SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000
words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.

A full-symmetry translation function. II. The introduction of positioned fragments. By JORDI RIUS and
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Abstract

A generalization of the full-symmetry τ translation function
[Rius & Miravitlles (1986). *Acta Cryst.* A42, 402–404] is
given that allows the explicit introduction of the positioned
part of the structure in its computation. This generalization
is useful for the structural expansion of molecular crystals
with more than one molecule in the asymmetric unit,
specially in those cases where the non-availability of high-
resolution diffraction data prevents the use of the tangent-
formula recycling of a single positioned fragment, *e.g.* in
the determination of crystal structures from powder diffrac-
tion data. Its application to four structures is shown.

Rius & Miravitlles (1986) described the reciprocal-space τ
translation function which places molecular fragments with
respect to all symmetry elements simultaneously using the
Fourier expansion of Harada, Lifchitz, Berthou & Jolles
(1981). Here a generalization of the τ function is introduced
that also considers the positioned part of the structure. This
generalization is useful for molecular crystals with more
than one molecule in the asymmetric unit, since it allows
one to take advantage of the molecular orientations found
in the rotation search. If the symmetry-independent
molecules are similar, a single rotation search furnishes all
correct orientations. Once the first molecular fragment is
positioned, another symmetry-independent oriented
molecular fragment can be placed with respect to it. This
procedure can be repeated iteratively in crystal structures
containing more than two independent molecules in the
asymmetric unit.

The principal application of this function lies in those
problems where only low-resolution data are available, *i.e.*
when the tangent-formula recycling of a single positioned
fragment is not possible. One example of this potential
application is the crystal-structure determination from pow-
der diffraction data only, since, as is well known, the better
resolved and consequently the more reliable indexed reflec-
tions of a powder spectrum are those appearing at low 2θ
angles.

The τ function is defined as

$$\tau(\mathbf{r}) = (1/V)\sum_{\mathbf{h}} |F'_o(\mathbf{h})|^2 |F'_c(\mathbf{h}, \mathbf{r})|^2 \tag{1}$$

$$= \operatorname{Re}(2/V)\sum_{\mathbf{h}} \left[\sum_j |F'_o(\mathbf{h})|^2 F_P(\mathbf{h}) S_j^*(\mathbf{h}) \right.$$

$$\times \exp\left(-i2\pi \mathbf{h}\mathbf{t}_j\right)\exp\left(-i2\pi \mathbf{h}_j \mathbf{r}\right)$$

$$+ \sum_j \sum_{k>j} |F'_o(\mathbf{h})|^2 S_j(\mathbf{h}) S_k^*(\mathbf{h})$$

$$\left. \times \exp\left(-i2\pi \mathbf{h}\mathbf{t}_{kj}\right) \exp\left(-i2\pi \mathbf{h}_{kj}\mathbf{r}\right) \right] \tag{2}$$

with

$$|F'_o(\mathbf{h})|^2 = |F_o(\mathbf{h})|^2 - |F_P(\mathbf{h})|^2 - \sum_l |S_l(\mathbf{h})|^2 - \sum_m^q f_m(\mathbf{h})^2, \tag{3}$$

where r = shift vector applied to the input oriented molecule
(hereafter called search fragment); $F_o(\mathbf{h})$ = observed struc-
ture factor; $S_j(\mathbf{h})$ = molecular structure factor computed
with the atomic coordinates obtained after applying the
rotation matrix R_j to the search fragment, referred to a
fixed local origin in the fragment; $\mathbf{t}_j$ = translation of the jth
space-group symmetry operation; $\mathbf{t}_{kj} = \mathbf{t}_k - \mathbf{t}_j$; $\mathbf{h}_{kj} =
\mathbf{h}(R_k - R_j)$; $\mathbf{h}_j = \mathbf{h}R_j$; $F_P(\mathbf{h})$ = structure factor computed
with the positioned atoms; q = number of atoms in the unit
cell not included in the calculation of $F_P(\mathbf{h})$ or $S_j(\mathbf{h})$.

