Electronic Supplementary Material for CrystEngComm

The Retcif procedure

Stage 1: read input *cif* file to retrieve refcode, space group symbol and symmetry operations, brute formula, cell parameters, number of chemical units, atom type and nuclear coordinates for all atoms present. The atomic coordinate list is rearrange with non-hydrogens first, the connectivity matrix is computed from original CSD coordinates, separate chemical units are recognized and each atom is assigned to one of them. The atom count is then compared with the retrieved brute formula; if the count is incorrect (some hydrogen coordinates not present) an error flag is hoisted. This stage handles only the atoms of organic chemistry, and assigns an 'unknown' mark if other atoms (e.g. metals) are present, setting a warning flag for the current crystal structure.
Stage 2: scan non-hydrogen atoms. There are separate procedures for each atom type (see also the Scheme).
2.1 Carbon atoms. Hydrogen atom assignment is considered for C≡CH acetylenic, $C{=}CH_2$ terminal methylene, $R\text{-}CH_2\text{-}R$ saturated methylene, R=CH-R unsaturated or aromatic, R_3CH methine, $R\text{-}CH_3$ methyl, R being any non-hydrogen atom compatible with the rules of valence. No action is of course required for quaternary R_4C carbons. All C-H distances are renormalized to 1.08 Å; then: a) acetylenic H is located along the C-C bond direction; b) terminal methylene H's are located assuming a planar configuration at the double bond , all angles 120°; c) methylene H's are located in a plane perpendicular to the RCR plane and bisecting the RCR angle, with a tetrahedral configuration; d) unsaturated H's are located in the RCR plane on the bisector of the RCR angle; e) methine H's are located assuming three identical RCH angles; f) methyl atoms are located in a tetrahedral configuration with tetrahedral angles, as close as possible to the original set of R'-R-C-H torsion angles, if available from the CSD; otherwise, staggered configurations are assumed.

The problem is to determine automatically which of the above is the case for each C atom in a molecule. If the CSD atom count is correct, the problem is solved by using the CSD connectivity to determine the type and number of hydrogen atoms to be assigned to the carbon atom under examination. If the atom-count error flag is on, the approximate valence saturation, *V*, is calculated on the basis of average C-R bond distances[1], the number of hydrogen atoms to be assigned being then 4-*V*, with appropriate roundoff. This last step is obviously not 100% safe, due both to valence vagaries, especially when R is nitrogen, and to errors or misinterpretations in the original X-ray coordinates.
2.2) Nitrogen atoms. The configuration at nitrogen atoms is variable, since various degrees of pyramidalization are possible. The absolute prediction of H-atom locations is therefore very difficult if not impossible. No attempt is made at such a prediction, and structures are accepted only if approximate positions for the hydrogen atoms are available in the CSD files, which is increasingly, indeed almost invariably the case in most recent X-ray structure determinations. The CSD connectivity is then used throughout, and an error flag is set if the atom count does not match (as above). Quaternary nitrogen of general formula $R_nN^+H_{4-n}$ is assigned 4-*n* hydrogen atoms, and is considered not to act as hydrogen bond acceptor. No action is taken for R_3N groups (this causes an error if the nitrogen atom is actually quaternary and hydrogen positions are not in the original *cif* file). Nitrogen is considered to act as hydrogen bond acceptor in R-NH-R or RNH_2 groups; amide hydrogens are recognized and marked as H-bond donors. No action is taken when the R=N-R connectivity is detected, as distinguished from the R-NH-R connectivity on the basis of the presence of H-atom coordinates in the original *cif* file. However, sometimes a R-N-R connectivity is detected on the basis of R-N bond distances, even in absence of H-atom coordinates; in such case, a hydrogen atom is assigned on the bisector of the RNR angle. This identification is sometimes uncertain. In the two latter configurations, nitrogen is considered as a H-bond acceptor and hydrogen as a H-bond donor. One hydrogen is assigned for the R=N-H terminal connectivity, and obviously no action is taken for C≡N or R-N=N terminal nitrogen atoms, which are not considered as H-bond acceptors. N-H distances are renormalized to 1.00 Å.
2.3) Oxygen atoms. The considerations made for nitrogen on the a priori predictability of H-atom positions hold also for oxygen; in this case too only the connectivity retrieved from the original CSD files is used for H-atom assignment. No action is taken for the R-O-R connectivity, and oxygen is considered not to act as H-bond acceptor (sometimes a questionable choice). Alcohol

and acid functions are recognized and marked as H-bond donor and acceptor groups. C=O, N=O, S=O and P=O oxygen is always considered as H-bond acceptor. COO- groups are recognized and assigned no hydrogen; except for the case of zwitterions (e.g. aminoacids and peptides) the carboxyl group is often a source of error because in many carboxylic acid crystals, there is disorder in the H-atom positions and C-O and C=O distances are apparently very similar. There is no possible (automatic) solution for this problem. S-OH and P-OH hydrogens are taken care of as alcohol hydrogens. All O-H distances are renormalized to 1.00 Å.

2.4) Other atomic species. S-H thiol hydrogens are assigned as for O-H hydrogens. No provision is made for hydrogen atoms attached to atoms other than C, O, N and SH, and an error message is generated when this happens, as well as in cases with erroneous, improper, or just unusual bonding situations.

Stage 3: final checks and output. The Retcif procedure works with any number of molecules in the asymmetric unit, identical or different in chemical composition. In Stage 3, the total atom count after the H-atom assignment procedures is matched with the brute formula retrieved from the CSD, generating error flags when appropriate. In spite of this and all other sieves, the whole procedure is not absolutely safe, because of many combinations of casual errors and of their accidental cancellation. The checking procedures have been kept very conservative, considering the abundance of crystal structures in the Database, so that many good structures are discarded, and a few bad ones are accidentally included. A "statistical noise" of the order of 1-3% of wrong structures is thus introduced in the retrieved samples. The Table summarizes the types of atoms and their codes.

Table. Atomic species and their labels

name	code number	bonding radius	intermolecular radius[a]		
hydrogen not H-bonding	1	0.30	1.10		
carbon	3	0.67	1.77		
nitrogen not HB acceptor	4	0.63	1.64		
oxygen not HB acceptor	5	0.66	1.58		
fluorine	6	0.72	1.46		
sulfur	9	1.04	1.81		
chlorine	10	0.99	1.76		
-COH oxygen	16	alcohol			
-COH hydrogen	25	alcohol			
-C=O oxygen	17	carboxylic acids and amides (carbonyls?)			
-COH oxygen	18	carboxylic acids			
-CO(OH) hydrogen	26				
-CO(NHR) nitrogen	19	amides			
-CO(NH_2) nitrogen	20				
(NHR) hydrogen	27	amides and amines			
(NH_2) hydrogen	28	amides and amines			
>C=S sulfur	21				
-NO_2 oxygen	22	nitro group			
nitrogen HB acceptor	23	aromatic ring, amine			

[a] R..S.Rowland, R.Taylor, J.Phys.Chem. 1996,100,7384, except for boron.

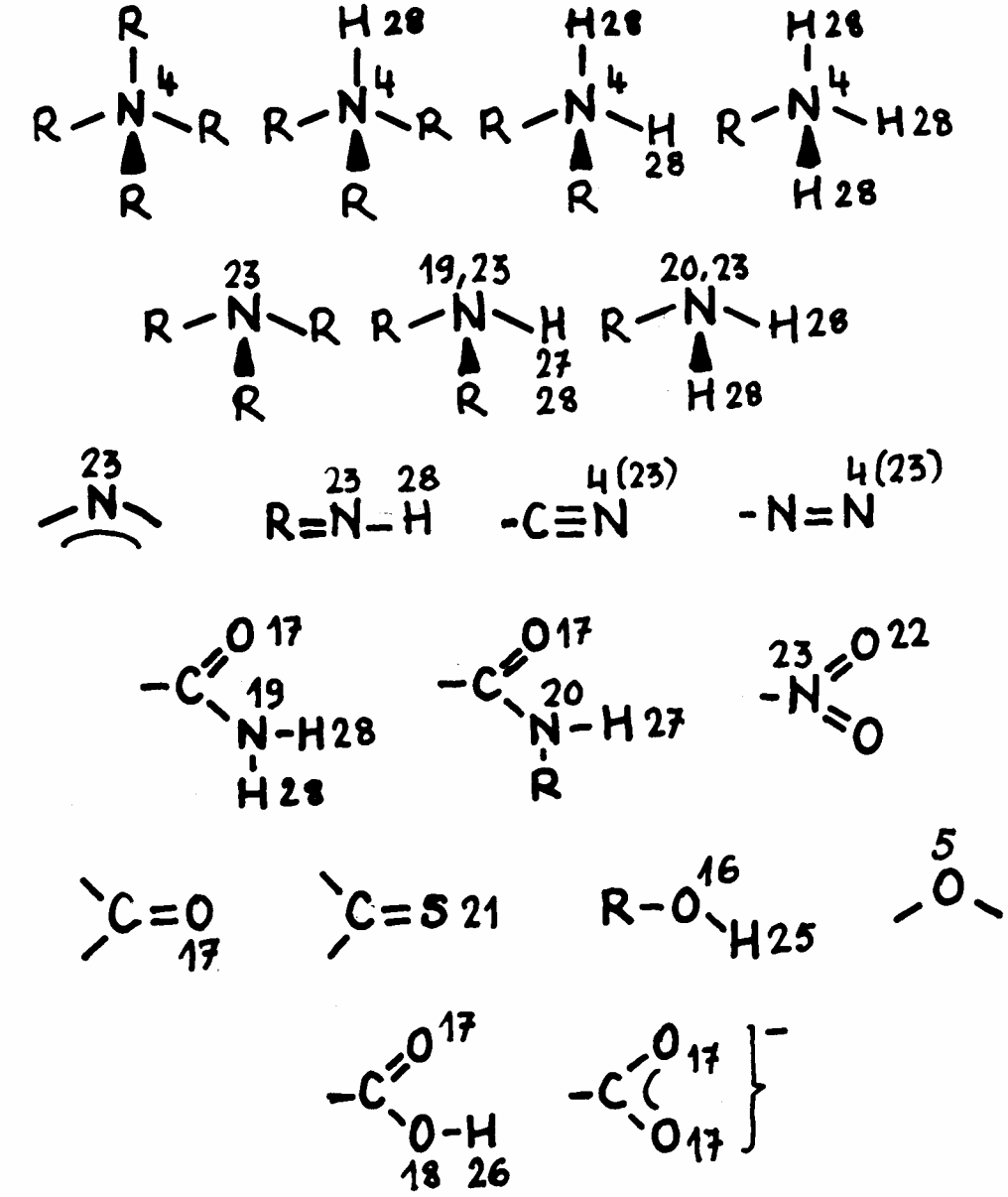
The Retcif procedure produces computer files that are standard input to the OPiX program package.[2] An intermediate file, with extension *oih* (OPiX- Implicit Hydrogen) file is generated with only the un-flagged crystals structures, unless an explicit override command is given, in which case the structural information is anyway written on file, ready for perusal and manual correction. A total override option is also available, in which atomic labels (*e.g*., hydrogen bond acceptor or not, etc.) are issued, but the original H-atom coordinates are written on the *oih* file without any attempt at hydrogen reassignment or normalization. This option is useful for neutron crystal structures. Deuterium is treated as hydrogen.

