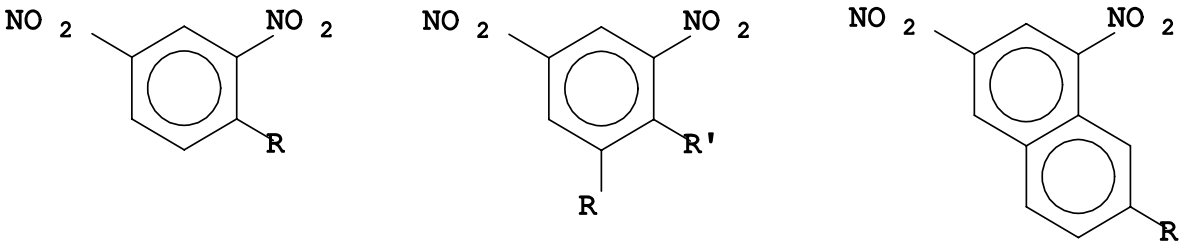
Date: 06 Aug. 2007

DIRDIF.ORBASE GALLERY

A visualization of a database of molecular fragments (file DIRDIF.ORBASE) which can be input to the program ORIENT for the solution of crystal structures using vector search methods.



Why using vector search or molecular replacement for small molecules?

- Because it makes sense to use available chemical information.
- If you have a good fragment, vector search is stronger than direct methods only.
- Because it is fun seeing your fragment growing.
- Because by using vector search you get familiar with it and you can use it when you need it: in some problem cases it is the only way to solve your structure.

And why not?

- It is easier than you might think it is.
- You do not need to be a crystallographer.
- The only thing to do before an automatic structure solution is selecting a proper fragment.

Your interactions with DIRDIF.ORBASE are:

Retrieving ready-to-use fragments: rigid fragments, or fragments with one or more preferred orientations (e.g. nitrobenzene, steroids) are available in this file. (Let your fingers do the walking!)

Storing your own fragments: when you work on a series of related compounds you can store your coordinates in a file DIRDIF.ORUSER (this is a 'personal' file, analogous to the system file DIRDIF.ORBASE).

Modifying a fragment to suit your specific needs (e.g. replace C by N, add a methylcarbon, fuse an aromatic ring).

How to use vector search?

When the vector search program ORIENT is called, a molecular fragment is used as input. The program determines its correct orientation, and the DIRDIF system passes automatically control to the program TRACOR to put the fragment on its correct position relative to the symmetry elements. Then control is passed on to the program PHASEX for phase refinement and phase expansion (using direct methods applied to difference structure factors). Finally the program FOUR organizes an automatic recycling procedure for completion of the structure.

Running the program ORIENT: the program reads the parameters of the fragment or model, from a file named ATMOD.

When you want to solve the structure with ORIENT in the automatic mode (instruction: DIRDIF CCODE ORIENT), the ATMOD file has to be present in advance.

When you run ORIENT interactively (instruction: DIRDIF CCODE) you either select a fragment in advance or during execution of the program. An existing ATMOD file can be modified, or a new ATMOD file can be selected from DIRDIF.ORUSER and/or DIRDIF.ORBASE.

How to use DIRDIF.ORBASE?

Retrieving and modifying fragments: The instruction DIRDIF CCODE ORBASE allows you to retrieve and/or modify a fragment in advance, see page 3 for edit instructions. The resulting fragment is stored in a file ATMOD.

Storing your own fragments: For your own structural research you can build up your private database in a file named DIRDIF.ORUSER which is analogous to DIRDIF.ORBASE. The file DIRDIF.ORUSER is one of the distributed files and its header contains instructions for the addition of your fragments. It contains some examples as well. The atomic parameters of your own fragment may be obtained by previously solved structures, the Cambridge Structural Database, molecular modeling, and so on.

Notes

- Do not hesitate to use a model with slightly deviating geometry: vector search methods do not depend critically on precise geometry.
- N-compounds: for many nitrogen compounds the geometry of the corresponding C-compound is sufficiently accurate.
- O-compounds: for many oxygen compounds the geometry of the corresponding C-compound is sufficiently accurate, unless the aromaticity is broken.
- S-compounds: for many sulphur compounds an out-of-ring replacement is sufficiently accurate, but some compounds with S in a ring are listed additionally.
- Warning! Most light-atom structures with S are favourably considered as heavy-atom structures and you had better solve it with PATTY (instruction: DIRDIF CCODE PATTY).
- Building up a large fragment in many steps is likely to introduce too large deviations in the geometry. Try instead to get the fragment from related structures or molecular modeling.

