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Structure-factor and least-squares expressions for cubic crystal systems with isotropic vibrations.*

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A set of expressions is presented for calculating structure-factors and least-squares coefficients for cubic structures with isotropic temperature factors. These expressions have been utilized in programming the Burroughs 220 and IBM 7090 computers to perform structure-factor least-squares calculations for any cubic space group; to direct the course of calculations for a particular space group, only the space group number need be designated. The expressions will complement those presented by Hybl & Marsh (1961) for the orthorhombic system; however, we will not now carry their treatment of anisotropic temperature factors into the cubic system because of the extreme complexity and unwieldiness of the resultant structure-factor expressions and because of the generally assumed isotropic nature of atoms in cubic structures. A set of expressions for tetragonal, trigonal, and hexagonal systems with anisotropic vibrations is being prepared for publication.

Table 1. *Definition of triple products and sums of triple products*

C = cos2π   S = sin2π

Group I	hx ky ℓz	hy kz ℓx	hz kx ℓy	
C ≡	Chx·Cky·Cℓz	+ Chy·Ckz·Cℓx	+ Chz·Ckx·Cℓy	≡ $c_1 + c_2 + c_3$
E ≡	Shx·Sky·Cℓz	+ Shy·Skz·Cℓx	+ Shz·Skx·Cℓy	≡ $e_1 + e_2 + e_3$
G ≡	Chx·Sky·Sℓz	+ Chy·Skz·Sℓx	+ Chz·Skx·Sℓy	≡ $g_1 + g_2 + g_3$
I ≡	Shx·Cky·Sℓz	+ Shy·Ckz·Sℓx	+ Shz·Ckx·Sℓy	≡ $i_1 + i_2 + i_3$
K ≡	Shx·Sky·Sℓz	+ Shy·Skz·Sℓx	+ Shz·Skx·Sℓy	≡ $k_1 + k_2 + k_3$
M ≡	Shx·Cky·Cℓz	+ Shy·Ckz·Cℓx	+ Shz·Ckx·Cℓy	≡ $m_1 + m_2 + m_3$
O ≡	Chx·Sky·Cℓz	+ Chy·Skz·Cℓx	+ Chz·Skx·Cℓy	≡ $o_1 + o_2 + o_3$
Q ≡	Chx·Cky·Sℓz	+ Chy·Ckz·Sℓx	+ Chz·Ckx·Sℓy	≡ $q_1 + q_2 + q_3$
Group II	**hy kx ℓz**	**hz ky ℓx**	**hx kz ℓy**	
D ≡	Chy·Ckx·Cℓz	+ Chz·Cky·Cℓx	+ Chx·Ckz·Cℓy	≡ $d_1 + d_2 + d_3$
F ≡	Shy·Skx·Cℓz	+ Shz·Sky·Cℓx	+ Shx·Skz·Cℓy	≡ $f_1 + f_2 + f_3$
H ≡	Chy·Skx·Sℓz	+ Chz·Sky·Sℓx	+ Chx·Skz·Sℓy	≡ $h_1 + h_2 + h_3$
J ≡	Shy·Ckx·Sℓz	+ Shz·Cky·Sℓx	+ Shx·Ckz·Sℓy	≡ $j_1 + j_2 + j_3$
L ≡	Shy·Skx·Sℓz	+ Shz·Sky·Sℓx	+ Shx·Skz·Sℓy	≡ $\ell_1 + \ell_2 + \ell_3$
N ≡	Shy·Ckx·Cℓz	+ Shz·Cky·Cℓx	+ Shx·Ckz·Cℓy	≡ $n_1 + n_2 + n_3$
P ≡	Chy·Skx·Cℓz	+ Chz·Sky·Cℓx	+ Chx·Skz·Cℓy	≡ $p_1 + p_2 + p_3$
R ≡	Chy·Ckx·Sℓz	+ Chz·Cky·Sℓx	+ Chx·Ckz·Sℓy	≡ $r_1 + r_2 + r_3$

All of the geometrical structure factors for the cubic system have been reduced to sums of triple products of sines and cosines. A total of 48 different triple products are utilized; these triple products and the 16 sums of 3 triple products are defined in Table 1. The triple products are divided into two groups. Space groups of symmetry T or T_h require expressions in group I only; furthermore, the derivatives with respect to the parameters x, y, and z (and, of course, B) of any triple product in group I (or II) are other triple products in group I (or II) multiplied by $\pm 2\pi \begin{pmatrix} h \\ k \\ l \end{pmatrix}$.