The *oih* file contains all independent coordinates for non-hydrogen atoms, always including entire molecules if Z'<1 (never the case in the present study). Hydrogen atom positions are represented in the form of sets of numerical codes that specify the connectivity and the desired bond lengths, bond angles, etc. These codes can be changed by the user by manually editing the files. A subsequent routine reads the *oih* files and generates the extension *oeh* (OPiX Explicit Hydrogen) files in which full H-atom *x, y, z* coordinates are stored. *oeh*-type files branch into all modules of the OPiX package for crystal structure analysis, atom-atom lattice energies, crystal structure generation and polymorph predictor, and for the PIXEL calculations modules (see below).

[1] A.G.Orpen, L.Brammer, F.H.Allen,O.Kennard,D.G.Watson,R.Taylor, in Structure Correlation, Ed. H.-B.Buergi and J.D.Dunitz, VCH, Weinheim 1994, Appendix A.
[2] A.Gavezzotti *OPiX, A computer program package for the calculation of intermolecular interactions and crystal energies*, University of Milano, 2003; see http://users.unimi.it/gavezzot. Distribution is free to academic users, subject to acknowledgement. Non a-academic users should contact the author at his e-mail address. See also A.Gavezzotti, *Z.Krist.* 2005, **220**, 499.

SCHEME

Automatic atom numbering in the Retcif procedure



Six-digit codes for the generation of hydrogen atom positions

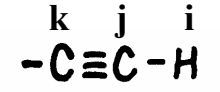
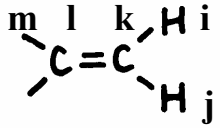
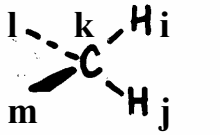
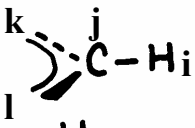
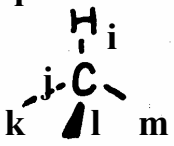
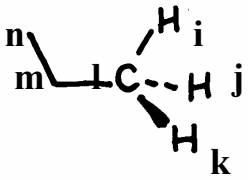
	i 0 0 j k 0	along CC direction
	i -1 0 k l m j -1 0 k l m	m-l-k-i torsion 0°, l-k-i angle 120° m-l-k-i torsion 180°, l-k-i angle 120°
	i j 0 k l m	on the C-C-C bisector plane HCH angle function of CCC angle
	i 0 0 k l m	on the C-C-C bisector
	i 0 j k l m	three identical C-C-H angles
	i -1 0 l m n j k	exptl. τ, C-C-H 109.47° id., τ+120° id., τ+240°

Table S1. Symmetry relationships found between two molecules in the asymmetric unit of Z'=2 crystals. Tolerance level 0.05 angstrom/atom

I inversion, 2 twofold axis, M mirror, S screw axis, G glide plane,
T pure translation

k,m: space group operations for the two molecules (sequence as in CSD)
R: distance between centers of mass
for S and G, T/s means screw or glide translation with average deviation
all distances in angstrom units

CSD refcode	space group	op.	k	m	R	asymmetry indices Is- and Is+ eq.3,4
#ACEJIC	'P c a 21'	I	1	1	4.27	0.026 0.027 0.025 1.950 3.776 5.304
#ACEJIC	'P c a 21'	S	1	3	6.03	T/s 2.759 0.025 dy,dz 0.025 0.026
#ACEQAB	'P 21/c'	G	1	3	7.26	T/s 5.791 0.037 dx 0.033
#ADUWOL	'P n a 21'	I	1	1	7.59	0.018 0.018 0.024 3.627 3.571 8.250
#ADUWOL	'P n a 21'	S	1	3	8.14	T/s 3.740 0.047 dy,dz 0.021 0.028
#AHELAA	'P 21/c'	G	1	2	19.27	T/s 18.822 0.017 dx 0.036
#AHGULP10	'P 21 21 21'	S	2	4	17.84	T/s 5.641 0.019 dy,dz 0.023 0.035
#AMBNAC01	'P 21/n'	G	1	4	11.25	T/s 6.884 0.015 dx 0.020
#AQEBAZ	'P 21'	S	1	2	14.46	T/s 10.392 0.024 dy,dz 0.038 0.031
#ASITOL	'P c a 21'	I	1	1	8.88	0.045 0.037 0.048 0.348 4.991 8.858
#ASITOL	'P c a 21'	S	1	4	25.18	T/s 12.687 0.048 dy,dz 0.020 0.021
#ATDZPY	'P 21/c'	S	1	3	7.75	T/s 4.366 0.013 dy,dz 0.030 0.017
#ATUWAN	'P n a 21'	G	1	3	6.91	T/s 3.195 0.037 dx 0.013
#AVEGOX	'P -1'	G	1	1	6.51	T/s 6.477 0.035 dx 0.027
#AVEGOX	'P -1'	S	1	2	19.62	T/s 5.584 0.028 dy,dz 0.027 0.041
#BAKYAO	'P 21/n'	T	2	4	33.19	0.041
#BANTAM	'P n a 21'	G	1	1	7.13	T/s 2.870 0.026 dx 0.030
#BANTAM	'P n a 21'	I	1	2	5.60	0.014 0.019 0.028 2.582 3.705 5.627
#BANTAM	'P n a 21'	S	1	3	11.22	T/s 8.378 0.021 dy,dz 0.024 0.029
#BEFFEX	'P 1'	I	1	1	5.39	0.046 0.036 0.045 4.494 4.749 5.271
#BEQCUW	'P -1'	G	1	1	8.43	T/s 3.086 0.025 dx 0.014
#BEQCUW	'P -1'	S	1	2	16.77	T/s 15.596 0.018 dy,dz 0.009 0.044
#BIRYIK10	'P 21/c'	G	1	4	13.76	T/s 13.351 0.011 dx 0.028
#BOSMAX	'P -1'	G	1	1	7.68	T/s 6.662 0.025 dx 0.037
#BOSMAX10	'P -1'	G	1	1	7.68	T/s 6.662 0.025 dx 0.037
#BUMJEY	'C c'	I	1	1	7.34	0.017 0.030 0.027 2.454 2.931 7.483
#BUMJEY	'C c'	S	1	3	12.19	T/s 6.626 0.043 dy,dz 0.030 0.029
#CAGGUN	'P c a 21'	S	2	3	16.41	T/s 5.725 0.035 dy,dz 0.016 0.029
#CALBIA	'P n a 21'	G	1	3	10.29	T/s 8.350 0.040 dx 0.024
#CALVIV	'I 2'	G	1	3	20.79	T/s 9.260 0.032 dx 0.022
#CARZEB	'P 21/c'	G	1	4	13.90	T/s 10.610 0.011 dx 0.004
#CASHOT02	'P 21/n'	G	1	1	5.03	T/s 5.002 0.011 dx 0.004
#CASHOT02	'P 21/n'	S	2	3	11.86	T/s 5.177 0.046 dy,dz 0.046 0.028
#CAWHAJ	'P 21'	S	1	1	6.46	T/s 3.213 0.043 dy,dz 0.038 0.030
#CAXPIB	'P c a 21'	G	2	4	10.69	T/s 8.574 0.020 dx 0.020
#CELPEO	'P 21'	S	2	1	13.39	T/s 9.378 0.038 dy,dz 0.030 0.035
#CEMLEL	'P 21/n'	T	1	3	9.47	0.040
#CEZTAC	'P 21/n'	G	2	1	8.81	T/s 6.845 0.044 dx 0.045
#CIHQIT	'P -1'	G	1	1	5.13	T/s 3.134 0.035 dx 0.020
#CITSON10	'P n a 21'	S	1	3	9.37	T/s 2.876 0.040 dy,dz 0.044 0.019
#CIVXOU10	'P 21/c'	T	1	3	17.26	0.031
#CIWBIT10	'P 21/c'	G	2	1	11.86	T/s 10.228 0.047 dx 0.013
#CIWPAZ10	'P -1'	G	1	2	14.21	T/s 13.813 0.050 dx 0.010
#CIZYOZ	'P -1'	G	1	1	6.13	T/s 2.640 0.043 dx 0.008
#CLPYMD	'P b c a'	G	1	2	11.03	T/s 3.933 0.019 dx 0.002
#CMBZAN20	'P 21/c'	G	1	4	13.08	T/s 11.274 0.037 dx 0.024
#COGDEH	'P 21/c'	G	1	3	7.84	T/s 4.744 0.031 dx 0.027
#COHDAE	'R 3'	2	1	1	6.12	2.579 0.032 0.031 0.020 3.778 6.497
#COHDAE	'R 3'	S	1	2	23.46	T/s 4.814 0.037 dy,dz 0.041 0.025
#COTRIM	'P 21/c'	S	1	1	4.74	T/s 2.658 0.037 dy,dz 0.027 0.018
#COTRIM	'P 21/c'	G	1	3	11.29	T/s 11.151 0.013 dx 0.025
#CUJQIH	'C 2'	2	1	1	7.50	0.042 3.386 0.039 1.389 0.030 7.493
#CUKCOA10	'P 21/c'	T	1	3	18.64	0.038
#CUTGAZ	'P 21'	G	1	2	13.11	T/s 12.883 0.034 dx 0.042
#DAHFOI	'P c a 21'	S	1	1	6.81	T/s 4.995 0.047 dy,dz 0.036 0.045
#DAHFOI	'P c a 21'	G	1	4	11.15	T/s 10.633 0.049 dx 0.015
#DAXBEJ	'P 21/a'	G	2	1	10.66	T/s 9.118 0.043 dx 0.033
#DCPYZO01	'I b a 2'	S	1	5	6.58	T/s 2.750 0.042 dy,dz 0.034 0.037
#DEDVEO	'P a'	S	2	1	9.61	T/s 8.745 0.036 dy,dz 0.011 0.010
#DEGNIN	'P 21 21 21'	G	1	2	13.56	T/s 11.370 0.037 dx 0.038
#DEMNUE	'P -1'	G	1	2	9.23	T/s 6.002 0.021 dx 0.022
#DIGXOG	'P 21 21 21'	G	1	1	5.95	T/s 5.358 0.040 dx 0.044
#DIGXOG	'P 21 21 21'	I	1	2	20.21	0.046 0.033 0.027 1.331 3.52520.163