COFRED EDITOR

This editor is a simple COmmon FRagment EDitor, which is called when executing:

DIRDIF CCODE ORBASE	or
DIRDIF CCODE	(for an interactive run of ORIENT).

In the editor the following instructions are possible:

H	Help
D C4	Delete atom C4.
R C4 S5	Rename or replace atom C4 by S5; Adjust bond length if end-of-chain.
R C4 N4 1.2	Replace atom C4 by N4 at distance 1.20 from parent atom if end-of-chain.
A C4 C	Add one or more C-atoms to C4. (The number of atoms added and their positions depend on the hybridization of the parent atom C4. The new atoms will be numbered automatically.)
A C4 C –T	Add one or more C-atoms to C4, forcing a specified hybridization. (The number of atoms added and their positions will be determined automatically.) Possible keys are:
	-T tetrahedral(sp3)
	-P planar (sp2)
	-L linear (sp)
A C4 =O	Add =O to atom C4 in planar hybridization.
A C4 –CN	Add -CN to atom C4.
A C4 -NO2	Add -NO2 to atom C4 (Beware of geometry!).
F C2 C3 5	Fuse a 5-membered aromatic ring to bond C2-C3 of an aromatic ring or planar system.
F C2 C3 6	Fuse a 6-membered aromatic ring to bond C2-C3 of an aromatic ring or planar system.
G C4	Supply geometrical information about atom C4.
S	Save (store present atoms in back-up array).
U	Undo (retrieve atoms stored at last save instruction).
X 35	Rotate model around horizontal axis by 35 degrees.
Y 35	Rotate model around vertical axis by 35 degrees.
Z 35	Rotate model in the plane of the screen.
Q	Quit: finish session. Any present H-atom will be removed. (The user will have the opportunity to accept or reject the model obtained so far.)

After finishing the session the parameters of the fragment are stored in a file ATMOD. When this file is used by the program ORIENT, these parameters are saved in a file called ATOLD.

CLASSIFICATION

The fragments are classified according to chemical classes as given in Molecular Structures and Dimensions Vol.A1, Ed. by Olga Kennard *c.s.*, Crystallographic Data Centre Cambridge (1972). As the 'rigidity' of the fragment is of greater importance than the chemical functionality, we occasionally deviate from these classes. Note that several classes have no entries, as fragments are not available, or are easily generated.

1	Aliphatic Carboxylic Acid Derivatives	34	Hetero-Nitrogen (>6-Rings Monocyclic)
2	Aliphatic Carboxylic Acid Salts	35	Hetero-Nitrogen (2 Fused Rings)
3	Aliphatic Amines	36	Hetero-Nitrogen(>2 Fused Rings)
4	Aliphatic N and S Compounds	37	Hetero-Nitrogen (Bridged Ring Systems)
5	Aliphatic Miscellaneous	38	Hetero-Oxygen
6	Enolates (Aliphatic and Aromatic)	30	Hetero-Sulphur and Hetero-Selenium
7	Nitriles (Al. & Ar.)	40	Hetero-(Nitrogen and Oxygen)
8	Urea Compounds (Al. & Ar.)	41	Hetero-(Nitrogen and Sulphur)
9	Nitrogen-Nitrogen Comp. (Al. &Ar.)	42	Hetero-Mixed Miscellaneous
10	Nitrogen-Oxigen Comp. (Al. & Ar.)	43	Barbiturates
11	Sulphur and Selenium Compounds	44	Pyrimidines and Purines
12	Carbonium Ions, Carbanions, Radicals	45	Carbohydrates
13	Benzoic Acid Derivatives	46	Phosphates
14	Benzoic Acid Salts	47	Nucleosides and Nucleotides
15	Benzene Nitro Compounds	48	Amino-Acids and Peptides
16	Anilines	49	Porphyrins and Corrins
17	Phenols and Ethers	50	Antibiotics
18	Benzoquinones	51	Steroids
19	Benzene Miscellaneous	52-57	Terpetines
20	Monocyclic Hydrocarbons (3,4,5-Rings)	58	Alkaloids
21	Monocyclic Hydrocarbons (6-Rings)	59	Miscellaneous Natural Products
22	Monocyclic Hydrocarbons (7, 8-Rings)	60	Molecular Complexes
23	Monocyclic Hydrocarbons (>8-Rings)	61	Clathrates
24	Naphtalene Compounds	62-66	B, Si, P, As, Sb, Bi Compounds
25	Naphtoquinones	67-68	Group IA, IIA, III Compounds
26	Anthracene Compounds	69-70	Ge, Sn, Pb, Te Compounds
27	Hydrocarbons (2 Fused Rings)	71	Transition-metal compounds
28	Hydrocarbons (3 Fused Rings)	72-75	Metal pi-Complexes
29	Hydrocarbons (4 Fused Rings)	76-86	Metal Complexes
30	Hydrocarbons (>4 Fused Rings)	87-99	Miscellaneous
31	Bridged Ring Hydrocarbons		
32	Hetero-Nitrogen (3,4,5-Rings Monocyclic)		
33	Hetero-Nitrogen (6-Rings Monocyclic)		

