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Patterson-Oriented Automatic Structure Determination. Utilizing Patterson Peaks

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Abstract

Methods for automatic structure determination [Pavelčík (1988). *Acta Cryst.* A**44**, 724-729] have been extended by routines utilizing Patterson peaks and a new version of the *XFPS* computer program [Pavelčík, Rizzoli & Andreetti (1990). Univ. of Parma, Italy, and Komensky Univ., Bratislava, Czechoslovakia] has been developed. The results of test calculations were compared with those of *SHELXS*86 [Sheldrick (1986). Univ. of Göttingen, Germany]. About 80% of heavy-atom structures can be solved automatically.

Introduction

The *XFPS* computer program (Pavelčík, 1986) was developed to perform semiautomatic calculations of a sharpened Patterson function, an atomic minimum superposition, a symmetry minimum function and various types of Fourier syntheses. The program is able, in an ideal case, to solve a heavy-atom structure in a single computer job with a sequence of instructions supplied by the user. Recently, the program has been extended by new routines such as a symmetry sum function (Pavelčík, 1989*a*), second- and third-order symmetry minimum functions, cross-vector and full-symmetry minimum translational functions (Pavelčík, 1988, 1991) and by an expert routine controlling a fully automated structure determination. The serious drawbacks of the automated procedure were: an oversimplified algorithm for solving structures in space groups *P*1, *Pc*, *Pm*, *Cc* and *Cm*; some errors in a procedure for generating the symmetry of the multiple implication function (Zimmermann, 1988; Pavelčík, 1990); and a restriction to use only on mainframe computers.

In this paper some new approaches to the Patterson deconvolution are described. These new methods are based on simultaneous use of the peaks of the symmetry minimum function, the Patterson peaks and the stored Patterson function. The *XFPS* program has been reorganized and developed as a program for fully automatic structure determination of heavy-atom compounds for both mainframe and personal computers (Pavelčík & Sivý, 1989; Pavelčík, Rizzoli & Andreetti, 1990; Pavelčík, Sivý, Rizzoli & Andreetti, 1992).

Procedures

Improvement of basic procedures

The Patterson synthesis, symmetry minimum function (SMF), atomic minimum superposition and Fourier syntheses are calculated as described previously (Pavelčík, 1986). The sharpening function has been changed to a function of two parameters,

$$|F_0|_S^2 = |F_0|^2(1+as^2)\exp(bs^2)\Big/\Big(\sum_i f_i\Big), \qquad (1)$$

where $s = (\sin \Theta)/\lambda$, f_i is the scattering curve and a and b are sharpening parameters. The Patterson peaks are output with heights, H', scaled by

$$H' = H\sum_i Z_i^2/P(000). \qquad (2)$$

H and $P(000)$ are the peak height and the origin of the Patterson function on an arbitrary scale, respectively; Z_i are atomic numbers. The output peak heights are in this way related to the product of their atomic numbers. The lengths of the Patterson vectors are also given as output.

For the Patterson or Fourier synthesis, a grid, given by the interlayer separation, res, is calculated by

$$\text{res} = (d_{\min}/3)(N_{\text{unique}}/N_{\text{obs}})^{1/3}, \qquad (3)$$

which reflects both the maximum diffraction angle and the quality of an experiment.

Symmetry

User-oriented programming requires program input to be as simple as possible. This led us to develop a computer routine that for generating equivalent positions requires only a space-group number as given in *International Tables for Crystallography* (1989).

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Various cell axes and origin selections (*International Tables for Crystallography*, 1989) are further restricted: The unique axis in a monoclinic cell is **b**; the centre of symmetry is at the cell origin; a rhombohedral cell is in the hexagonal setting only. The group elements are obtained with the help of the space-group generators (Wondratschek, 1989) but the number of generators is kept to an absolute minimum of three (excluding the lattice translations and the centre of symmetry). The first generator is the 1, 2, 4^+, $\bar{4}^+$, 3^+, 6^+ or $\bar{6}^+$ axis parallel to the z direction and the translation vector is given as $(t_x/4, t_y/4, t_z/4)$ or $(0, 0, t_z/6)$ for hexagonal axes. The second generator is $(s_1x+t_1/4, s_2y+t_2/4, s_3z+t_3/4)$ or $(s_1y, s_2x, s_3z+t_3/6)$ for trigonal or hexagonal systems, related to a direction different from z. The s_i are $+1$ or -1. The third generator is a threefold body-diagonal rotation axis indicating a cubic group.