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#DIHCOM   'P -1'         G   1  1  6.24 T/s  4.035  0.007 dx  0.008
#DIHCOM   'P -1'         S   1  2 13.64 T/s  9.372  0.013 dy,dz  0.004  0.010
#DIHCOM10 'P -1'         G   1  1  6.24 T/s  4.035  0.007 dx  0.008
#DIHCOM10 'P -1'         S   1  2 15.54 T/s  9.362  0.033 dy,dz  0.008  0.005
#DOJVED   'P b c a'      S   1  3 14.06 T/s  9.967  0.034 dy,dz  0.019  0.045
#DOJVED   'P b c a'      G   1  7 18.62 T/s 18.398  0.015 dx  0.022
#DOJVED10 'P b c a'      S   1  3 14.06 T/s  9.967  0.034 dy,dz  0.019  0.045
#DOJVED10 'P b c a'      G   1  7 18.62 T/s 18.398  0.015 dx  0.022
#DOLQEA   'P -1'         G   1  2 18.46 T/s 12.684  0.049 dx  0.048
#DONJEV   'P 21/c'       T   1  2 33.93 0.046
#DTYROS   'P 21'         I   1  1  6.30 0.000 0.000 0.001 2.055 2.934 6.238
#DTYROS   'P 21'         G   1  2  7.96 T/s  3.150  0.000 dx  0.001
#DUJMAW   'P -1'         G   1  1  6.16 T/s  4.395  0.033 dx  0.036
#EABBIS   'P -1'         S   1  1  6.84 T/s  4.899  0.035 dy,dz  0.022  0.036
#EBOCIH   'P 21/c'       G   1  1  5.59 T/s  5.528  0.028 dx  0.024
#EBOCIH   'P 21/c'       S   1  3  8.75 T/s  5.249  0.039 dy,dz  0.026  0.027
#EBONAK   'P -1'         2   1  1  4.11 0.009 3.148 0.009 2.428 0.009 4.111
#EBONAK   'P -1'         G   1  2  7.37 T/s  7.368  0.024 dx  0.006
#ECUNIA   'P 21 21 21'   G   1  2  9.77 T/s  9.327  0.024 dx  0.006
#EGURIH   'P 21 21 21'   G   1  2 12.37 T/s 11.313  0.043 dx  0.024
#EHOLIW   'P 32'         S   1  2 22.71 T/s 11.011  0.013 dy,dz  0.013  0.013
#EHOWIH02 'P 21/c'       S   1  1  4.82 T/s  2.847  0.029 dy,dz  0.010  0.035
#EHOWIH02 'P 21/c'       G   1  2  5.95 T/s  4.560  0.009 dx  0.017
#EKELIP   'P 21'         I   1  1  5.64 0.024 0.022 0.040 3.840 3.725 5.658
#EKENUD   'P 21/c'       G   1  1  7.00 T/s  2.473  0.049 dx  0.028
#EKUNIH   'P 21/n'       I   1  1  7.99 0.020 0.023 0.025 3.113 4.491 8.000
#EKUNIH   'P 21/n'       S   1  2 23.89 T/s  7.176  0.019 dy,dz  0.019  0.022
#EKUNIH   'P 21/n'       T   1  3 15.98 0.025
#EKUNIH   'P 21/n'       G   1  4 31.06 T/s 30.835  0.020 dx  0.013
#ELEXIC   'P 21/c'       S   1  2 12.12 T/s  3.255  0.034 dy,dz  0.018  0.034
#ELEXIC   'P 21/c'       G   2  3  7.80 T/s  6.397  0.027 dx  0.022
#ELOSIH   'P -1'         G   1  2  8.27 T/s  5.848  0.036 dx  0.035
#EPOPDO   'P 21/c'       G   1  2 11.52 T/s  8.132  0.040 dx  0.016
#EPOPDO   'P 21/c'       S   1  4 13.26 T/s  7.420  0.032 dy,dz  0.034  0.039
#EPOPDO01 'P 21/c'       G   1  2  7.89 T/s  3.887  0.015 dx  0.015
#EQOKUQ   'P c'          G   1  2 19.96 T/s  7.721  0.038 dx  0.037
#ETASIB   'P c a b'      G   1  3 10.79 T/s  3.217  0.029 dx  0.006
#ETASIB   'P c a b'      2   1  7  8.12 1.233 0.044 0.022 0.031 2.301 8.119
#ETASIB   'P c a b'      S   2  4 15.45 T/s 13.757  0.043 dy,dz  0.020  0.043
#ETICIT   'P c a 21'     S   1  1  8.41 T/s  2.290  0.046 dy,dz  0.017  0.030
#ETUWIZ   'P 21/n'       T   1  2 12.76 0.045
#EVIMOL   'P -1'         G   1  2 13.59 T/s 13.211  0.037 dx  0.021
#EYOTUH   'P -1'         G   1  1  9.00 T/s  8.671  0.009 dx  0.008
#EYOTUH   'P -1'         2   1  2 26.29 3.029 0.008 0.007 0.009 5.02126.295
#FACGIA   'P c a 21'     G   2  3 13.15 T/s 11.591  0.042 dx  0.032
#FAHJON   'P c a b'      T   3  8 23.94 0.038
#FAHJON10 'P c a b'      T   3  8 23.94 0.040
#FANRUI   'C 2 2 21'     S   1  1  7.45 T/s  3.778  0.036 dy,dz  0.015  0.014
#FAWREB   'P -1'         G   1  1  6.74 T/s  5.803  0.025 dx  0.025
#FAWREB   'P -1'         S   1  2 11.10 T/s  4.249  0.035 dy,dz  0.032  0.012
#FAZVOS   'P 21/c'       T   1  2 17.09 0.031
#FEDVOA   'P 21'         2   1  2  9.41 2.323 0.030 0.025 0.022 2.157 9.403
#FELYUQ   'P 21/n'       T   2  4 35.72 0.041
#FEMPUI   'P 21/n'       G   1  2  8.48 T/s  6.899  0.036 dx  0.044
#FEMPUI   'P 21/n'       T   1  3 10.46 0.044
#FETSON   'P 21/c'       G   2  1 13.09 T/s  9.483  0.039 dx  0.020
#FEXRIK   'P 21'         I   1  2  9.29 0.039 0.041 0.040 1.990 5.378 9.009
#FIDHIK   'P 21 21 21'   2   1  1  5.51 3.111 0.026 0.049 0.039 3.871 5.493
#FIDHIK   'P 21 21 21'   S   1  3  9.74 T/s  3.140  0.039 dy,dz  0.025  0.033
#FIKGOV   'P 21/a'       G   1  2 23.58 T/s 22.466  0.036 dx  0.036
#FIKGOV   'P 21/a'       S   2  3 17.12 T/s 10.001  0.043 dy,dz  0.037  0.039
#FISFES   'P n a 21'     S   3  1  5.65 T/s  2.982  0.031 dy,dz  0.036  0.043
#FOCFEJ   'P 21/c'       G   2  1 23.08 T/s 22.687  0.047 dx  0.046
#FOCHIP   'P a'          I   1  1  5.70 0.031 0.032 0.028 2.613 4.840 7.034
#FOKMIC   'P -1'         S   1  1  8.69 T/s  8.393  0.012 dy,dz  0.005  0.011
#FOKMIC   'P -1'         G   1  2 21.77 T/s  8.962  0.005 dx  0.006
#FOMDAN   'P -1'         G   1  1  5.67 T/s  3.228  0.041 dx  0.020
#FOWVUI   'P -1'         2   1  1  6.06 2.436 0.030 0.031 0.028 5.056 6.817
#FOWVUI   'P -1'         G   1  2 13.34 T/s 13.245  0.039 dx  0.038
#GAFLEF   'P 21 21 21'   G   1  3 12.85 T/s  6.361  0.032 dx  0.002
#GAFLEF   'P 21 21 21'   S   3  2  7.17 T/s  5.520  0.031 dy,dz  0.024  0.025
#GALDED   'P 21/c'       T   2  3 15.20 0.050
#GAMKOU   'P 21/c'       G   1  1  7.28 T/s  6.170  0.027 dx  0.033
#GAMKOU   'P 21/c'       S   1  3 10.58 T/s  8.481  0.036 dy,dz  0.013  0.010
#GAXJIY   'P n a 21'     G   2  3  9.16 T/s  7.127  0.012 dx  0.029
#GAXJIY   'P n a 21'     S   3  1 11.19 T/s  2.553  0.035 dy,dz  0.032  0.035
#GECCUM   'P 21/c'       T   1  3 13.89 0.016
#GIGSOE   'P 21 21 21'   G   1  4 17.45 T/s 17.119  0.046 dx  0.029
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#GIYBUL   'P -1'          G   1  1  7.73 T/s  5.659  0.049 dx  0.009
#GIZQAH   'P 21/c'        I   1  1  3.84 0.014 0.037 0.021 3.164 2.607 3.887
#GIZQAH   'P 21/c'        G   1  2 17.05 T/s 15.787  0.017 dx  0.010
#GIZQAH   'P 21/c'        T   1  3 12.98 0.012
#GIZQAH   'P 21/c'        S   1  4 18.84 T/s 15.456  0.018 dy,dz  0.009  0.029
#GIZQEL   'P -1'          G   1  2 19.21 T/s 18.859  0.048 dx  0.008