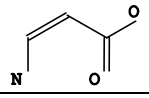
Acknowledgements. Fragments were obtained from published structure determinations, or from a connectivity search in the Cambridge Structural Database. Fragments were also prepared with MODELKS 2.96 (Steliou, Univ. of Montreal, Canada, Jan. 1991) and Chem-X (Chemical Design Ltd., Oxford, UK, July 1991) as made available through the CAOS/CAMM Center, Univ. of Nijmegen.

Revised edition (Apr. 1994): R.M.Beurskens, Univ. of Nijmegen. Update: June 1994.
Latest edition (Aug. 2007): J.M.M. Smits, Radboud University Nijmegen.

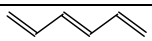
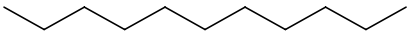
DIRDIF.ORBASE GALLERY

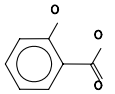
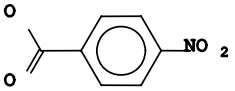
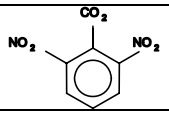
'd.a.: 5' denotes a dihedral angle of 5 degrees

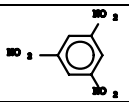
0.001	MONOS	Test model (7-atom fragment of model 41.41)		

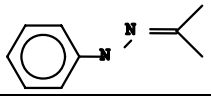
1.	For anhydrides, see class 38.			
1.11	D-Tartaric acid	$COOH(CHOH)_2COOH$		
1.12	Ethylacetate	$CH_3COOC_2H_5$		
1.13	Valeric acid	$CH_3(CH_2)_3COOH$		
1.14	Valeric acid amide	$CH_3(CH_2)_3CONH_2$		
1.21	Aminobutenoate			

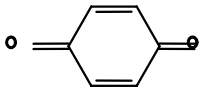
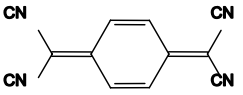
3.11	Butylamine	$CH_3(CH_2)_3NH_2$		

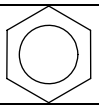
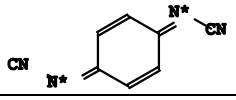
5.11	Butanole	$CH_3(CH_2)_3OH$		
5.12	Butadiene (trans conformer)			
5.13	Butadiene (cis conformer)			
5.21	Hexatriene			
5.31	Undecane			

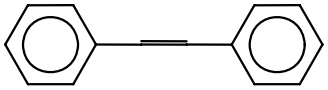
13.11	Hydroxybenzoic acid			
13.12	Nitrobenzoic acid			
13.21	Dinitrobenzoic acid			

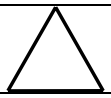
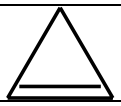
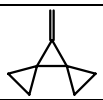
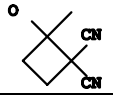
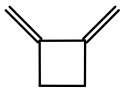
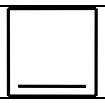
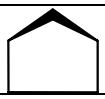
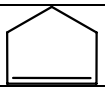
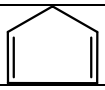
15.11	TNB			

