ₂	(R,S)-2-Cyano-2-pentafluorophenyl-butyrac acid ethyl ester	III/35b 2.2:1345
22714 Vol. F	C ₁₃ H ₁₁ N 153-78-6	Fluoren-2-ylamine	III/35b 3.2:1507
22715 Vol. F	C ₁₃ H ₁₁ NO 93-98-1	N-phenyl-benzamide	III/35b 3.2:1509; III/35e 2.2.1:1570
22738 Vol. F	C ₁₃ H ₁₂ O ₂ S 3112-88-7	Benzylsulfonyl-benzene	III/35e 2.2.5:4328
22787 Vol. F	C ₁₃ H ₁₅ F ₂ NO ₄	4- <i>tert</i> -Butoxycarbonylamino-2,6-difluoro-benzoic acid methyl ester	III/35b 2.2:1375
22788 Vol. F	C ₁₃ H ₁₅ F ₃	(E)-(3,3-Dimethyl-2-trifluoromethyl-but-1-enyl)-benzene	III/35b 2.2:1376
22809 Vol. F	C ₁₃ H ₁₆ F ₂ S	(1-Difluoromethylene-hexylsulfanyl)-benzene	III/35b 2.2:1383
22844 Vol. F	C ₁₃ H ₁₇ NO	3-Diethylamino-1-phenyl-propenone	III/35e 2.2.1:1630
22935 Vol. F	C ₁₃ H ₂₀ Se 76376-91-5	Heptyl-phenyl-selenide	III/35c4 2.2:1473
23096 Vol. F	C ₁₄ H ₅ ClF ₄	1-Chloro-2,3,5,6-tetrafluoro-4-phenylethynyl-benzene	III/35b 2.2:1423
23106 Vol. F	C ₁₄ H ₈ O ₃ 129-43-1	1-Hydroxy-anthraquinone	III/35e 2.2.1:1641
23108 Vol. F	C ₁₄ H ₈ O ₄ 117-10-2	1,8-Dihydroxy-anthraquinone	III/35e 2.2.1:1642
23117 Vol. F	C ₁₄ H ₉ NO ₂ 82-45-1	1-Amino-anthraquinone	III/35e 2.2.1:1651
23124 Vol. F	C ₁₄ H ₁₀ O ₃ 93-97-0	Benzoic acid anhydride	III/35e 2.2.1:1669
23131 Vol. F	C ₁₄ H ₁₁ F 390-75-0	1,1-Diphenyl-2-fluoro-ethene	III/35b 2.2:1441, 1442
23134 Vol. F	C ₁₄ H ₁₁ FOS	(R,S)-2-Fluoro-1-phenyl-2-phenylsulfanyl-ethanone	III/35b 2.2:1445
23144 Vol. F	C ₁₄ H ₁₂ F ₄ N ₂ O ₄	(R,S)-4-Cyano-4-(2,3,5,6-tetrafluoro-4-nitro-phenyl)-hexanoic acid methyl ester	III/35b 2.2:1461
23174 Vol. F	C ₁₄ H ₁₃ FO 337-72-4	2-Fluoro-1,1-diphenyl-ethanol	III/35b 2.2:1467
23176 Vol. F	C ₁₄ H ₁₃ N 2272-45-9	N-benzylidene- <i>p</i> -toluidine	III/35b 3.2:1556
23194 Vol. F	C ₁₄ H ₁₄ N ₄ O ₂ 55252-43-2	4-Nitro-4'-(N,N-dimethylamino)azobenzene	III/35b 3.2:1569
23234 Vol. F	C ₁₄ H ₁₅ N ₃ 60-11-7	Dimethyl-(4-phenylazo-phenyl)-amine	III/35b 3.2:1574
23437 Vol. F	C ₁₄ H ₂₆ F ₄ O	(R,S)-2-Fluoro-1-(2,2,2-trifluoroethoxy)-dodecane	III/35b 2.2:1502
23578 Vol. F	C ₁₅ H ₁₀ O 886-38-4	2,3-Diphenyl-2-cyclopropene-1-one	III/35e 2.2.1:1738