#GIZSOX   'P 21 21 21'    I   1  1  7.09 0.031 0.011 0.016 1.626 2.840 6.982
#GIZSOX   'P 21 21 21'    G   1  2 10.17 T/s  5.446  0.031 dx  0.025
#GUTFIK   'P 21/n'        G   1  1  7.07 T/s  3.487  0.033 dx  0.027
#GUTFIK   'P 21/n'        T   1  2 20.95 0.038
#GUTFIK   'P 21/n'        I   1  4 18.86 0.029 0.033 0.030 2.576 3.69818.849
#HACFUM   'P c a 21'      S   2  1 15.41 T/s  2.769  0.021 dy,dz  0.045  0.014
#HACGAT   'P b c 21'      G   1  3  9.51 T/s  7.993  0.046 dx  0.039
#HACNII   'P 21 21 21'    T   1  3 23.22 0.044
#HAGGIG   'P 21/n'        2   1  1  3.17 0.049 0.014 5.672 3.170 3.307 0.013
#HAKHOR   'P c a 21'      S   1  1  9.74 T/s  2.727  0.036 dy,dz  0.014  0.029
#HAKHOR   'P c a 21'      I   1  3 11.78 0.023 0.025 0.027 3.230 5.25611.765
#HAKHOR   'P c a 21'      G   3  2 10.83 T/s  5.840  0.046 dx  0.028
#HAPXEB   'P 21/c'        S   1  2 16.22 T/s  3.217  0.044 dy,dz  0.028  0.033
#HAPXEB   'P 21/c'        G   1  4 23.69 T/s 23.166  0.028 dx  0.025
#HATMEU   'P 21/c'        G   1  1  5.77 T/s  5.766  0.019 dx  0.018
#HATMEU   'P 21/c'        S   1  4 25.74 T/s 16.971  0.029 dy,dz  0.022  0.036
#HAYKUO01 'P 21/c'        S   1  2 22.76 T/s  8.897  0.039 dy,dz  0.030  0.030
#HAYKUO01 'P 21/c'        G   1  3 15.69 T/s 11.924  0.044 dx  0.019
#HELVUP   'P 21/c'        I   1  1  3.94 0.035 0.033 0.030 2.152 3.223 3.938
#HELVUP   'P 21/c'        T   1  3  8.46 0.025
#HELVUP   'P 21/c'        S   1  4 10.28 T/s  2.687  0.009 dy,dz  0.006  0.031
#HEVNUR   'P 21 21 21'    G   1  1  6.74 T/s  6.366  0.024 dx  0.008
#HIBLAF   'P 21/c'        I   1  2 28.37 0.048 0.024 0.039 2.200 5.21328.363
#HIBLAF   'P 21/c'        T   1  4 14.98 0.033
#HIBLAF   'P 21/c'        S   2  4 37.98 T/s  7.174  0.034 dy,dz  0.043  0.036
#HIMMAL   'P 21/n'        G   1  1  4.75 T/s  4.681  0.042 dx  0.027
#HIMMAL   'P 21/n'        S   1  3 12.43 T/s  2.583  0.024 dy,dz  0.040  0.022
#HIYJAA   'P n a 21'      G   1  2 11.51 T/s  8.166  0.024 dx  0.019
#HIYJAA   'P n a 21'      S   1  3 11.23 T/s  3.524  0.028 dy,dz  0.027  0.037
#HMPYTH   'P 21/c'        G   1  3  7.15 T/s  3.939  0.032 dx  0.027
#HNBOCL   'P 21/n'        T   1  3 11.48 0.048
#HOHRIF01 'P 21/c'        G   1  1  4.46 T/s  2.706  0.019 dx  0.035
#HOHRIF01 'P 21/c'        S   2  4 39.28 T/s  7.339  0.029 dy,dz  0.019  0.009
#HOQQIN   'P -1'          G   1  1  6.45 T/s  6.171  0.005 dx  0.004
#HOQQIN   'P -1'          S   1  2 10.26 T/s  8.831  0.017 dy,dz  0.008  0.014
#HOSNIM   'P n a 21'      I   1  1  5.80 0.039 0.025 0.032 1.198 4.058 5.783
#HOSNIM   'P n a 21'      G   1  2 17.59 T/s  6.890  0.024 dx  0.013
#HOSNIM   'P n a 21'      S   2  4 13.04 T/s  8.341  0.024 dy,dz  0.007  0.028
#HUXHOX   'P 21 21 21'    G   3  4 14.65 T/s 14.633  0.039 dx  0.040
#HUZCAG   'P -1'          G   1  2 11.35 T/s 11.180  0.033 dx  0.020
#IBEFAX   'P 21/n'        G   1  1  4.67 T/s  4.580  0.046 dx  0.030
#IBEFAX   'P 21/n'        S   1  3 13.80 T/s  3.892  0.037 dy,dz  0.041  0.026
#IBEFAX   'P 21/n'        T   1  4 15.97 0.035
#IBULUM   'P 21/n'        I   1  1  4.86 0.034 0.028 0.034 2.573 3.759 4.689
#IBULUM   'P 21/n'        T   1  3 12.26 0.039
#IBULUM   'P 21/n'        S   2  1 14.91 T/s  4.044  0.034 dy,dz  0.043  0.043
#ICOCAE   'P n a 21'      S   2  4 11.58 T/s  3.822  0.043 dy,dz  0.027  0.045
#ICOGIQ   'P -1'          G   1  1  5.57 T/s  5.566  0.050 dx  0.015
#ICULIB   'P 21/c'        T   2  4 15.26 0.049
#IDOTAX   'P n a 21'      G   1  1  5.78 T/s  4.451  0.035 dx  0.040
#IDOTAX   'P n a 21'      S   4  2 11.97 T/s  3.510  0.014 dy,dz  0.008  0.032
#IDUKEX   'P c a 21'      S   4  1 12.15 T/s  4.669  0.046 dy,dz  0.049  0.031
#IJUNUW   'P 21 21 21'    S   1  2 18.95 T/s  7.637  0.045 dy,dz  0.037  0.039
#IJUNUW   'P 21 21 21'    T   3  1 19.14 0.043
#IMIVOP   'P b c a'       G   1  5  8.37 T/s  7.755  0.037 dx  0.021
#IPAKEP   'P 21'          S   1  2 12.74 T/s  9.710  0.038 dy,dz  0.010  0.009
#IQAHIR   'P -1'          G   1  1  7.20 T/s  4.451  0.003 dx  0.004
#IQAHIR   'P -1'          S   1  2 13.01 T/s 11.336  0.005 dy,dz  0.006  0.003
#IREYIN   'P b c a'       T   1  7 10.81 0.024
#ISADIP   'P 21/n'        T   1  3  8.14 0.033
#IXENUU   'P 1'           S   1  1  8.51 T/s  5.005  0.033 dy,dz  0.010  0.016
#IYIDAV   'P -1'          G   1  1  6.47 T/s  5.933  0.027 dx  0.018
#IYIDAV   'P -1'          S   1  2 16.62 T/s  3.383  0.033 dy,dz  0.029  0.033
#IZAWUB   'P 2/c'         G   1  1  6.18 T/s  4.959  0.017 dx  0.005
#IZECUL   'P 21/n'        T   2  4 12.55 0.049
#IZEDUM   'P 21 21 21'    G   2  4 25.69 T/s 19.647  0.025 dx  0.028
#IZUFOY   'P -1'          S   1  1  9.37 T/s  2.164  0.050 dy,dz  0.030  0.030
#IZUMEV   'P 21 21 21'    T   4  2 17.30 0.039
#JAFKAD   'P -1'          S   1  1  7.14 T/s  3.739  0.008 dy,dz  0.008  0.007
#JAFKAD   'P -1'          G   1  2 11.99 T/s  9.397  0.002 dx  0.003
#JANYON   'P 21'          G   1  1  8.00 T/s  7.868  0.023 dx  0.047
#JARDEM   'P c a 21'      S   1  1  5.38 T/s  4.108  0.018 dy,dz  0.032  0.033
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#JARDEM   'P c a 21'     G   1  4  9.91 T/s  4.705  0.021 dx  0.016
#JATCOW   'P c c n'      T   1  5  9.55 0.034
#JATTOO   'P -1'         G   1  1  6.85 T/s  4.302  0.032 dx  0.024
#JAYPOP   'P 21/c'       S   1  1  6.82 T/s  2.570  0.021 dy,dz  0.008  0.020
#JAYPOP   'P 21/c'       G   1  4  7.60 T/s  4.578  0.034 dx  0.015
#JAZBIV   'P b c a'      G   1  2 10.91 T/s 10.900  0.027 dx  0.018
#JAZBIV   'P b c a'      S   3  8 31.59 T/s 23.659  0.047 dy,dz  0.038  0.033
#JEFTAQ   'P 21'         S   1  2 10.12 T/s  2.669  0.030 dy,dz  0.025  0.025
#JEHJAI   'P 21/n'       G   1  2 14.04 T/s  8.570  0.034 dx  0.027
#JELBAE   'P b n 21'     I   1  1  5.93 0.047 0.025 0.025 2.367 5.017 5.399
#JELBAE   'P b n 21'     S   1  4 17.63 T/s  3.125  0.028 dy,dz  0.032  0.032
#JELBAE   'P b n 21'     G   2  1  6.55 T/s  2.808  0.045 dx  0.043
#JIGREW   'P 21'         S   1  2  7.05 T/s  3.621  0.042 dy,dz  0.013  0.015