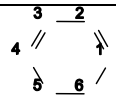
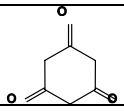
16.21	Azine derivative			

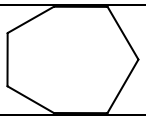
18.11	Benzoquinone			
18.21	Tetracyano-p-quinodimethane (TCNQ)			

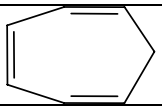
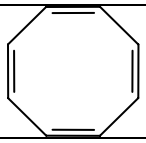
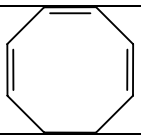
19.11	Benzene			
19.21	Dicyanamidebenzene dianion			

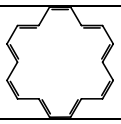
19.31	Tolane	

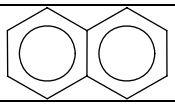
20.11	Cyclopropane			
20.12	Cyclopropene			
20.13	Cyclopropene-dispiro derivative			
20.21	Cyclobutane (flat)			
20.22	Cyclobutane (twist)			
20.23	LOXY			
20.24	Dimethylene-cyclobutane			
20.31	Cyclobutene			
20.41	Cyclopentane (twist-envelope)			
20.51	Cyclopentene			
20.61	Cyclopentadiene			

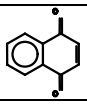
21.11	Cyclohexane (chair)			
21.12	Cyclohexane (twist-boat)			
21.21	Cyclohexene			
21.31	1,4-Cyclohexadiene (flat)			
21.32	1,3-Cyclohexadiene			
21.41	Phloroglucinol			

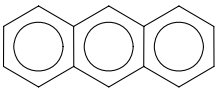
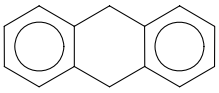
22.111	Cycloheptane, chair			
22.112	Same, twist-chair			

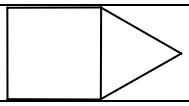
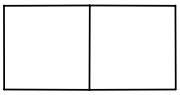
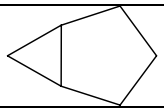
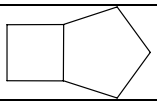
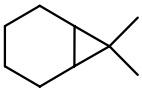
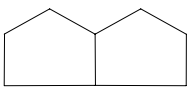
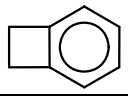
22.113	Same, bed			
22.114	Same, twist-bed			
22.21	Cycloheptatriene			
22.22	Same, other conf.			
22.31	Cyclooctatetraene			
22.32	1,3,5-Cyclooctatriene			
22.33	Same, other conf.			

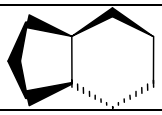
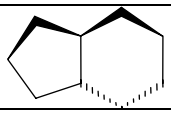
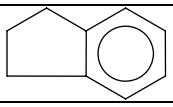
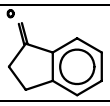
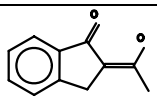
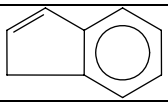
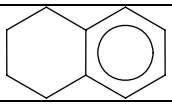
23.11	(18)-Annulene			

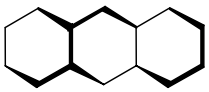
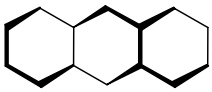
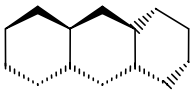
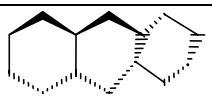
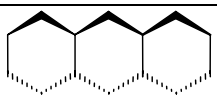
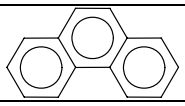
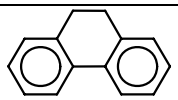
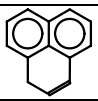
24.11	Naphthalene			

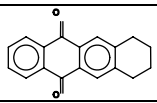
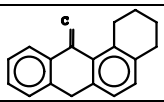
25.11	Naphthoquinone			

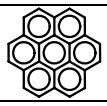
26.11	Anthracene			
26.211	Dihydroanthracene, d.a.: 4			
26.212	Same, d.a.: 42			
26.213	Same, d.a.: 65			