Table 2. *Derivatives of triple products*

All derivatives to be multiplied by 2π.
For example, read hm_1 as $2\pi hm_1$

	Group I x	Group I y	Group I z		Group II x	Group II y	Group II z
c_1	$-hm_1$	$-ko_1$	$-lq_1$	d_1	$-kp_1$	$-hn_1$	$-lr_1$
c_2	$-lq_2$	$-hm_2$	$-ko_2$	d_2	$-lr_2$	$-kp_2$	$-hn_2$
c_3	$-ko_3$	$-lq_3$	$-hm_3$	d_3	$-hn_3$	$-lr_3$	$-kp_3$
e_1	ho_1	km_1	$-lk_1$	f_1	kn_1	hp_1	$-ll_1$
e_2	$-lk_2$	ho_2	km_2	f_2	$-ll_2$	kn_2	hp_2
e_3	km_3	$-lk_3$	ho_3	f_3	hp_3	$-ll_3$	kn_3
g_1	$-hk_1$	kq_1	lo_1	h_1	kr_1	$-hl_1$	lp_1
g_2	lo_2	$-hk_2$	kq_2	h_2	lp_2	kr_2	$-hl_2$
g_3	kq_3	lo_3	$-hk_3$	h_3	$-hl_3$	lp_3	kr_3
i_1	hq_1	$-kk_1$	lm_1	j_1	$-kl_1$	hr_1	ln_1
i_2	lm_2	hq_2	$-kk_2$	j_2	ln_2	$-kl_2$	hr_2
i_3	$-kk_3$	lm_3	hq_3	j_3	hr_3	ln_3	$-kl_3$
k_1	hg_1	ki_1	le_1	l_1	kj_1	hh_1	lf_1
k_2	le_2	hg_2	ki_2	l_2	lf_2	kj_2	hh_2
k_3	ki_3	le_3	hg_3	l_3	hh_3	lf_3	kj_3
m_1	hc_1	$-ke_1$	$-li_1$	n_1	$-kf_1$	hd_1	$-lj_1$
m_2	$-li_2$	hc_2	$-ke_2$	n_2	$-lj_2$	$-kf_2$	hd_2
m_3	$-ke_3$	$-li_3$	hc_3	n_3	hd_3	$-lj_3$	$-kf_3$
o_1	$-he_1$	kc_1	$-lg_1$	p_1	kd_1	$-hf_1$	$-lh_1$
o_2	$-lg_2$	$-he_2$	kc_2	p_2	$-lh_2$	kd_2	$-hf_2$
o_3	kc_3	$-lg_3$	$-he_3$	p_3	$-hf_3$	$-lh_3$	kd_3
q_1	$-hi_1$	$-kg_1$	lc_1	r_1	$-kh_1$	$-hj_1$	ld_1
q_2	lc_2	$-hi_2$	$-kg_2$	r_2	ld_2	$-kh_2$	$-hj_2$
q_3	$-kg_3$	lc_3	$-hi_3$	r_3	$-hj_3$	ld_3	$-kh_3$

Note the cyclic relationship.