#JIMVUW01 'P 21/a'       G   1  3  9.73 T/s  9.485  0.050 dx  0.024
#JIRDOD   'P n a 21'     I   1  1  7.15 0.040 0.042 0.044 1.965 3.729 8.149
#JIRDOD   'P n a 21'     G   2  3 12.51 T/s 11.403  0.037 dx  0.049
#JIRDOD   'P n a 21'     S   3  4 15.32 T/s  3.893  0.037 dy,dz  0.034  0.049
#JISWAJ   'P -1'         S   1  1  6.91 T/s  4.660  0.029 dy,dz  0.023  0.023
#JISWAJ   'P -1'         G   1  2  9.93 T/s  8.847  0.023 dx  0.015
#JOXFIL   'P 21/n'       T   2  3 13.60 0.026
#JUKSAJ   'P 21/n'       S   2  1  8.51 T/s  2.858  0.038 dy,dz  0.050  0.029
#KAKJOV   'P 21/a'       G   1  1  5.35 T/s  4.220  0.037 dx  0.021
#KAKJOV   'P 21/a'       S   1  3 13.40 T/s  2.375  0.023 dy,dz  0.025  0.036
#KAKJOV01 'P 1 1 21/b'   G   1  1  5.37 T/s  4.236  0.032 dx  0.019
#KAKJOV01 'P 1 1 21/b'   S   1  3 13.44 T/s  2.392  0.030 dy,dz  0.023  0.030
#KAXBUH   'P 2/c'        T   2  4 26.51 0.033
#KESWOU   'P 21/n'       T   1  3  6.74 0.041
#KETZAK   'P 21/n'       2   1  1  6.69 2.767 0.014 0.031 0.023 4.467 6.666
#KETZAK   'P 21/n'       G   1  3 14.95 T/s 14.777  0.016 dx  0.027
#KOPGUR   'P -1'         G   1  2 15.33 T/s 11.856  0.036 dx  0.027
#KUFVAI   'P 21/c'       G   1  3 10.77 T/s  7.741  0.042 dx  0.028
#LAKHOU   'P 21/n'       G   1  4 21.81 T/s 21.057  0.013 dx  0.024
#LAKJOW   'P 21/n'       T   1  3 13.51 0.040
#LAKJOW   'P 21/n'       G   2  1 16.11 T/s 11.168  0.034 dx  0.020
#LASJIZ   'P n'          I   1  1  5.33 0.034 0.046 0.045 3.879 4.327 5.251
#LATWUZ   'P -1'         S   1  1  8.57 T/s  4.963  0.003 dy,dz  0.002  0.003
#LATWUZ   'P -1'         G   1  2 13.91 T/s 11.480  0.003 dx  0.004
#LEDZEZ   'P -1'         G   1  1  5.25 T/s  3.636  0.032 dx  0.015
#LEQJAS   'P n a 21'     G   1  2 10.28 T/s  7.183  0.025 dx  0.013
#LEQJAS   'P n a 21'     S   2  4 11.66 T/s  4.171  0.024 dy,dz  0.024  0.019
#LIKDUE   'P 21/n'       G   1  4  8.83 T/s  7.287  0.043 dx  0.037
#LIKDUE   'P 21/n'       S   2  1 21.16 T/s  8.532  0.045 dy,dz  0.035  0.044
#LUTPOF   'P -1'         G   1  1  8.41 T/s  4.013  0.004 dx  0.005
#LUTPOF   'P -1'         S   1  2 11.04 T/s  8.060  0.004 dy,dz  0.002  0.004
#MALJAL   'P 21/c'       G   1  4  9.20 T/s  8.118  0.014 dx  0.017
#MALJAL   'P 21/c'       S   2  1 14.34 T/s  7.442  0.018 dy,dz  0.014  0.009
#MALOAM   'P 21/c'       G   1  1  6.57 T/s  6.229  0.035 dx  0.039
#MATTUW   'P 21'         2   1  1  7.47 2.402 0.033 0.030 0.046 3.498 7.445
#MATZEN   'P -1'         G   1  2 13.07 T/s  4.987  0.049 dx  0.042
#MAWCUJ   'P -1'         G   1  1  6.58 T/s  6.331  0.022 dx  0.028
#MAWCUJ   'P -1'         S   1  2 12.59 T/s  6.350  0.040 dy,dz  0.018  0.026
#MERFIY   'P -1'         G   1  1  7.34 T/s  5.357  0.043 dx  0.027
#MIBWAV   'P 21'         S   1  1  9.12 T/s  5.149  0.019 dy,dz  0.023  0.018
#MIPKAX01 'P b c a'      G   1  2 26.66 T/s 21.425  0.022 dx  0.014
#MIPKAX01 'P b c a'      S   1  6 13.47 T/s  6.328  0.020 dy,dz  0.035  0.022
#MIYKEK   'C c'          S   2  4 10.44 T/s  3.899  0.046 dy,dz  0.037  0.035
#MODHIW   'P 21 21 21'   G   1  3 11.81 T/s 10.745  0.041 dx  0.018
#MUKGAA   'P 21/c'       G   1  1  5.85 T/s  2.747  0.004 dx  0.003
#MUKGAA   'P 21/c'       S   1  3  7.24 T/s  5.387  0.007 dy,dz  0.009  0.008
#MUKTIV   'P 21/c'       T   1  2 10.37 0.027
#MUKTIV   'P 21/c'       S   1  3 10.96 T/s  4.740  0.039 dy,dz  0.036  0.047
#NAHPIV   'P -1'         S   1  1  8.87 T/s  8.032  0.018 dy,dz  0.020  0.027
#NAJCUX   'P 1'          G   1  1  6.86 T/s  4.967  0.041 dx  0.041
#NAMWII   'P -1'         G   1  1  7.07 T/s  6.857  0.018 dx  0.013
#NAMWII   'P -1'         S   1  2 22.14 T/s  7.077  0.014 dy,dz  0.019  0.013
#NAMZOQ   'P 21/c'       G   1  1  7.58 T/s  4.118  0.039 dx  0.022
#NAMZOQ   'P 21/c'       S   2  3  7.75 T/s  3.630  0.034 dy,dz  0.030  0.026
#NAWPIL   'P 21/n'       G   1  3 10.20 T/s  8.857  0.047 dx  0.031
#NEFPUJ   'P 21/n'       S   1  1  7.94 T/s  3.658  0.027 dy,dz  0.029  0.048
#NEFPUJ   'P 21/n'       G   1  3 20.56 T/s 20.539  0.046 dx  0.020
#NEGJEO   'P -1'         G   1  1  7.10 T/s  3.728  0.035 dx  0.028
#NETJUR   'P 21/c'       G   1  1  6.08 T/s  5.155  0.031 dx  0.043
#NETROT   'P 21 21 21'   T   1  3 15.18 0.047
#NEWTAK   'P 21/n'       S   2  4 28.04 T/s 13.420  0.037 dy,dz  0.037  0.037
#NEZNEL   'P 21/n'       S   1  1  6.33 T/s  3.546  0.013 dy,dz  0.018  0.013
#NEZNEL   'P 21/n'       G   1  3  6.34 T/s  6.336  0.013 dx  0.001
#NIJGIW   'C 2'          G   1  1  8.54 T/s  4.129  0.016 dx  0.018
#NOYVEC   'P -1'         G   1  1  9.00 T/s  4.923  0.036 dx  0.032
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#NUBFIZ   'P c a 21'     S   1  3 19.15 T/s  3.084  0.034 dy,dz  0.042  0.050
#NUTWEE   'P 21 21 21'   G   1  3 14.76 T/s  6.306  0.024 dx  0.021
#OBIBAC   'P n a 21'     S   2  1 15.23 T/s 12.918  0.041 dy,dz  0.040  0.046
#OHOWUD   'P c a 21'     G   1  2 20.58 T/s 17.482  0.038 dx  0.023
#OHOWUD   'P c a 21'     S   2  4  9.25 T/s  3.636  0.034 dy,dz  0.040  0.026
#OJECUB   'P 41'         S   1  1  7.01 T/s  4.622  0.032 dy,dz  0.020  0.023
#OLIZUE   'P -1'         G   1  1  6.39 T/s  6.256  0.015 dx  0.011
#OMAZAD   'P 21/c'       G   1  2 23.21 T/s 22.078  0.027 dx  0.031
#OMAZAD   'P 21/c'       T   1  3  9.32 0.048
#OXTZOL   'P b c a'      2   1  1  3.77 0.013 1.502 0.011 1.806 0.016 3.620
#OXTZOL   'P b c a'      G   1  2 14.11 T/s 10.052  0.005 dx  0.007
#OXTZOL   'P b c a'      T   1  4 12.95 0.004
#OXTZOL   'P b c a'      S   1  7  4.95 T/s  3.583  0.003 dy,dz  0.007  0.013
#OXTZOL   'P b c a'      I   1  8  9.06 0.018 0.011 0.005 0.924 1.622 9.046
#OXTZOL01 'P b c a'      2   1  1  3.69 0.023 1.509 0.009 1.783 0.027 3.534
#OXTZOL01 'P b c a'      I   1  2  9.93 0.017 0.007 0.013 0.401 2.116 9.920
#OXTZOL01 'P b c a'      G   1  4 13.92 T/s 10.072  0.006 dx  0.007
#OXTZOL01 'P b c a'      T   1  6  8.45 0.014
#OXTZOL01 'P b c a'      S   1  7  4.89 T/s  3.582  0.002 dy,dz  0.005  0.015
#PABRIT   'P -1'         2   1  1  5.26 2.893 0.010 0.005 0.010 3.744 5.285