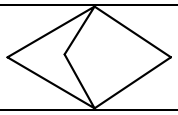
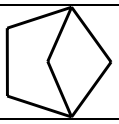
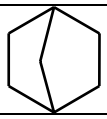
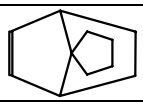
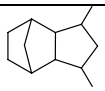
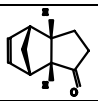
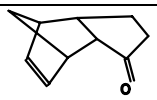
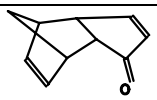
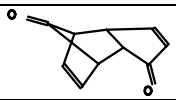
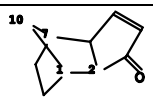
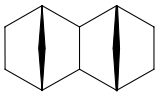
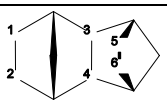
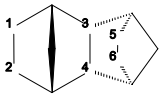
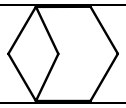
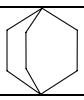
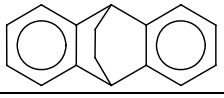
27.11	Bicyclo[2.1.0]pentane			
27.21	Bicyclo[2.2.0]hexane			
27.22	Bicyclo[3.1.0]hexane			
27.31	Bicyclo[3.2.0]heptane			
27.32	DiMe Bicyclo[4.1.0]heptane			
27.41	Bicyclo[3.3.0]octane			
27.45	Benzocyclobutane			

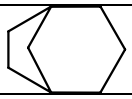
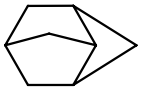
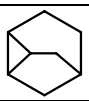
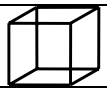
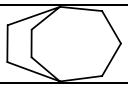
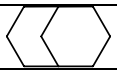
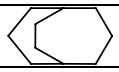
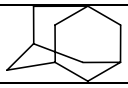
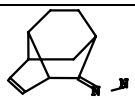
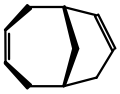
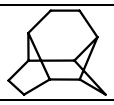
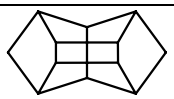
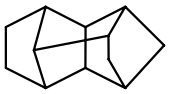
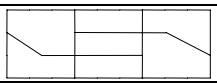
27.51	cis-Hydrindane			
27.52	trans-Hydrindane			
27.53	Indane = Benzocyclopentane			
27.55	Indan-1-on			
27.56	Acylindanone			
27.57	Indene			
27.61	Tetralin			

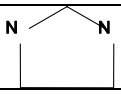
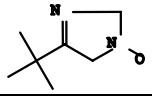
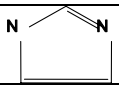
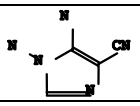
28.21	cis-anti-cis-Perhydroanthracene			
28.22	cis-syn-cis-Perhydroanthracene			
28.23	cis-trans-Perhydroanthracene			
28.24	trans-anti-trans-Perhydroanthracene			
28.25	trans-syn-trans-Perhydroanthracene			
28.31	Phenanthrene			
28.32	Dihydrophenanthrene			
28.41	Phenalene (aromatic)			

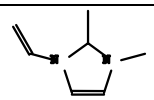
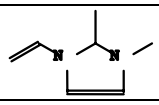
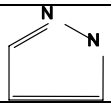
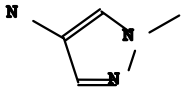
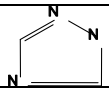
29.31	Tetrahydrobenzo anthrachinone			
29.41	Tetrahydrobenzo anthrone (d.a.: 32)			

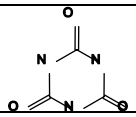
30.31	Coronene			

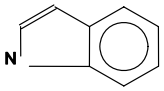
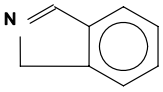
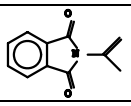
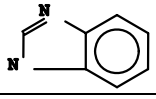
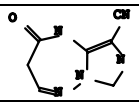
31.01	Bicyclo[1.1.1]pentane			
31.11	Bicyclo[2.1.1]hexane			
31.21	Bicyclo[2.2.1]heptane = Norbornane			
31.22	Norbornene			
31.23	Norbornene-spiro derivative			
31.251	Fused Norbornane-pentane			
31.252	Same			
31.253	Same			
31.254	Same			
31.26	BULAC	 =		
31.27	CARBET			
31.28	DIENON			
31.29	DOLS1			
31.31	Fused Norbornanes			
31.32	Fused Norbornanes			
31.331	Same, C5=C6			
31.332	Same, C3=C4			
31.333	Same, C1=C2, C5=C6			
31.341	Fused Norbornanes			
31.342	Same, C3=C4			
31.41	Bicyclo[3.1.1]heptane			
31.51	Bicyclo[2.2.2]octane			
31.521	Dibenzobicyclooctane, bridge: single bond (1.55)			
31.522	Same, aromatic bond (1.39)			
31.523	Same, double bond (1.30)			