The symmetry of any space group can be packed into 32 bits. The following items are stored for each space group: code for the lattice type P, I, R, F, A, B, C (3 bits), code for the centre of symmetry (1 bit), code for the rotation matrix of the first generator (3 bits), t_x, t_y, t_z (7 bits), s_1, s_2, s_3, t_1, t_2, t_3 (10 bits) and code for the third generator (1 bit).

The subroutine of the crystal symmetry generator (in Fortran77) represents only 70 lines, of which 29 lines are data definition containing 230 INTEGER*4 words of packed symmetry information (the routine has also been developed as an independent program, *XSPGR*, available on request, suitable for other crystallographic programs as well as for the teaching of space groups).

Preselection routines

The SMF gives in some cases correct peaks buried among background peaks. This is particularly true for structures with intermediate heavy atoms such as Cl, P or S in organic compounds. Also, quasispecial coordinates (*e.g.* 0.5, 0.25) often lead to ambiguous interpretation of the Harker vectors and to spurious peaks in the SMF. In such cases preselection functions are useful to suppress the false peaks of the SMF. The preselection routines are based on the second- or third-order symmetry minimum function, denoted the SOSMF (Pavelčík, 1988). Because full three-dimensional calculation of such a function would be computationally demanding, two fast approximations to this function were developed. The equivalent origin approximation has already been described (Pavelčík, 1988).

Another approximation based on the Patterson peaks is presented here. The SOSMF can be reformulated as a figure of merit for peaks $\mathbf{r}_i$ of the SMF (potential atoms) as

$$H(\mathbf{r}_i)=\int_V \min_s P[\mathbf{r}_i-(R_s\mathbf{x}+\mathbf{t}_s)]\,\mathrm{d}\mathbf{x}, \qquad (4)$$

where R_s are rotational and $\mathbf{t}_s$ translational parts of the symmetry operators, respectively. From another point of view this function can be regarded as a cumulative function (Ramachandran & Srinivasan, 1970) of the atomic minimum superposition. The Patterson peak approximation is given by

$$H(\mathbf{r}_i)=\sum_k \min_s P[\mathbf{r}_i-(R_s\mathbf{x}_{ki}+\mathbf{t}_s)], \qquad (5)$$

where $\mathbf{x}_{ki}=\mathbf{r}_i+\mathbf{u}_k$ and $\mathbf{u}_k$ are Patterson peaks. The summation is over all Patterson peaks higher than a product of atomic numbers of the lightest heavy atom. If $\mathbf{u}_k$ is a cross vector belonging to atom $\mathbf{r}_i$ and another atom in the structure, then an important contribution is expected. A weighted modification of this function can be written as

$$\begin{aligned}H(\mathbf{r}_i)=\sum_k &\Big[\min_s P(\mathbf{r}_i-R_s\mathbf{r}_i-\mathbf{t}_s)\Big]\\ &\times\Big[\min_s P(\mathbf{x}_{ki}-R_s\mathbf{x}_{ki}-\mathbf{t}_s)\Big]\\ &\times\Big[\min_s P(\mathbf{r}_i-R_s\mathbf{x}_{ki}-\mathbf{t}_s)\Big]. \qquad (6)\end{aligned}$$

The first two terms represent self-vectors. All the required Patterson values can be easily obtained from a stored Patterson function by a look-up table. In contrast to the equivalent-origin approximation, this approach is applicable to all space groups and is particularly useful for the Pc, Pm, Cc, $R3$, $R3c$ and $R3m$ space groups.