#PABRIT   'P -1'         G   1  2 11.31 T/s 11.218  0.005 dx  0.004
#PAMBOO   'P b c a'      T   3  2 18.91 0.041
#PAMBOO01 'P b c a'      T   4  3 18.91 0.043
#PAPCUF   'P b c a'      T   2  7 20.47 0.033
#PAPCUF   'P b c a'      G   3  4 13.34 T/s 11.772  0.044 dx  0.045
#PSULHZ11 'P 21/a'       G   1  3  8.18 T/s  7.649  0.036 dx  0.011
#PUVVUX01 'P c a 21'     G   1  2  6.74 T/s  3.902  0.009 dx  0.010
#PUVVUX01 'P c a 21'     S   1  3 11.74 T/s  2.547  0.016 dy,dz  0.020  0.014
#PYRFUR   'P c a 21'     S   1  2 10.66 T/s  4.383  0.047 dy,dz  0.036  0.043
#PYRZOL05 'P 21 c n'     G   2  1 12.27 T/s 11.496  0.016 dx  0.000
#QADVEW   'C c'          2   1  1  6.99 0.008 4.487 0.011 2.965 0.010 6.965
#QADVEW   'C c'          G   1  2  8.01 T/s  4.127  0.024 dx  0.024
#QADVEW   'C c'          S   1  3 12.63 T/s  4.843  0.036 dy,dz  0.043  0.021
#QALBOU   'P c a 21'     I   1  1  6.53 0.015 0.029 0.033 2.449 4.970 6.525
#QALBOU   'P c a 21'     G   1  2  8.29 T/s  6.048  0.030 dx  0.046
#QALBOU   'P c a 21'     S   1  4 13.71 T/s  3.895  0.026 dy,dz  0.040  0.019
#QALBUB   'P 1'          2   1  1  3.79 0.040 4.603 0.019 3.787 0.04014.637
#QAQDUH   'P -1'         G   1  1  6.94 T/s  5.827  0.003 dx  0.003
#QAQDUH   'P -1'         S   1  2  8.75 T/s  4.810  0.011 dy,dz  0.011  0.007
#QIGFOB   'C 2/c'        T   3  7 20.53 0.046
#QIMMAA01 'P 21/c'       G   1  1  6.93 T/s  6.722  0.048 dx  0.034
#QOBPOM   'P b c 21'     2   1  1  4.71 1.499 0.029 0.033 0.038 4.968 5.434
#QOHMOP   'P n a 21'     G   2  1 14.25 T/s  9.849  0.035 dx  0.043
#QUJKUB   'P 21/n'       G   1  1  5.97 T/s  3.851  0.038 dx  0.034
#QUKVUN01 'P -1'         G   1  2 12.80 T/s 12.256  0.006 dx  0.011
#RAJKOC   'P 21/c'       S   2  4 22.09 T/s 14.717  0.012 dy,dz  0.028  0.037
#RATGOJ   'P c a 21'     G   1  4  8.85 T/s  8.806  0.031 dx  0.013
#RAVSUC   'P -1'         G   1  1  5.64 T/s  4.587  0.042 dx  0.023
#REFYOR   'P 21/c'       G   2  1 12.24 T/s 10.282  0.049 dx  0.039
#REMYEN   'P 21'         S   1  1  6.87 T/s  3.384  0.023 dy,dz  0.019  0.018
#REVNUB   'P 21/c'       G   1  2 13.28 T/s 11.257  0.039 dx  0.049
#RIGCUF   'P 21'         S   1  1 10.13 T/s  7.414  0.031 dy,dz  0.012  0.024
#RIGVEI   'P 2/n'        G   1  3 17.00 T/s 10.012  0.014 dx  0.019
#RIKVEM   'P 21'         S   1  1  7.38 T/s  3.496  0.019 dy,dz  0.016  0.019
#RIMFUO   'P 21/a'       S   1  3 20.59 T/s  2.347  0.039 dy,dz  0.044  0.046
#RIQQUD   'P -1'         G   1  1 10.43 T/s  8.266  0.019 dx  0.023
#SAGNUJ   'P 21/c'       G   1  1  6.10 T/s  2.715  0.017 dx  0.025
#SANRIJ   'P 21/c'       S   2  3  6.59 T/s  2.642  0.038 dy,dz  0.036  0.024
#SARQOQ   'P 21'         I   1  1  5.45 0.045 0.030 0.034 2.431 4.979 5.303
#SARZEP   'P 21/c'       S   2  4 24.12 T/s 10.949  0.041 dy,dz  0.023  0.020
#SASXOA   'P 21/n'       T   1  2 13.08 0.024
#SEBLER   'P c a 21'     S   2  1  7.50 T/s  7.015  0.035 dy,dz  0.040  0.040
#SEBLER   'P c a 21'     G   4  1 10.63 T/s  3.987  0.049 dx  0.045
#SEDNAQ   'P 21/c'       2   1  1  8.01 0.447 0.013 0.018 0.043 3.490 7.988
#SEDNAQ   'P 21/c'       G   1  3 16.26 T/s 16.091  0.015 dx  0.036
#SEFGIU   'P 21/n'       I   1  1  5.12 0.024 0.027 0.026 2.731 4.261 4.802
#SEFGIU   'P 21/n'       T   1  3 14.03 0.022
#SEFGIU   'P 21/n'       G   2  1  8.78 T/s  7.085  0.037 dx  0.034
#SEFGIU   'P 21/n'       S   2  3 14.82 T/s  5.493  0.048 dy,dz  0.050  0.023
#SEGBIP   'P 21/n'       G   2  1 17.31 T/s 10.086  0.048 dx  0.034
#SEGBIP   'P 21/n'       S   2  3 22.53 T/s 11.749  0.035 dy,dz  0.030  0.045
#SEZNAM   'P -1'         G   1  2 11.82 T/s  9.233  0.030 dx  0.037
#SINSIR   'P 1 1 21/n'   I   1  1  8.52 0.017 0.015 0.022 2.502 3.819 8.515
#SINSIR   'P 1 1 21/n'   G   1  2  8.97 T/s  3.880  0.017 dx  0.015
#SINSIR   'P 1 1 21/n'   T   1  3 19.64 0.016
#SINSIR   'P 1 1 21/n'   S   1  4 25.73 T/s 23.386  0.022 dy,dz  0.018  0.030
#SIVYEB   'P -1'         G   1  2 15.73 T/s 14.233  0.046 dx  0.032
#SOYMOI   'P 21/c'       G   1  2 11.42 T/s 10.599  0.018 dx  0.009
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#SOYMOI   'P 21/c'       S   1  4 10.18 T/s  6.076  0.020 dy,dz  0.014  0.013
#SUCGUS   'P c a 21'     I   1  1  5.95 0.021 0.018 0.041 2.569 2.763 5.924
#SUCGUS   'P c a 21'     S   1  3 12.23 T/s  3.271  0.014 dy,dz  0.039  0.026
#SUCGUS   'P c a 21'     G   2  3  7.84 T/s  4.903  0.042 dx  0.033
#SUCHED   'P n a 21'     S   1  2 13.67 T/s  4.089  0.047 dy,dz  0.035  0.047
#SUCHED   'P n a 21'     I   1  4  8.13 0.039 0.050 0.050 2.248 3.072 8.108
#TAKREC01 'P -1'         S   1  1  7.04 T/s  2.635  0.020 dy,dz  0.017  0.014
#TAKREC01 'P -1'         G   1  2 12.67 T/s 12.579  0.017 dx  0.019
#TALWUY   'P 21/n'       G   1  3 17.06 T/s 14.714  0.047 dx  0.012
#TASDUN   'C c'          2   1  1  6.78 2.413 0.007 0.006 0.005 4.068 6.754
#TASDUN   'C c'          G   1  2 18.32 T/s  5.515  0.029 dx  0.028
#TASDUN   'C c'          S   1  3  8.34 T/s  3.158  0.022 dy,dz  0.006  0.007
#TCBENZ   'P 21/c'       G   1  2  6.57 T/s  3.170  0.013 dx  0.003
#TCBENZ02 'P 21/c'       G   1  2 14.68 T/s 12.291  0.016 dx  0.002
#TCBENZ02 'P 21/c'       S   1  4 11.41 T/s  6.742  0.007 dy,dz  0.006  0.021
#TEBBUX   'P 21/n'       S   1  1  7.34 T/s  3.060  0.011 dy,dz  0.024  0.014
#TEBBUX   'P 21/n'       G   1  3 11.39 T/s  6.152  0.015 dx  0.010
#TEMBES01 'P c a 21'     G   1  4  8.34 T/s  6.747  0.046 dx  0.046
#THNAPQ   'P 21/c'       G   1  1  7.03 T/s  6.522  0.038 dx  0.018
#THNAPQ   'P 21/c'       S   1  4 18.23 T/s  3.143  0.043 dy,dz  0.022  0.020
#TICYAF   'P 21/c'       G   1  1  7.33 T/s  7.221  0.025 dx  0.029
#TIHFIZ   'P -1'         G   1  2 11.29 T/s  6.512  0.035 dx  0.038
#TOMYEZ   'P c a 21'     I   1  1  6.27 0.045 0.040 0.043 1.977 3.580 6.126
#TONQUI01 'P -1'         2   1  1  4.56 0.029 4.011 0.022 2.556 0.025 5.112
#TUDROZ   'P b c a'      G   1  1  7.96 T/s  7.025  0.049 dx  0.044