$|F'_o(\mathbf{h})|^2$ are the Fourier coefficients of the observed Patter-
son function without the Patterson function of the posi-
tioned part and without the self-Patterson function of the
search fragment (and symmetry-related ones). The last term
in (3) subtracts the contribution from the q atoms to the
Patterson origin peak (Beurskens, Gould, Bruins Slot &
Bosman, 1987).

$|F'_c(\mathbf{h}, \mathbf{r})|^2$ are the Fourier coefficients of the calculated
cross-Patterson function without those cross-Patterson
peaks due to interactions between the atoms in the posi-
tioned part. $|F'_o(\mathbf{h})|^2$ and $|F'_c(\mathbf{h}, \mathbf{r})|^2$ are equal only for $q = 0$
and if $\mathbf{r}$ is the correct shift vector. The correct shift vector
is always characterized by a strong positive maximum in τ.

The generalization of the τ function to consider the
positioned part of the structure is reflected in the appear-
ance of the double summation in (2),

$$\operatorname{Re}(2/V)\sum_{\mathbf{h}} \sum_j |F'_o(\mathbf{h})|^2 F_P(\mathbf{h}) S_j^*(\mathbf{h})$$

$$\times \exp\left(-i2\pi \mathbf{h}\mathbf{t}_j\right)\exp\left(-i2\pi \mathbf{h}_j \mathbf{r}\right) \tag{4}$$

which nearly represents the convolution of the inverted
search fragment with the modified α function (Ramachan-
dran & Srinivasan, 1970) and vanishes when no part of the
structure is known. This is an automated interpretation of
the modified α function when the geometry of the molecular
search fragment is known. If a fragment is already posi-
tioned, the τ asymmetric unit will be, in general, the whole
unit cell (except for non-primitive lattices).

Table 1. *Data and results of the application of the τ function to four test examples*

τ_c = height of correct peak; τ_w = height of highest-ranked τ wrong peak.

Code name	MUNICH1*	NEWQB†	MBH2‡	TNP§
Molecular formula	$C_{29}H_{16}$	$C_{24}H_{20}N_2O_5$	$C_{15}H_{24}O_3$	$C_5H_3N_5O_8$
Space group	C2	P1̄	P1	Pbca
Z	8	4	3	16
Number of observed reflections [$F > 2\sigma(F)$]	1115	2573	1577	492
Model size	20	8	18	10
Scattering fraction				
(positioned part)	0·49	0·13	0·32	0·23
(search fragment)	0·49	0·13	0·32	0·23
τ_c	1000	1000	1000	1000
τ_w	687	747	546	960
Rank number of correct τ peak	1	1	1	1

* Szeimies-Seebach, Harnisch, Szeimies, Van Meersche, Germain & Declercq (1978).
† Grigg, Kemp, Sheldrick & Trotter (1978).
‡ Poyser *et al.* (1986).
§ Cromer, Coburn, Ryan & Wasserman (1986).

To improve the resolution of the τ function, the $|F'_o(\mathbf{h})|^2$ are sharpened, and $F_p(\mathbf{h})$ as well as the molecular structure factors are derived using point atoms with thermal motion. Although the τ function has been defined with F values, it can be easily modified to use E values. The implementation of (4) in a program that computes the τ function is extremely easy, since it only represents the addition of N new Fourier terms for each reflection ($N/2$ for centrosymmetric space groups, N = number of symmetry operations).

Test calculations

Four test structures with more than one molecule in the asymmetric unit have been selected to illustrate how τ places the search fragment with respect to the previously positioned part of the structure, even with low-resolution data. Although also performed, the first step, *i.e.* the positioning of search fragments when no positioned atoms are present, is not discussed here, since this case was discussed by Rius & Miravitlles (1986).

The test structures are tricyclo[3.1.0.0^{2,6}]hex-1(6)-ene (MUNICH1), methyl 4-(2-furyl)-6,8-dioxo-2,7-diphenyl-3,7-diazabicyclo[3.3.0]octane-2-carboxylate (NEWQB), the sesquiterpene alcohol punctotin D (MBH2) and 1-methyl-2,3,4,5-tetranitropyrrole (TNP). Relevant crystal and test data are given in Table 1. The fragments used in the tests were derived by applying arbitrary rotations and translations to the refined atomic coordinates.