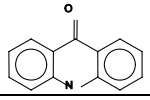
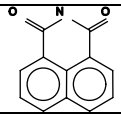
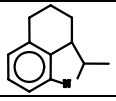
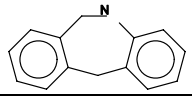
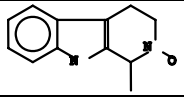
31.55	Bicyclo[3.2.1]octane			
31.56	Tricyclooctane			
31.57	DELE8			
31.58	Cubane			
31.61	Bicyclo[3.2.2]nonane			
31.64	Bicyclo[3.3.1]nonane			
31.71	Bicyclo[3.3.2]decane			
31.74	Adamantane			
31.75	NN=decane			
31.79	Bicyclodecane			
31.81	Tetracycloundecane			
31.83	Dodecahedrane (pentagonal dodecahedron)			
31.84	Pentacyclododecane			
31.86	Hexacyclododecane			
31.88	Diamantane C14			
31.91	Buckminster-fullerene (C60 ball)			

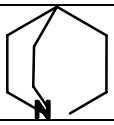
32.21	Pyrrolidine			
32.31	Pyrrole			
32.41	Imidazolidine			
32.43	N-oxyimidazol derivative			
32.51	Imidazole			
32.52	Imidazolyl derivative			

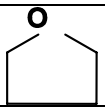
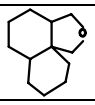
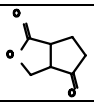
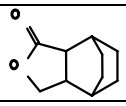
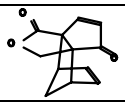
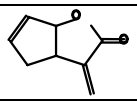
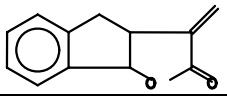
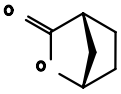
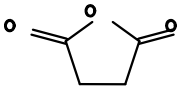
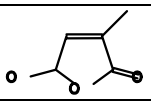
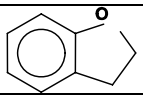
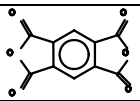
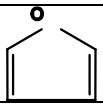
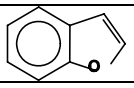
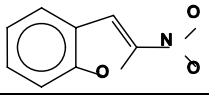
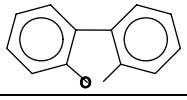
32.53	Imidazolium-ion			
32.54	Same			
32.61	Pyrazole			
32.62	Pyrazole derivative			
32.81	1,2,4-Triazole			

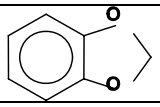
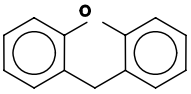
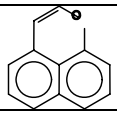
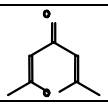
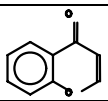
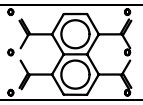
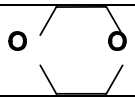
33.	For pyridines, see benzene derivatives			
33.31	Dihydropyridine			
33.51	1,3,5-Triazine (flat)			
33.52	Trioxotriazine			

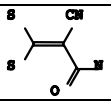
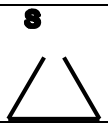
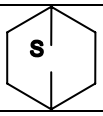
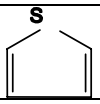
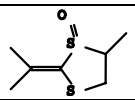
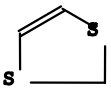
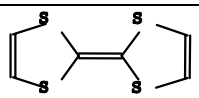
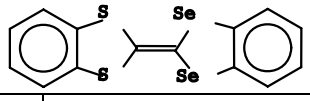
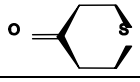
35.11	Indole			
35.21	2H-Isoindole			
35.22	STRIAN			
35.31	Benzimidazole			
35.51	Imidazotriazepine			