Another preselection routine is based on R-factor calculation using E values. The $R_i(E)$ factors for individual peaks are calculated by Pavelčík (1988). If the number of input peaks is twice (or more times) the number of heavy atoms then it is possible to delete some false peaks by selecting only peaks for which

$$R_i(E)\le 0.99\langle R(E)\rangle. \qquad (7)$$

Generators of atomic fragments

Once (preselected) peaks of the SMF are known, the next step in the Patterson deconvolution is to build tentative heavy-atom fragments. This is usually a multisolution process. To build a fragment, one peak (the pivot peak) of the SMF is fixed. The fragment can be built either by equivalent origin shifts applied to the peaks of the SMF (Pavelčík, 1988) or by a new fragment generator utilizing Patterson peaks, which is described here. This method is suitable for low-symmetry space groups with an infinite number of equivalent origins in one or two dimensions. For a given pivot peak $\mathbf{r}_i$ of the SMF, the tentative atomic positions are generated by

$$\mathbf{r}_j=\mathbf{r}_i+R_s\mathbf{u}_k, \qquad (8)$$

where $\mathbf{u}_k$ are Patterson peaks in the asymmetric part of the Patterson function. The atomic position is accepted only if equations

$$P(\mathbf{r}_j - R_s\mathbf{r}_j - \mathbf{t}_s) > P_{\text{lim}} \tag{9}$$

and

$$P(\mathbf{r}_j - R_s\mathbf{r}_i - \mathbf{t}_s) > P_{\text{lim}} \tag{10}$$

are satisfied for all symmetry operators. This means that all self- and cross-vectors must be greater in magnitude than a preselected value.

In the space group $P1$ the SMF is reduced to a single point and no symmetry can be used for Patterson deconvolution. The algorithm was modified accordingly. In $P1$ the heaviest atom is fixed at the origin. A pivot atom is fixed by one Patterson peak, $\mathbf{u}_i$ (all high peaks are successively used as pivot peaks in the multisolution process). All other Patterson peaks, $\mathbf{u}_k$, are tried as possible atomic positions. The atom position is accepted only if

$$P(\mathbf{u}_k) > P_{\text{lim}} \tag{11}$$

and

$$P(\mathbf{u}_i - \mathbf{u}_k) > P_{\text{lim}}. \tag{12}$$

The fragment generated by any of the generators forms the input into the cross-vector function. The advantage of using combined SMF peaks, Patterson peaks and a stored Patterson function, in comparison to methods using Patterson peaks only, is that the appearance of only one symmetry-related cross-vector as a Patterson peak is sufficient to generate a tentative atomic position (other symmetry-related cross-vectors may be in the overlapped regions).

Cross-vector functions

In fragment generators, only cross-vectors between the pivot atom and potential new atoms are checked. In the cross-vector function all cross-vectors among all atoms of the fragment are checked and atoms having no or only weak cross-vectors are removed from the atom list. One cross-vector function has already been described (Pavelčík, 1988). This procedure has recently been slightly modified in such a way that atoms generated from the same peak of the SMF (in the fragment generated by equivalent origin shifts) may be treated optionally as independent atoms. This may help to solve structures with atoms in special or quasispecial positions (pseudosymmetry, translational ambiguity).

Another cross-vector function, called the weighted cross-vector function, is described here. This alternative was developed for structures in which the background level in the normalized Patterson function approaches the product of atomic numbers of heavy atoms (*e.g.* organic molecules with Cl, P, S as heavy atoms). For atoms in the fragment, a table of all symmetry-minimum interactions, SMI or I_{ij}, (Pavelčík, 1988) is calculated. Instead of fixing the best cross-linked atom as in the unweighted cross-vector function, the atom that is not well cross-linked is deleted from the atom list. This is done in the following way. For each atom, a sum of the SMIs is calculated,

$$ZZ_i = \sum_j I_{ij}. \tag{13}$$

In the next step, the weighted characteristic is given by

$$wZZ_i = \sum_j ZZ_j I_{ij}. \tag{14}$$

The weighted sum is high for groups of atoms that are all well linked. The atom with the smallest value of wZZ_i is deleted from the atom list and the ZZ_i are recalculated. The process is repeated until the number of atoms in the fragment is equal to the number (max) supplied by user.