MUNICH1 is an example of a non-centrosymmetric structure with a centred unit cell and with two identical molecules in the asymmetric unit (τ asymmetric unit for the second step: 0, $\mathbf{a}/2$; 0, $\mathbf{b}$; 0, $\mathbf{c}$). The search fragment is a complete molecule. As can be seen in Table 1, the translation search is quite satisfactory.

NEWQB has been selected to show the application of τ to a centrosymmetric crystal structure. The search fragment

is not very large here. Even in this case, the result is excellent.

MBH2 has been chosen to show the behaviour of τ when the second summation in (2) vanishes. It is also an example of how τ can be employed iteratively. Only the intermediate step, *i.e.* the positioning of the second molecule with respect to the first one, is indicated in Table 1.

TNP illustrates the case of a high-symmetry space group. The result given in Table 1 was obtained with low-resolution data, *i.e.* $[(\sin\theta)/\lambda]^2_{max} = 0·10 \text{ Å}^{-2}$.

All calculations were performed with *ROTSEARCH* (Rius & Miravitlles, 1987).

References

BEURSKENS, P. T., GOULD, R. O., BRUINS SLOT, H. J. & BOSMAN, W. P. (1987). *Z. Kristallogr.* In the press.
CROMER, D., COBURN, M., RYAN, R. & WASSERMAN, M. (1986). *Acta Cryst.* C42, 1428-1430.
GRIGG, R., KEMP, J., SHELDRICK, G. M. & TROTTER, J. (1978). *J. Chem. Soc. Chem. Commun.* pp. 1109-1111.
HARADA, Y., LIFCHITZ, A., BERTHOU, J. & JOLLES, P. (1981). *Acta Cryst.* A37, 398-406.
POYSER, J. P., EDWARDS, R., ANDERSON, J., HURSTHOUSE, M., WALKER, N., SHELDRICK, G. & WALLEY, A. (1986). *J. Antibiot.* 39, 167-169.
RAMACHANDRAN, B. N. & SRINIVASAN, R. (1970). *Fourier Methods in Crystallography*, edited by M. J. BUERGER, pp. 86-87. New York: John Wiley.
RIUS, J. & MIRAVITLLES, C. (1986). *Acta Cryst.* A42, 402-404.
RIUS, J. & MIRAVITLLES, C. (1987). *J. Appl. Cryst.* 20, 261-264.
SZEIMIES-SEEBACH, U., HARNISCH, J., SZEIMIES, G., VAN MEERSCHE, M., GERMAIN, G. & DECLERCQ, J.-P. (1978). *Angew. Chem. Int. Ed. Engl.* 17, 848-850.

International Union of Crystallography

Report of the Executive Committee for 1986

Meetings

The Union sponsored the following meetings held during 1986: Winter School on Teaching, Characterization and Properties of Epitaxial Electronic Materials, Trieste, Italy, 13–24 January 1986; Gordon Research Conference on Electron Distributions and Chemical Bonding, Plymouth, USA, 30 June–4 July 1986; First International Symposium on Shaped Crystal Growth, Budapest, Hungary, 22–25 July 1986; Symposium on Organic Crystal Chemistry, Poznań-Rydzyna, Poland, 1–4 August 1986 (satellite meeting of ECM-10); One-day Tutorial Workshop on Inorganic Molecular Crystals, Wrocław, Poland, 4 August 1986 (satellite meeting of ECM-10); Tenth European Crystallographic Meeting, Wrocław, Poland, 5–9 August 1986; Satellite Conference on Crystal Growth and Liquid Crystals, Łódź, Poland, 11–13 August 1986 (satellite meeting of ECM-10); International Summer School on Crystallographic Computing, Leipzig, German Democratic Republic, 11–20 August 1986; Research Course on Neutron Diffraction Techniques in Crystal Structure Determination, Studsvik and Uppsala, Sweden, 18–29 August 1986; Workshop on Crystallography in Molecular Biology: Structure of Biological Macromolecules, Poushchino, USSR, 4–13 September 1986; International Symposium on Molecular Structure: Chemical Reactivity and Biological Activity, Beijing, People's Republic of China, 15–19 September 1986; Symposium on Computational Methods in Chemical Design: Molecular Modelling and Computer Graphics, Schloss Elmau, Federal Republic of Germany, 19–26 October 1986; International School on Solar Cell Materials and Applications, Fayoum, Arab Republic of Egypt, 19–26 October 1986.