#TUKWOL01 'P n a 21'     S   1  1  5.06 T/s  2.516  0.015 dy,dz  0.021  0.029
#TUKWOL01 'P n a 21'     G   2  3  9.08 T/s  8.006  0.038 dx  0.016
#TUKWOL01 'P n a 21'     I   4  2 11.13 0.036 0.046 0.038 1.247 2.30011.009
#UBEDUA   'P c'          I   1  1  6.57 0.027 0.022 0.027 2.297 4.390 7.528
#UBEDUA   'P c'          S   2  1  8.91 T/s  5.588  0.046 dy,dz  0.024  0.025
#UBEREY   'P 21'         G   1  1  5.09 T/s  2.247  0.050 dx  0.013
#UCECAG   'P 21/c'       T   1  2 10.35 0.043
#UCECAG   'P 21/c'       G   2  4 24.36 T/s  7.608  0.040 dx  0.004
#UCECAG01 'P 21/c'       T   1  2 12.96 0.040
#UCECAG01 'P 21/c'       G   2  4 26.72 T/s 13.508  0.024 dx  0.009
#UCIQIH   'P 21/c'       G   1  3  7.34 T/s  7.321  0.046 dx  0.006
#UDAQAS   'P 21/c'       G   1  1  7.51 T/s  4.512  0.023 dx  0.047
#UDAQAS   'P 21/c'       S   1  3 16.06 T/s 11.114  0.016 dy,dz  0.020  0.026
#UGUZEB   'P 21'         S   1  1  6.90 T/s  3.018  0.019 dy,dz  0.019  0.022
#UMUNEV   'P -1'         S   1  1  7.60 T/s  4.047  0.039 dy,dz  0.039  0.009
#UMUNEV   'P -1'         G   1  2 21.73 T/s 20.925  0.033 dx  0.038
#VAFMUK   'C c'          G   1  1  7.36 T/s  2.707  0.040 dx  0.037
#VAKROP   'P -1'         G   1  1  4.53 T/s  4.202  0.011 dx  0.024
#VALGOE   'P 21/n'       G   1  1  6.44 T/s  3.434  0.017 dx  0.016
#VALGOE   'P 21/n'       S   1  3  9.98 T/s  2.205  0.016 dy,dz  0.015  0.011
#VASLAD   'P n a 21'     I   1  1  5.06 0.027 0.019 0.028 2.479 3.896 4.963
#VASLAD   'P n a 21'     G   1  2  6.17 T/s  4.060  0.015 dx  0.019
#VASLAD   'P n a 21'     S   1  3  9.22 T/s  7.740  0.016 dy,dz  0.024  0.028
#VASLAD   'P n a 21'     2   1  4  9.52 0.033 3.831 0.033 2.086 0.020 9.521
#VASZUK   'P -1'         G   1  1  6.42 T/s  4.099  0.028 dx  0.041
#VATJUW   'P 21/c'       T   2  4 22.86 0.023
#VATKEH   'P 21/c'       S   1  2 19.20 T/s 14.313  0.036 dy,dz  0.041  0.048
#VATKEH   'P 21/c'       G   1  4 15.38 T/s 14.648  0.042 dx  0.036
#VAYJAG01 'P -1'         S   1  1  7.61 T/s  4.581  0.024 dy,dz  0.018  0.007
#VAYJAG01 'P -1'         G   1  2 10.89 T/s  6.295  0.034 dx  0.015
#VAYJAG02 'P -1'         G   1  1  6.07 T/s  6.075  0.028 dx  0.017
#VAYJAG02 'P -1'         S   1  2  9.90 T/s  2.288  0.047 dy,dz  0.036  0.023
#VEMSAH   'P 1'          2   1  1  5.03 3.679 0.012 0.008 0.009 4.976 4.491
#VIBKAS   'P 21/c'       S   1  1  5.54 T/s  2.977  0.037 dy,dz  0.045  0.041
#VIBKAS   'P 21/c'       G   1  3 14.99 T/s 12.999  0.016 dx  0.029
#VOVVAD   'P c a 21'     I   1  2 12.32 0.044 0.018 0.037 1.901 3.14112.340
#VOVVAD   'P c a 21'     S   2  3 26.87 T/s  3.086  0.045 dy,dz  0.041  0.032
#VUSMOL   'P -1'         G   1  1  6.13 T/s  5.015  0.046 dx  0.033
#VUSMOL   'P -1'         S   1  2 12.13 T/s  6.679  0.021 dy,dz  0.015  0.020
#VUSREG   'P -1'         2   1  1  7.75 0.016 4.046 0.013 3.219 0.014 7.834
#VUSREG   'P -1'         G   1  2 16.70 T/s 11.247  0.016 dx  0.010
#VUSREG10 'P -1'         2   1  1  7.75 0.016 4.046 0.013 3.219 0.014 7.834
#VUSREG10 'P -1'         G   1  2 16.70 T/s 11.247  0.016 dx  0.010
#WAHLEX   'P -1'         2   1  1  4.66 0.007 4.217 0.008 2.999 0.009 5.485
#WAHLEX   'P -1'         G   1  2 11.29 T/s 10.467  0.006 dx  0.004
#WARTEO   'P -1'         2   1  1  6.89 0.034 3.038 0.040 2.662 0.029 6.922
#WECXAE   'P 21/c'       2   1  1  7.92 0.242 0.045 0.033 0.028 2.605 7.921
#WECXAE   'P 21/c'       G   1  3  8.42 T/s  7.804  0.042 dx  0.018
#WECXAE   'P 21/c'       T   2  4 17.10 0.045
#WEDSED   'P 1'          2   1  1  6.17 0.031 5.266 0.023 3.459 0.019 6.183
#WEDSEE   'P n a 21'     I   1  1  6.02 0.027 0.014 0.018 1.270 4.863 5.838
#WEDSEE   'P n a 21'     G   1  2  8.33 T/s  5.999  0.029 dx  0.011
#WEDSEE   'P n a 21'     S   1  4 13.79 T/s 12.317  0.017 dy,dz  0.020  0.012
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#WETSAP   'P 21'         S   1  1  6.51 T/s  4.528  0.026 dy,dz  0.017  0.033
#WINPUE   'P n'          G   1  1  6.67 T/s  3.972  0.032 dx  0.029
#WINPUE   'P n'          S   1  2  9.50 T/s  7.623  0.023 dy,dz  0.013  0.043
#WIPJEK   'P 21/c'       T   2  4 27.87 0.036
#WIQFOR   'P n a 21'     S   2  1 16.75 T/s 11.169  0.033 dy,dz  0.046  0.045
#WITLOA   'P b c a'      S   1  6 12.03 T/s  6.374  0.038 dy,dz  0.041  0.044
#WOCGEA   'P -1'         G   1  1  4.71 T/s  2.889  0.024 dx  0.013
#WOGQOY   'P 21/n'       G   1  1  5.34 T/s  3.975  0.037 dx  0.031
#WOMXIF   'P 21/c'       G   1  1  6.87 T/s  4.713  0.005 dx  0.005
#WOMXIF   'P 21/c'       S   1  2  9.61 T/s  6.788  0.009 dy,dz  0.011  0.007
#WUNKAR   'P -1'         G   1  1  7.02 T/s  4.356  0.020 dx  0.023
#WUVTUC   'P 21 21 21'   S   1  4 15.21 T/s 10.272  0.047 dy,dz  0.035  0.044
#XADTUR   'P c a 21'     S   1  1  6.75 T/s  2.343  0.044 dy,dz  0.025  0.032
#XADTUR   'P c a 21'     I   1  3  6.90 0.037 0.022 0.039 1.321 2.931 6.782
#XAKZIS   'P 21/c'       G   1  1  4.80 T/s  3.483  0.015 dx  0.050
#XAQDID   'P c a 21'     G   1  1  5.17 T/s  4.027  0.043 dx  0.014
#XAQDID   'P c a 21'     S   1  3 10.46 T/s  6.947  0.016 dy,dz  0.021  0.018
#XASHII   'P -1'         G   1  1  5.42 T/s  5.117  0.011 dx  0.003
#XASHII   'P -1'         S   1  2 13.66 T/s  3.304  0.015 dy,dz  0.014  0.015
#XEFLUQ   'P 21'         S   1  2 20.77 T/s  5.092  0.040 dy,dz  0.017  0.022
#XEFNAX   'P 1'          G   1  1  6.10 T/s  3.334  0.017 dx  0.027
#XEZGEO   'P -1'         S   1  1  6.54 T/s  3.139  0.023 dy,dz  0.016  0.003
#XEZGEO   'P -1'         G   1  2 12.09 T/s  8.785  0.009 dx  0.004
#XILDUR   'P 21/n'       T   2  3  7.05 0.042
#XOZFIB   'P 21 21 21'   I   1  1  5.14 0.040 0.031 0.036 2.376 3.984 5.016
#XOZFIB   'P 21 21 21'   G   1  3  9.03 T/s  8.983  0.034 dx  0.022
#YACGAK   'C c'          2   1  1  4.43 2.015 0.007 0.006 0.007 3.365 3.980
#YACGAK   'C c'          S   1  2  9.91 T/s  2.634  0.009 dy,dz  0.006  0.005
#YACGAK   'C c'          G   1  3  5.48 T/s  3.990  0.007 dx  0.005
#YAHYIP   'P 1'          G   1  1  9.39 T/s  9.187  0.008 dx  0.006