23587 Vol. F	C ₁₅ H ₁₁ F ₃ OS	(R,S)-1,1,1-Trifluoro-3-phenyl-3-phenylsulfanyl-propan-2-one	III/35b 2.2:1518
23611 Vol. F	C ₁₅ H ₁₂ O ₂ 120-46-7	1,3-Diphenyl-1,3-propanedione	III/35e 2.2.1:1786
23963 Vol. F	C ₁₆ H ₁₁ F ₃ OS	(Z)-4,4,4-Trifluoro-1-phenyl-2-phenylsulfanyl-but-2-en-1-one	III/35b 2.2:1596
23964 Vol. F	C ₁₆ H ₁₁ F ₃ O ₂	(Z)-4,4,4-Trifluoro-2-phenoxy-1-phenyl-but-2-en-1-one	III/35b 2.2:1599
23973 Vol. F	C ₁₆ H ₁₂ N ₂ O 842-07-9	2-Hydroxy-1-phenylazo-naphthalene	III/35e 2.2.1:1827
24029 Vol. F	C ₁₆ H ₁₅ FO ₂ S	(E)-(1-Fluoro-4-phenyl-but-1-ene-1-sulfonyl)-benzene	III/35b 2.2:1629
24084 Vol. F	C ₁₆ H ₁₈ N ₄ O ₂ 80631-72-7	4-Nitro-4'-(N,N-diethylamino)azo-benzene	III/35b 3.2:1646
24107 Vol. F	C ₁₆ H ₁₉ N ₃ 87986-73-0	Diethyl-(4-phenylazo-phenyl)-amine	III/35b 3.2:1649
24115 Vol. F	C ₁₆ H ₂₀ O ₂ Si 2553-19-7	Diethoxy-diphenyl-silane	III/35e 2.2.2:3138
24384 Vol. F	C ₁₇ H ₁₆ F ₃ NO ₂	(R)-3,3,3-Trifluoro-2- <i>p</i> -tolylamino-propionic acid benzyl ester	III/35b 2.2:1675
24399 Vol. F	C ₁₇ H ₁₇ FO ₂ S	(E)-(1-Fluoro-2-methyl-4-phenyl-but-1-ene-1-sulfonyl)-benzene	III/35b 2.2:1681
24591 Vol. F	C ₁₈ H ₁₅ ClSn 639-58-7	Chloro-triphenyl-stannane	III/35c4 2.2:1831
24602 Vol. F	C ₁₈ H ₁₆ O ₂ 84-47-9	2- <i>tert</i> -Butylanthraquinone	III/35e 2.2.1:1915
24625 Vol. F	C ₁₈ H ₁₉ F ₃ O ₄	2,2-Bis-(3,4-dimethoxyphenyl)-1,1,1-trifluoroethane	III/35b 2.2:1716
24730 Vol. F	C ₁₈ H ₂₈ O ₂ Si ₃ 17977-72-9	1,1,3,3,5,5-Hexamethyl-1,5-diphenyl-trisiloxane	III/35e 2.2.6:4514
25024 Vol. F	C ₂₀ H ₁₆ F ₂	(R,S)-1,2-Difluoro-1,1,2-triphenyl-ethane	III/35b 2.2:1745
25026 Vol. F	C ₂₀ H ₁₇ FO	(R,S)-2-Fluoro-1,1,2-triphenyl-ethanol	III/35b 2.2:1746

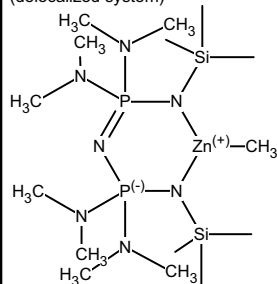
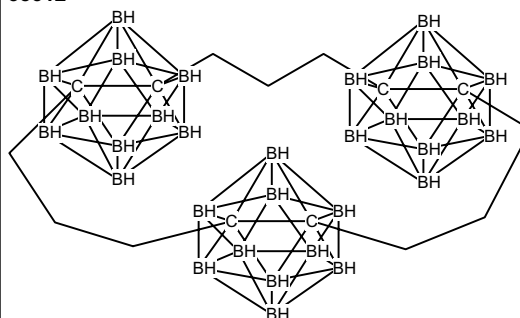
Appendix: Large Drawings

<p>36422 (delocalized system)</p> 	<p>36591</p> 
<p>36648</p> 	<p>36907</p> 
<p>36936</p> 	<p>36937</p> 
<p>37071 (delocalized system)</p> 	<p>37081</p> 
<p>37169</p> 	<p>37203</p> 
<p>37204</p> 	<p>37205</p> 

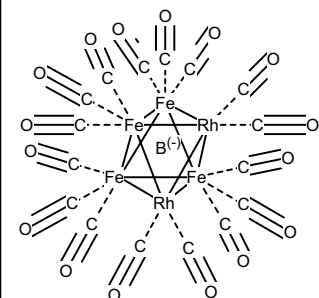
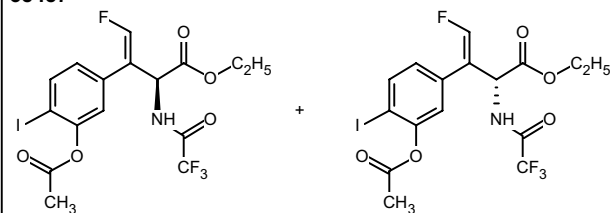
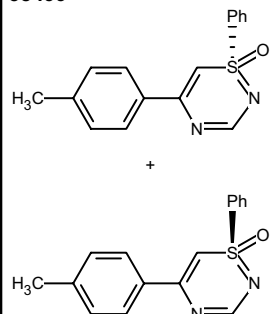
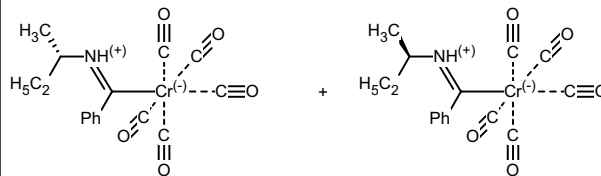
37470**37634****37696****37705****37839****38101****38211****38243****38260****38262**

38263**38287****38310**

(delocalized system)

**38312****38314**

(mixture of cis- and trans- isomers)

**38487****38499****38536**

Compounds with 13 to 162 Carbon Atoms (Supplement
to Subvolume C and F)

Bauhofer, C.; Peters, G.; Weigner, P.

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