R(Patt) factor

Each solution of the Patterson function given by the cross-vector function is subject to an R-factor calculation. Because of the small size of a fragment (two or three heavy atoms in general), the Patterson-function-derived R factor is preferred. Patterson-function values are influenced only by given cross-vectors and accidental overlaps (local character) and they are less affected by the unknown part of the structure than the $|F|^2$ values. The Patterson vectors are generated for all atoms in the unit cell, $\mathbf{u}_{ijkl} = (R_k\mathbf{r}_i + \mathbf{t}_k) - (R_l\mathbf{r}_j + \mathbf{t}_l)$, where k, l represent symmetry operations

$$R(\text{Patt}) = \sum |P_0 - P_c| / \sum P_0. \tag{15}$$

P_0 are values of the normalized Patterson function. The P_c are calculated from the atomic numbers. The overlap of atoms is taken into account (some vectors are overlapped due to symmetry),

$$P_c = \sum_j Z_i Z_j \exp(-\Delta r_{ij}^2/\text{hw}_s). \tag{16}$$

Summation is over all overlapping vectors and Δr_{ij} is the distance between vectors. The factor $\exp(-\Delta r^2/\text{hw}_s)$ is an empirical function; hw_s is the parameter given by

$$\text{hw}_s = [P(000)/P_s(000)]^{2/3}\text{hw}_0. \tag{17}$$

$P(000)$ and $P_s(000)$ are origin peaks of the unsharpened and sharpened Patterson functions respectively. hw_0 is an empirical constant related to the half-width of the unsharpened Patterson peak at the origin and the constant was set to $\text{hw}_0 = 0.25$ Å^2.

Automatic procedure

The general strategy for structure determination is the same as decscribed previously (Pavelčík, 1988).

Considerable improvements were achieved for space groups in which the origin is not fixed by the symmetry in one or two dimensions. In this case the superposition based on a single Patterson vector was replaced by four procedures. These are: the SOSMF in the Patterson peak approximation; the fragment generator based on Patterson peaks; the cross-vector function; and the atomic minimum superposition. In the space group $P1$ with three or more heavy atoms in the cell, the simple superposition was replaced by a special routine described above and by multiple-atom superposition. The overall strategy is shown in Fig. 1.

Test calculations and discussion

The parameter b of the sharpening function (1) was optimized to give the best result in the superposition. The optimization seems to be more important for structures with intermediate heavy atoms. The optimization for VULM (Table 1) in which superposition is based on four Cl atoms gave optimum results at $b = -1$ and optimization for LILI (Table 2), with superposition based on eight light atoms, gave optimum results at $b = 2$, indicating that light structures correspond to a possibility of higher sharpening. Parameter a was fixed at 6, as recommended by Jacobson (1970).

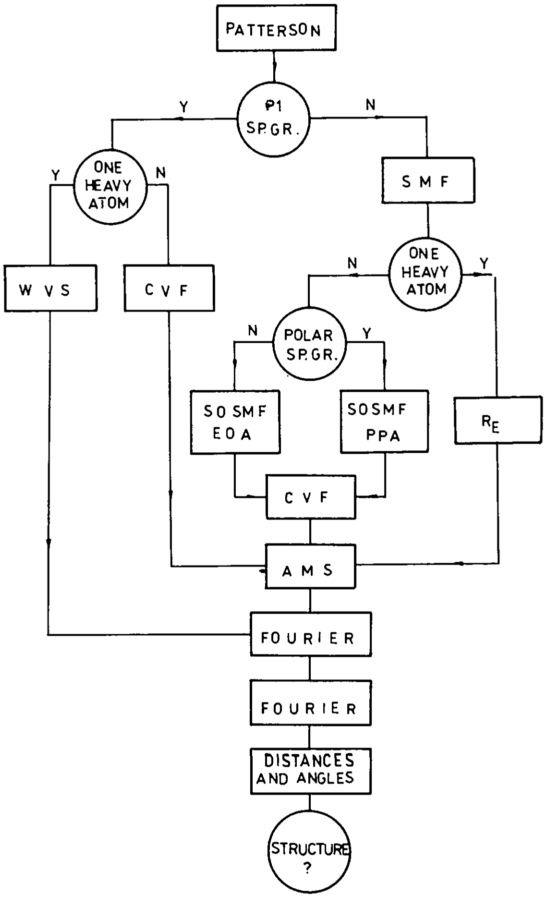

Fig. 1. Flow chart of the automatic structure determination. SMF: symmetry minimum function; WVS: weighted vector superposition; SOSMF: second-order symmetry minimum function; EOA: equivalent-origin approximation with fragment generator by equivalent-origin shift; PPA: Patterson peak approximation with fragment generator by Patterson peaks; CVF: cross-vector function; AMS: atomic minimum superposition. Y: yes; N: no.

Table 1. *Crystal data for heavy-atom structures and results of automatic solution*

XFPS option SOLV and *SHELXS*86 option PATT. Y: solved; N: not solved.