#YAJQIK   'P 21/c'       S   1  2 20.81 T/s  9.413  0.040 dy,dz  0.038  0.036
#YAJQIK   'P 21/c'       G   1  4 25.41 T/s 24.350  0.037 dx  0.024
#YAKCIW   'P 21/c'       S   1  1  7.44 T/s  2.804  0.031 dy,dz  0.029  0.033
#YAKCIW   'P 21/c'       G   2  3 17.37 T/s 15.989  0.028 dx  0.032
#YALBIX   'P -1'         G   1  1  6.61 T/s  4.157  0.035 dx  0.029
#YALBIX   'P -1'         S   1  2 11.21 T/s  2.636  0.027 dy,dz  0.032  0.037
#YAPBAT   'P 1'          I   1  1  6.83 0.042 0.038 0.035 2.651 3.185 9.660
#YAVCON   'P 21/a'       S   1  4 13.10 T/s  9.181  0.019 dy,dz  0.022  0.024
#YAVCON   'P 21/a'       2   2  4 23.29 2.060 0.036 0.029 0.044 2.35923.286
#YAVJOU   'P 21/a'       G   1  4 18.05 T/s 17.415  0.034 dx  0.036
#YAXYOL   'P -1'         G   1  1  7.32 T/s  5.298  0.041 dx  0.033
#YAXYOL   'P -1'         S   1  2 15.76 T/s  6.214  0.029 dy,dz  0.037  0.047
#YEBQAX   'P 21/c'       G   1  4 12.12 T/s 11.475  0.033 dx  0.020
#YEBQAX   'P 21/c'       S   2  1  7.90 T/s  4.031  0.034 dy,dz  0.043  0.038
#YEFHOH   'P c a 21'     S   1  3 12.89 T/s  2.558  0.031 dy,dz  0.014  0.022
#YEGHIB   'P 21/c'       G   1  2 17.83 T/s 17.383  0.047 dx  0.049
#YEJNAC   'P 21/n'       T   1  2 11.72 0.045
#YEKFOJ   'P -1'         G   1  1  8.68 T/s  5.245  0.028 dx  0.025
#YEPFEE   'P -1'         G   1  1  3.71 T/s  3.437  0.023 dx  0.008
#YEPYEX   'P 21 21 21'   T   4  1 14.56 0.030
#YICFAR   'P 21/a'       G   1  3 13.78 T/s 13.442  0.028 dx  0.002
#YITNUK   'P -1'         2   1  1  7.05 2.083 0.006 0.010 0.006 4.084 7.904
#YITNUK   'P -1'         G   1  2 14.38 T/s 13.901  0.007 dx  0.006
#YOSHOD10 'P 1 1 21/a'   S   1  2 16.51 T/s 13.829  0.010 dy,dz  0.008  0.036
#YUHHUE   'P 2 21 21'    G   4  1 14.35 T/s 12.322  0.039 dx  0.041
#YUHHUE01 'P 21 21 2'    G   1  4 12.55 T/s 12.331  0.037 dx  0.045
#YUXLUY   'P 21/n'       G   2  3 19.54 T/s 18.470  0.032 dx  0.023
#ZAKNEE   'P 21'         S   1  1  8.03 T/s  4.170  0.029 dy,dz  0.037  0.031
#ZAYGUB   'C 2/c'        G   1  3 19.77 T/s  8.656  0.049 dx  0.026
#ZEGCUJ   'P 21/c'       G   1  4 11.14 T/s 11.144  0.040 dx  0.011
#ZIKWAR   'P 21 21 21'   S   3  1  8.89 T/s  2.148  0.049 dy,dz  0.048  0.039
#ZIZFET   'P 21/n'       G   1  1  4.84 T/s  3.214  0.020 dx  0.036
#ZIZFET   'P 21/n'       S   2  4 20.28 T/s  7.426  0.040 dy,dz  0.025  0.012
#ZOGQAN04 'P n a 21'     I   1  1 11.40 0.035 0.015 0.022 1.683 3.84611.402
#ZOGQAN04 'P n a 21'     S   1  3 11.27 T/s  3.463  0.022 dy,dz  0.024  0.021
#ZOXYIU   'P 21'         G   1  1  5.91 T/s  3.741  0.033 dx  0.032
#ZOXYIU   'P 21'         I   1  2 15.21 0.028 0.029 0.030 3.185 2.58315.212
#ZOYLUU   'P 21/n'       G   1  4  9.62 T/s  7.610  0.043 dx  0.018
#ZUHXEF   'P 21/c'       G   2  3 11.85 T/s  8.774  0.044 dx  0.037
#ZULDOZ   'P n a 21'     G   1  2  6.34 T/s  6.343  0.026 dx  0.007
#ZUMLEY   'P 21/n'       G   1  3 12.94 T/s  6.731  0.045 dx  0.015
#ZUMMAV   'P c'          G   1  1  8.59 T/s  3.108  0.033 dx  0.026
#ZZZMUC09 'P c a 21'     S   2  1  8.43 T/s  3.713  0.030 dy,dz  0.039  0.048
#ZZZMUC09 'P c a 21'     G   2  4  7.05 T/s  4.795  0.027 dx  0.044
#ZZZPRC02 'P 21/c'       G   2  4 26.10 T/s 18.648  0.032 dx  0.028
total, tot.sym, M, 2, I, T, S, G  1850   354    0   31   42   53  164  238
```

Table S2. A list of crystal structures where extra symmetry between molecules in the asymmetric unit has been detected at the tolerance level of 0.02 Å/atom

assigned space group	extra symmetry and possible supergroup[a]	CSD refcodes
$P\bar{1}$	S, G $P2_1/c$	DIHCOM,FOKMIC,HOQQIN, IQAHIR, JAFKAD,LATWUZ,LUTPOF,NAMWII, QAQDUH,XASHII
$P\bar{1}$	2, G $P2/c$	EYOTUH,PABRIT,VUSREG,WAXLEX
$P2_1/c$	S, G $Pbca$	CARZEB,CASHOT02,EHOWIH02,EPOPDO01, GAMKOU,GIZQAH,HATMEU,JAYPOP, MALJAL,MUKGAA,NEZNEL,SINSIR, SOYMOI,TCBENZ,TEBBUX,TICYAF, YICFAR,WOMFIX,VALGOE
$P2_1/c$	T, $C2/c$	EKUNIH,GECCUM,GIZQAH,IBEFAX,SINSIR
$P2_1$	I, $P2_1/c$	DTYROS
	S, G $P2_12_12_1$	JANYON,RIKVEM,WETSAP

T translation, I inversion, S screw axis, G glide plane.

Table S3 Different symmetries and aggregation modes for substituted acetic acid crystals.

R group in R-COOH	aggregation mode	CSD refcodes
CH_3	catemer Z'=1	ACETAC
CH_2F,CCl_3,CF_3 CH_2Br,CHBrF, $CClF_2$,CH_2NO_2, CBr_3,$CH_2Cl(\alpha)$, CH_3CH_2	cyclic Z'=1	FACETC, TCACAD02, TFACET, BRMACA, BARBAX, NAGWAT, NTRACD, WADFIR, CLACET02, PRONAC
$CFCl_2$ $CH_2Cl(\beta)$	catemer Z'=2	NAGVUM, CLACET01
$C(CH_2Cl)_3$	cyclic Z'=2	CAYKUI

Fig. S1. Shows the set-up for the detection of translational symmetry: all vectors joining equivalent atoms in the two molecules (red lines) must be identical in length and direction; the vector joining the centers of mass (blue line) is taken as reference. τ_1 and τ_2 show a possible source of minor conformational difference.

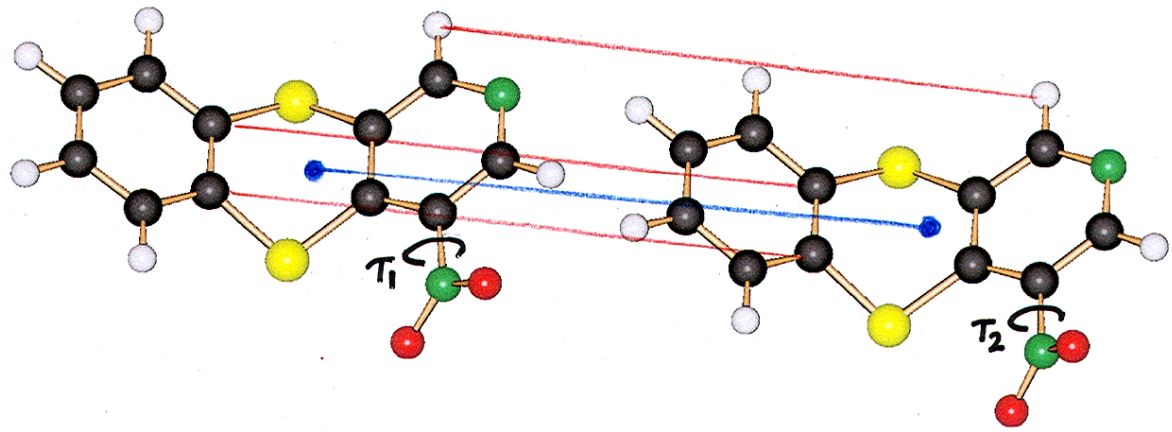

Fig. S2. Shows the set-up for the detection of centrosymmetry: all vectors joining equivalent atoms in the two molecules (red lines) must pass through the center of mass of the dimer. τ_1 and τ_2 show a possible source of minor conformational difference.

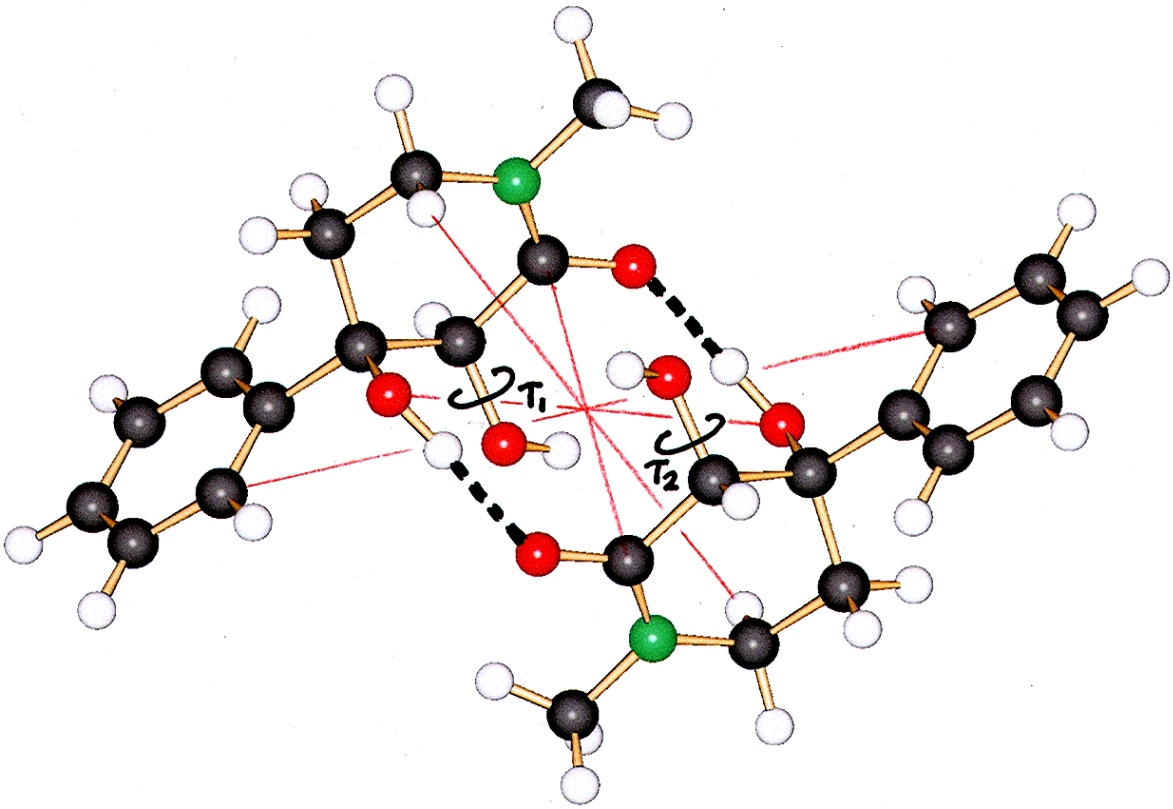

Fig. S3. Shows the set-up for the detection of mirror or glide symmetry: the midpoints of all vectors joining equivalent atoms in the two molecules (red lines) must lie on the mirror (glide) plane (black polygon). The blue line shows the perpendicular to the plane (*x*-axis). For mirror symmetry, there is no global translation in the *yz* plane; for glide symmetry there is a global translation in the *yz* plane (the glide translation).

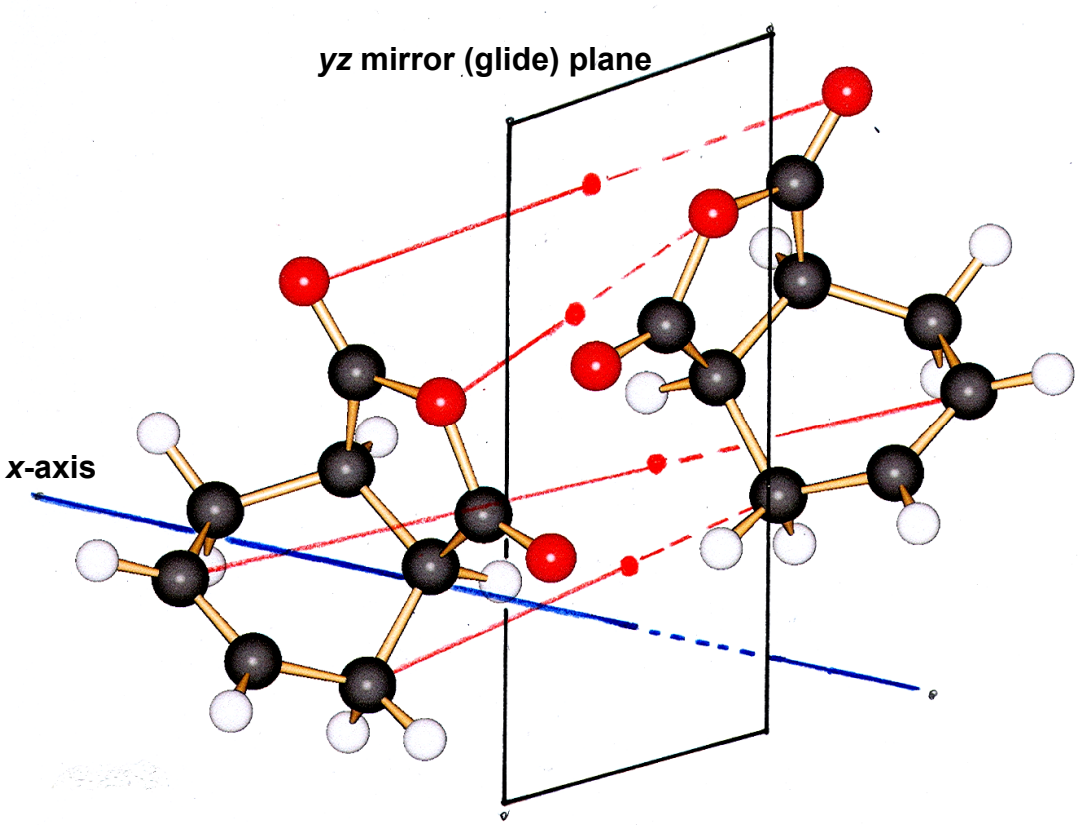

Fig. S4. Shows the set-up for the detection of twofold or screw symmetry: the midpoints of all vectors joining equivalent atoms in the two molecules (red lines) must lie on the twofold (screw) axis (*x*-axis). For twofold symmetry, there is no global translation along the *x*-axis; for screw symmetry there is a global translation along the *x*-axis (the screw translation).