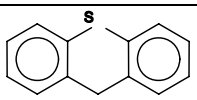
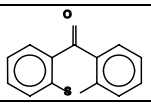
36.21	Oxohydroacridine			
36.31	Naphthalimide			
36.32	Ergolin-fragment			
36.411	Dibenzoazacycloheptadiene, fold-line: N-C			
36.412	Same, fold-line: C-C			
36.51	BEWIJS			

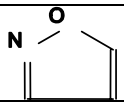
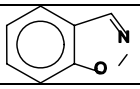
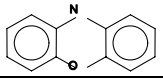
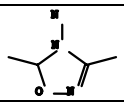
37.21	Azabicyclooctane			

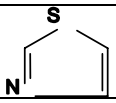
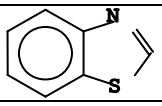
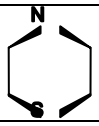
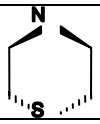
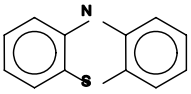
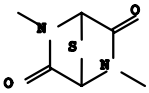
38.11	Oxirane			
38.21	Oxetane			
38.31	Tetrahydrofuran			
38.32	VADER			
38.33	FENBUT			
38.34	GAMDEL			
38.35	FENLAK			
38.36	MANG1			
38.37	MANG4			
38.38	Camphanic-lacton			
38.41	Succinic anhydride			
38.42	STRIA			
38.43	Dihydrobenzofuran			
38.44	PMDA			
38.51	Furan			
38.52	Benzofuran			
38.53	Nitrobenzofuran			
38.54	Dibenzofuran			

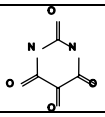
38.61	Benzodioxole			
38.62	1,3-Dioxole			
38.72	Xanthene			
38.73	Oxaphenalene			
38.74	Dimethylpyrone (flat)			
38.75	Benzopyrone			
38.76	NTDA			
38.81	1,4-Dioxane (chair)			
38.82	Pyran			

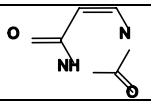
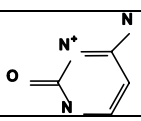
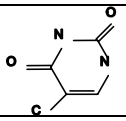
39.01	NOVOA			
39.11	Thiirane			
39.21	Thietane			
39.31	Thiabicycloheptane			
39.32	Thiophen			
39.34	SULFOX			
39.35	1,3-Dithiole			
39.36	TTF-Cation			
39.37	SSe-fulvalene			
39.41	Thiacyclohexanon, bed			
39.42	Same, chair			

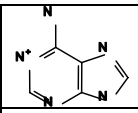
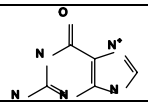
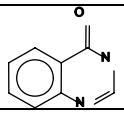
39.511	Thioxanthene, d.a.: 4			
39.512	Same, d.a.: 40			
39.52	Thioxanthone			

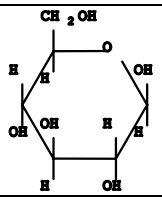
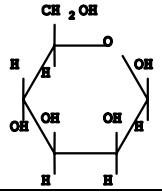
40.11	Isoxazole			
40.22	Benzisoxazole			
40.311	Phenoxazine, d.a: 5			
40.312	Same, d.a.: 33			
40.41	Oxazo			

41.11	Thiazole			
41.12	Benzothiazole			
41.22	Thiazocyclohexane bed, one C-C: aromatic (1.39)			
41.23	Same chair, C-C: single bonds (1.51)			
41.311	Phenothiazine, d.a.: 5			
41.312	Same, d.a.: 29			
41.313	Same, d.a.: 42			
41.41	MONOSX			

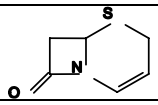
43.21	Alloxan			

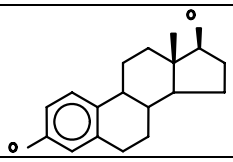
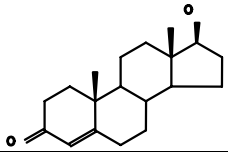
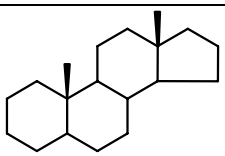
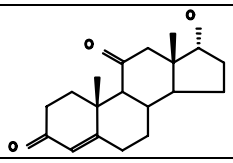
44.11	Uracil			
44.12	Cytosine protonated			
44.13	Thymine			