Code	Space group	Formula	Z	*XFPS*	*SHELXS*86	Reference
BAVO	$P2_12_12_1$	$Ba(VO_3)_2.H_2O$	4	Y	N	1
FUNG	$Pccn$	$C_{17}H_{22}ClN_2O_4PS_2$	8	Y	N	2
HAVE	$P2_1/c$	$C_7H_{15}N_2O_7P$	4	Y	N	3
HAVE	$P2_1$	$C_7H_{15}N_2O_7P$	4	N	N	3
HAVE	Pc	$C_7H_{15}N_2O_7P$	4	Y	N	3
PYOX	$P\bar{1}$	$C_{14}H_{12}Cl_4CuN_2O_6$	2	Y	N	4
PYOX	$P1$	$C_{14}H_{12}Cl_4CuN_2O_6$	2	Y	N	4
CUSA	$P\bar{1}$	$C_{17}H_{13}CuKN_2O_3S$	2	Y	Y	5
BETA	$C2/c$	$C_{18}H_{29}ClN_2O_5$	8	Y	N	6
KEID	$P\bar{1}$	$C_{14}H_{24}CoKN_4O_{12}$	2	N	Y	7
CUIM	$P2_1/c$	$C_{13}H_{18}CuN_3O_3$	4	Y	Y	8
CUMOS	$C2/c$	$C_{36}H_{66}Cu_2MoN_2S_6$	4	Y	Y	9
MGHEX	$P3_1$	$C_{56}H_{80}Cl_2MgN_{16}O_{20}$	3	N	N	10
AZET	$Pca2_1$	$C_{21}H_{16}ClNO$	8	N	N	10
APAPA	$P4_12_12$	$C_{30}H_{49}N_{15}O_{22}P_2$	8	N	N	10
BOBBY	$P2_13$	$C_6H_6CaNNaO_6$	4	Y	Y	10
SELENID	$P2_1$	$C_{22}H_{28}O_2Se$	2	Y	Y	10
MORF	$P2_1/c$	$C_7H_{11}Cl_3N_2O_2$	4	Y	Y	11
DAMO	$Pbca$	$C_{15}H_{50}B_4Cu_2F_{16}N_{10}$	8	Y	N	12
VULM	$P2_12_12_1$	$C_{18}H_{30}ClNO_2$	4	Y	Y	13

References: [1] Ulická, Pavelčík & Huml (1987); [2] Vrábel, Pavelčík, Kellö, Miertuš, Konečný & Lokaj (1987); [3] Pavelčík, Havetta & Paterek (1989); [4] Pavelčík, Žemlička, Kettmann & Krätsmár-Šmogrovič (1987); [5] Sivý, Pavelčík, Krätsmár-Šmogrovič, Žemlička & Seressova (1990); [6] Kettmann & Csöllei (1989); [7] Pavelčík, Novomesky, Soldánová & Polynova (1988); [8] Sivý, Plesch, Krätsmár-Šmogrovič, Svajlenova & Kettmann (1989); [9] Acott, Garner, Nicholson & Clegg (1983); [10] Sheldrick (1982); [11] Vrábel, Pavelčík, Kellö, Miertuš, Konečný & Lokaj (1985); [12] Sivý, Valach, Koreň, Macášková, Pavelčík & Sivý (1989); [13] Kettmann, Pavelčík, Majer & Rybár (1989).

Table 2. *Crystal data for non-heavy-atom structures*

Code	Space group	Formula	Z	Reference
LILI	$P2_12_12_1$	$C_{10}H_{14}N_2O_2$	4	14
SUAC	$P2_12_12_1$	$C_{27}H_{38}O_{12}$	4	15
DIAM	$P4_2/n$	$C_{14}H_{20}O$	8	10
DIOL	$I\bar{4}2d$	$C_{10}H_{18}O_2$	16	10
BED	$I4$	$C_{26}H_{26}N_4O_4$	8	10
NO55	$Fdd2$	$C_{20}H_{24}N_4$	16	10
TPH	$C222_1$	$C_{24}H_{20}N_2$	12	10
TURIO	$P6_322$	$C_{15}H_{24}O_2$	12	10
IUCR6	$P6_122$	C_2OS	6	16
IUCR7	$I\bar{4}3d$	$C_{16}O_{36}S_{48}$	1	16

References: [10] Sheldrick (1982); [14] Pavelčík (1989*b*); [15] Pavelčík, Havetta & Suchý (1985); [16] Ahmed, Cruickshank, Larson & Stewart (1972).