The Executive Committee met at Foxhill, near Chester, England, in July 1986. The most important items of business dealt with were (1) approval of the audited accounts for 1985; (2) subscription rates and other matters concerning the journals, including the appointment of Professor C. E. Bugg to succeed Dr S. C. Abrahams as Editor of *Acta Crystallographica* at the XIV General Assembly in Perth in August 1987; (3) other publications of the Union; (4) initiation of an agreement with Oxford University Press to start the IUCr/OUP Book Series; (5) establishment of a Book Series Committee to develop the IUCr/OUP Book Series; (6) the General Fund estimates and proposal for the level of the unit contribution for the next triennium; (7) sponsorship of meetings; (8) financial support for young scientists attending meetings receiving IUCr sponsorship; (9) free circulation of scientists; (10) discussion of the arrangements for the XIV General Assembly and Congress with the Congress Programme Committee; (11) level of financial support for the above Congress, including assistance for Commission Chairman, Editors and Co-editors; (12) review of the activities of the Commissions; (13) application by the JCPDS-ICDD to become a Scientific Associate of the Union; (14) nominations for Officers of the Union, and Chairman and members of the Commissions; (15) upgrad-ing the office technology in the Union office in Chester; (16) refurbishment of these premises.

The Finance Committee met at the Chester office in January and then at Foxhill immediately prior to the Executive Committee meeting in July.

Publications

Volume 42 of *Acta Crystallographica* and Volume 19 of the *Journal of Applied Crystallography* were published, as were Volumes 48B and 52A of *Structure Reports*. A short-run reprint of *International Tables for Crystallography* Volume A was made, to keep this volume in print until a new edition could be published in 1987. No more volumes of *Molecular Structures and Dimensions* have been published since Volume 15, which was published in 1984.

Adhering Bodies

The latest list of Adhering Bodies of the Union, and the names and addresses of the Secretaries of the National Committees, is given in Table 1.

Work of the Commissions

Commission on Journals

Volumes 42 of *Acta Crystallographica* (*Acta*) and 19 of the *Journal of Applied Crystallography* (*JAC*) were produced and published in 1986. The total number of papers published in *Acta* increased 4% while those in *JAC* decreased 4% compared with 1985, see Table 2. A total of 1201 papers were submitted to *Acta* in 1986 compared with 1075 in 1985, 1138 papers being sent for publication in 1986 and 920 in 1985. Corresponding figures for *JAC* were 143 papers submitted in 1986 and 144 in 1985, with 117 papers sent for publication in 1986 and 127 in 1985. A substantial backlog in processing manuscripts developed during the year due to the resignation of the previous Technical Editor and the death of the Deputy Technical Editor, see *Acta* (1987). A**43**, 137–139. By year's end, considerable progress had been made toward eliminating the backlog.

The average length of all articles in *Acta* increased very slightly in 1986 to 3·4 pages from 3·3 pages in 1985, reversing the previous downward trend. The largest increase was in Section A from 5·5 pages in 1985 to 6·0 pages in 1986. The average length in *JAC* decreased from 5·1 pages in 1985 to 4·7 pages in 1986. Median publication time, the average elapsed time between the published acceptance and nominal publication dates, was 5·7 months for *Acta* A and B and 4·8 months for *Acta* C and *JAC*. Corresponding publication times in 1985 were 5·0, 5·6, 3·8 and 5·1 months. The increased time in *Acta* A was caused in part by the Ewald issue of November 1986. The remaining increases in publication time were due to the temporary understaffing in the Technical Editor's office and these are expected to return to normal in 1987.