The sums in group I are directly related to sums in group II: C transforms to D, E to F, G to H, I to J, . . . *etc.*, simply by interchanging h and k (see Table 1). The derivatives of a sum can be written down immediately by inspection of Table 2 where the derivatives of each

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Table 3. *Structure factor expressions for the cubic space groups*

For each space group the two right-hand columns contain the geometric factors A and B according to the parity classification in the left-hand column. For the holohedral space groups T_h and O_h, the origin is taken at a center of symmetry; the B terms then vanish and only the A terms are given

No. 195: T^1 - P23

All planes	4C	-4K

No. 196: T^2 - F23

h,k,l all even or all odd	16C	-16K

No. 197: T^3 - I23

h+k+l even	8C	-8K

No. 198: T^4 - P2₁3

h+k	k+l		
2n	2n	4C	-4K
2n	2n+1	-4G	4M
2n+1	2n	-4I	4O
2n+1	2n+1	-4E	4Q

No. 199: T^5 - I2₁3

h+k	k+l (h+k+l even)		
2n	2n	8C	-8K
2n	2n+1	-8G	8M
2n+1	2n	-8I	8O
2n+1	2n+1	-8E	8Q

No. 200: T_h^1 - Pm3

All planes	8C

No. 201: T_h^2 - Pn3

h+k	k+l	
2n	2n	8C
2n	2n+1	-8E
2n+1	2n	-8G
2n+1	2n+1	-8I

No. 202: T_h^3 - Fm3

h,k,l all even or all odd	32C

No. 203: T_h^4 - Fd3

h+k	k+l	l+h	
4n	4n	4n	32C
4n	4n+2	4n+2	-32E
4n+2	4n	4n+2	-32G
4n+2	4n+2	4n	-32I
4n	4n	4n+2	16(C-E-G+I)
4n	4n+2	4n	16(C-E+G-I)
4n+2	4n	4n	16(C+E-G-I)
4n+2	4n+2	4n+2	-16(C+E+G+I)

No. 204: T_h^5 - Im3

h+k+l even	16C

No. 205: T_h^6 - Pa3

h+k	k+l	
2n	2n	8C
2n	2n+1	-8G
2n+1	2n	-8I
2n+1	2n+1	-8E

No. 206: T_h^7 - Ia3

h+k	k+l (h+k+l even)	
2n	2n	16C
2n	2n+1	-16G
2n+1	2n	-16I
2n+1	2n+1	-16E

No. 207: O^1 - P432

All planes	4(C+D)	-4(K-L)

No. 208: O^2 - P4₂32

h+k+l = 2n	4(C+D)	-4(K-L)
h+k+l = 2n+1	4(C-D)	-4(K+L)

No. 209: O^3 - F432

h, k, l all even or all odd	16(C+D)	-16(K-L)

No. 210: O^4 - F4₁32

h, k, l	h + k + l		
all even	4n	16(C+D)	-16(K-L)
all odd	4n + 1	16(C-L)	-16(K-D)
all even	4n + 2	16(C-D)	-16(K+L)
all odd	4n + 3	16(C+L)	-16(K+D)

No. 211: O^5 - I432

h + k + l = 2n	8(C+D)	-8(K-L)

No. 212: O^6 - P4₃32

h	k	l	h+k+l		
2n	2n	2n	4n	4(C+D)	-4(K-L)
2n+1	2n+1	2n+1	4n+1	4(C-L)	-4(K-D)
2n	2n	2n	4n+2	4(C-D)	-4(K+L)
2n+1	2n+1	2n+1	4n+3	4(C+L)	-4(K+D)
2n+1	2n+1	2n	4n	-4(G+J)	4(M-P)
2n	2n	2n+1	4n+1	-4(G-P)	4(M-J)
2n+1	2n+1	2n	4n+2	-4(G-J)	4(M+P)
2n	2n	2n+1	4n+3	-4(G+P)	4(M+J)
2n	2n+1	2n+1	4n	-4(I+F)	4(O-R)
2n+1	2n	2n	4n+1	-4(I-R)	4(O-F)
2n	2n+1	2n+1	4n+2	-4(I-F)	4(O+R)
2n+1	2n	2n	4n+3	-4(I+R)	4(O+F)
2n+1	2n	2n+1	4n	-4(E+H)	4(Q-N)
2n	2n+1	2n	4n+1	-4(E-N)	4(Q-H)
2n+1	2n	2n+1	4n+2	-4(E-H)	4(Q+N)
2n	2n+1	2n	4n+3	-4(E+N)	4(Q+H)