The *XFPS* program has been tested on structures of various symmetry, unit-cell content and complexity and compared with *SHELXS*86 (Sheldrick, 1986) [based on *SHELX*84 (Sheldrick, 1985)]. The tests for mainframe *XFPS*89 (and mainframe *SHELXS*86) are given in Table 1. Some parts of the program were also tested on structures not containing heavy atoms because we did not have enough heavy-atom test structures for higher symmetry and rare space groups. These are given in Table 2. Comparison of symmetry minimum functions and symmetry sum functions are given in Table 3 and results of testing of preselection routines on the mainframe are given in Table 4. In these tests the Patterson function was calculated with an interlayer separation of 0.25 Å. For the SOSMF the peaks higher than $0.8Z$ were used, but the maximum number of peaks was limited to 100 (Z is the atomic number of the lightest heavy atom considered). The results of test calculations performed with the MS-DOS PC version are given in Table 5. The efficiency of a fully automated structure determination with *XFPS* (option SOLV) was compared with the results of *SHELXS*86 MS-DOS (option PATT). The results of the fully automated structure determinations are quite encouraging, but there is still a place for further development.

Table 3. *Results and comparison of symmetry minimum function, SMF, symmetry sum function, SSF, and symmetry sum function with origin-removed Patterson function, SSFOR*

Code	Heavy atoms	SMF	SSF	SSFOR
BAVO	Ba, 2V	2, 5, 8	1, 4, 7	1, 4, 7
FUNG	Cl, 2S, P	1, 2, 24, 31	6, 46, 77, 79	6, 53, 66, 81
PYOX	Cu, 4Cl	3, 27, 32, 34, 65	2, 18, 26, 33, 40	1, 17, 26, 31, 32
CUSA	Cu, K, S	3, 26, 46	2, 24, 40	2, 26, 36
MORF	3Cl	2, 6, 10	2, 4, 14	2, 4, 17
DAMO	2Cu	1, 2	4, 6	4, 6
KEID	2Co	1	1	2
CUMOS	Mo, Cu, 3S	1, 3, 7, 18, 22	3, 12, 36, 44, 66	3, 9, 36, 42, 69
AZET	2Cl	1, 7	2, 9	2, 8
APAPA	2P	2, 9	4, 16	2, 9
BOBBY	Ca, Na	1	1	1

Table 4. *Results for the second-order symmetry minimum function*

EO: equivalent-origin approximation; EOC: equivalent-origin approximation followed by convergence-function searching for max. atoms (max. is number of atoms in the asymmetric part of the unit cell plus 1); PP: Patterson peak approximation; PPW: weighted Patterson peak approximation.
Values in brackets are numbers in the peak list that were deleted by the procedure or that have zero contribution.

Code	EO	EOC	PP	PPW
BAVO	1, 2, 4	1, 2, 4	1, 3, 6	2, 3, 5
FUNG	1, 2, 5, 16	1, 2, 4, (33)	1, 2, 5, 15	2, 3, 8, 9
PYOX	3, 4, 11, 14, 56	4, (10, 11, 25, 50)	3, 23, 27, 37	2, 19, 20, (37)
CUSA	1, 2, 3	1, 2, 3	1, 2, 3	1, 2, 3
MORF	1, 2, 3	1, 2, 3	1, 2, (16)	1, 2, (16)
DAMO	1, 2	1, 2	1, 2	1, 2
KEID	-	-	1	1
CUMOS	1, 2, 5, 7, 10	1, 2, 3, 4, (7)	1, 2, 5, 7, 9	1, 2, 5, 6,7
AZET	1, 8	2, (11)	1, 15	1, 15
APAPA	9, 94	(19, 94)	4, 33	4, 5
BOBBY	-	-	1	1

Table 5. *Crystal data for heavy-atom structures and results of automatic solution with the PC version of XFPS*

XFPS option SOLV and *SHELXS*86 option PATT were used.
Y: solved; *N*: not solved.