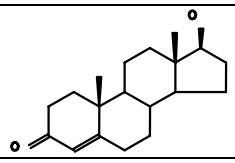
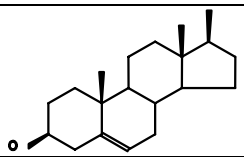
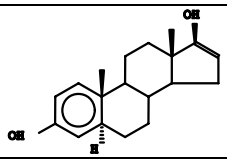
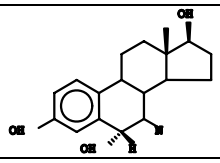
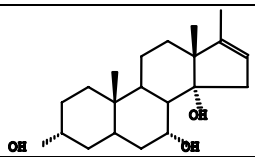
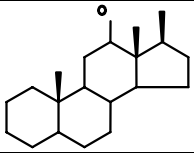
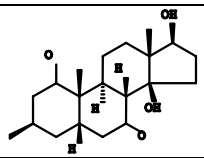
44.21	Adenine protonated			
44.22	Guanine protonated			
44.31	Benzopyrimidone			

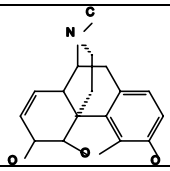
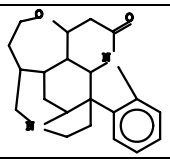
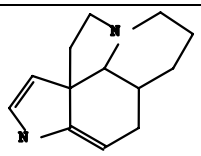
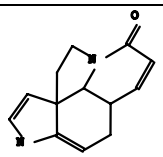
45.11	beta-D-Ribose and 45.111			
45.12	alpha-D-Ribose and 45.121			
45.21	beta-Fructopyranose			
45.51	beta-D-Glucopyranose			
45.52	alpha-D-Glucopyranose			
45.61	beta-D-Mannopyranose			
45.71	beta-D-Arabinopyranose			

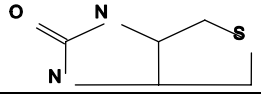
48.11	Glycine (pi = 5.97)	NH_2CH_2COOH		
48.21	gamma-Aminobutyric acid zwitterion	$NH_3^+(CH_2)_3COO^-$		

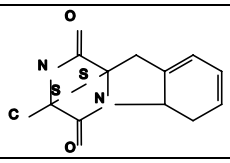
50.11	Cephalosporin-C			

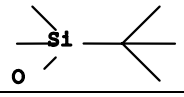
51.11	Estradiol			
51.12	Testosterone			
51.13	5a-Steroid			
51.14	Cortisone			

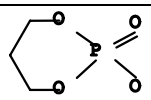
51.15	Progesterone skeleton			
51.16	Cholesterol skeleton			
51.17	Ster1			
51.18	Ster2			
51.19	Ster3			
51.20	Ster4			
51.21	Ster5			

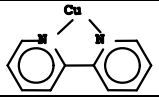
58.11	Morphine skeleton			
58.21	Strychnine			
58.22	Same: cation			
58.51	Vincadifform.			
58.52	Oxotabersonine			

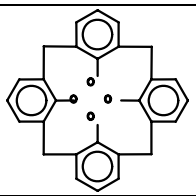
59.11	(+)Biotin skeleton			

59.21	Gliotoxin skeleton			

63.11	Silano derivative (staggered)			

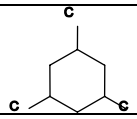
64.31	CLAM2			

67.51	Cu-bipyridine			

90.	Calixarenes			
90.01	HUMMEL			
	six more different geometries: 90.02, 90.03, 90.04, 90.05, 90.06, 90.07			

DIRDIF.ORUSER GALLERY

Molecular fragments in DIRDIF.ORUSER analogous to those in DIRDIF.ORBASE (see header lines of the file DIRDIF.ORUSER for instructions and suggestions for use). The distributed file may contain additional fragments.

0.1	IODINE	I_2		
0.2	PHENA			
0.3	PO4	PO_4		
0.4	GOLD	$AuPC_3$		
0.5	PF6	PF_6		
8	BASKET	A basket-shaped fragment used in supramolecular chemistry.		