Code	Space group	Formula	*Z*	*XFPS*	*SHELXS*86	Reference
ES67A	$P2_1/c$	$C_{13}H_{19}Cl_6Ta$	2	*Y*	*Y*	17
ES67	$P2_1/c$	$C_{13}H_{19}Cl_6Ta$	4	*Y*	*Y*	17
FC1014	$I422$	$C_{176}H_{208}O_{20}W_4$	1	*Y*	*Y*	17
FC999	$P4/n$	$C_{95}H_{114}O_{10}W$	1	*Y*	*Y*	17
FC969	$C2/c$	$C_{128}H_{112}O_{32}W_4$	1	*Y*	*Y*	17
MCO	$Fd\bar{3}m$	$MnCr_2O_4$	8	*Y*	*N*	18
STR	$P2_1/c$	$C_{30}H_{13}Co_2FeMnO_{11}$	4	*Y*	*N*	19
PV206	$P2_1/n$	$C_{38}H_{34}N_2Zr$	8	*Y*	*N*	20
PV214	$P\bar{1}$	$C_{24}H_{22}ClOZr$	2	*Y*	*Y*	20
PV213	$P\bar{1}$	$C_{68}H_{100}K_2N_4O_{16}$	1	*Y*	*N*	20
JR171	$P\bar{1}$	$C_{57}H_{63}N_4O_4V$	2	*Y*	*Y*	20
JR143	$P2_1/c$	$C_{36}H_{60}N_4V_2$	4	*Y*	*N*	20
TC107	$P2_1/n$	$C_{24}H_{28}Mo_2O_8Ti_2$	2	*Y*	*Y*	20
PV220	$P2_1/c$	$C_{29}H_{22}ClCrO_6PZr$	4	*Y*	*Y*	20
PV216	Cc	$C_{29}H_{22}ClCrNO_6Zr$	4	*Y*	*Y*	20
JR193	$P1$	$C_{56}H_{88}N_2O_{24}Zr$	1	*N*	*N*	20
WL480	$P\bar{1}$	$C_{58}H_{84}Cl_2O_5Ti_2$	2	*N*	*N*	20
FC955	$P2_1/n$	$C_{64}H_{70}Cl_2O_4W$	4	*Y*	*N*	20
ZAGA11	$P\bar{1}$	$C_{28}H_{38}Cl_2N_2O_6P_2Pd$	1	*Y*	*Y*	21

References: [17] Rizzoli (1990); [18] Bocelli (1990); [19] Bocelli & Sterzo (1990); [20] Chiesi-Villa, Guastini & Rizzoli (1990); [21] Matijašić (1990).

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An Attempt to Describe One-Dimensional Incommensurate Composite Structure as Phason-Defected One-Dimensional Quasiperiodic Structure*

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Abstract

An incommensurate phase with one-dimensional (1D) incommensurate composite structure newly discovered in an Al-Cu-Fe alloy coexists with the structurally related commensurate phase. Both of them can be described as a phason-defected 1D fictitious quasicrystal. The 1D quasicrystal is obtained by cutting a six-dimensional (6D) crystal with physical space. With the increase of a particular linear phason strain, the section of the 6D crystal transfers firstly to the incommensurate phase and then to the commensurate phase.

1. Introduction

There are different types of incommensurate structures, for example, incommensurate modulated structure (de Wolff, 1974), incommensurate composite structure (Janner & Janssen, 1980) and quasiperiodic structure (Shechtman, Blech, Gratias & Cahn 1984). They can easily be distinguished one from another by means of diffraction data. The diffraction peaks of an incommensurate modulated structure can be divided into two groups: main peaks and satellite peaks. The main peaks form a periodic lattice that corresponds to the average structure and each main peak is accompanied by satellite peaks. The incommensurate composite structure consists of two or more substructures. Each of them gives an independent set of periodic diffraction peaks to form the major reflections. The minor reflections originate from the mutual interaction among different substructures. In this sense, both incommensurate modulated structures and incommensurate composite structures are to some extent related to three-dimensional (3D) periodicity. The quasicrystal possesses quasiperiodicity in both real and reciprocal spaces that is not related to 3D periodicity (Schechtman *et al.*, 1984). Thus far, the incommensurate modulated structure, the incommensurate composite structure and the quasicrystal structure are recognized as completely different incommensurate structures and no information about the structural relationship among them has been

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