No. 213: O^7 - P4₁32

h	k	l	h+k+l		
2n	2n	2n	4n	4(C+D)	-4(K-L)
2n+1	2n+1	2n+1	4n+1	4(C+L)	-4(K+D)
2n	2n	2n	4n+2	4(C-D)	-4(K+L)
2n+1	2n+1	2n+1	4n+3	4(C-L)	-4(K-D)
2n+1	2n+1	2n	4n	-4(G+J)	4(M-P)
2n	2n	2n+1	4n+1	-4(G+P)	4(M+J)
2n+1	2n+1	2n	4n+2	-4(G-J)	4(M+P)
2n	2n	2n+1	4n+3	-4(G-P)	4(M-J)
2n	2n+1	2n+1	4n	-4(I+F)	4(O-R)
2n+1	2n	2n	4n+1	-4(I+R)	4(O+F)
2n	2n+1	2n+1	4n+2	-4(I-F)	4(O+R)
2n+1	2n	2n	4n+3	-4(I-R)	4(O-F)
2n+1	2n	2n+1	4n	-4(E+H)	4(Q-N)
2n	2n+1	2n	4n+1	-4(E+N)	4(Q+H)
2n+1	2n	2n+1	4n+2	-4(E-H)	4(Q+N)
2n	2n+1	2n	4n+3	-4(E-N)	4(Q-H)

No. 214: O^8 - I4₁32

h	k	l	h+k+l		
2n	2n	2n	4n	8(C+D)	-8(K-L)
2n	2n+1	2n+1	4n	-8(I+F)	8(O-R)
2n+1	2n	2n+1	4n	-8(E+H)	8(Q-N)
2n+1	2n+1	2n	4n	-8(G+J)	8(M-P)
2n	2n	2n	4n+2	8(C-D)	-8(K+L)
2n	2n+1	2n+1	4n+2	-8(I-F)	8(O+R)
2n+1	2n	2n+1	4n+2	-8(E-H)	8(Q+N)
2n+1	2n+1	2n	4n+2	-8(G-J)	8(M+P)

No. 215: T_d^1 - P$\bar{4}$3m

All planes	4(C+D)	-4(K+L)

No. 216: T_d^2 - F$\bar{4}$3m

h, k, l all even or all odd	16(C+D)	-16(K+L)

No. 217: T_d^3 - I$\bar{4}$3m

h + k + l = 2n	8(C+D)	-8(K+L)

No. 218: T_d^4 - P$\bar{4}$3n

h + k + l = 2n	4(C+D)	-4(K+L)
h + k + l = 2n+1	4(C-D)	-4(K-L)

No. 219: T_d^5 - F$\bar{4}$3c

h, k, l all even	16(C+D)	-16(K+L)
h, k, l all odd	16(C-D)	-16(K-L)

No. 220: T_d^6 - I$\bar{4}$3d

h	k	l	h+k+l		
2n	2n	2n	4n	8(C+D)	-8(K+L)
2n	2n+1	2n+1	4n	-8(I+F)	8(O+R)
2n+1	2n	2n+1	4n	-8(E+H)	8(Q+N)
2n+1	2n+1	2n	4n	-8(G+J)	8(M+P)
2n	2n	2n	4n+2	8(C-D)	-8(K-L)
2n	2n+1	2n+1	4n+2	-8(I-F)	8(O-R)
2n+1	2n	2n+1	4n+2	-8(E-H)	8(Q-N)
2n+1	2n+1	2n	4n+2	-8(G-J)	8(M-P)

No. 221: O_h^1 - Pm3m

All planes	8(C+D)

No. 222: O_h^2 - Pn32

h	k	l	
2n	2n	2n	8(C+D)
2n	2n+1	2n+1	-8(G+H)
2n+1	2n+1	2n	-8(E+F)
2n+1	2n	2n+1	-8(I+J)
2n+1	2n+1	2n+1	8(C-D)
2n+1	2n	2n	-8(G-H)
2n	2n	2n+1	-8(E-F)
2n	2n+1	2n	-8(I-J)

No. 223: O_h^3 - Pm3n

h + k + l = 2n	8(C+D)
h + k + l = 2n+1	8(C-D)

No. 224: O_h^4 - Pn3m

h+k	k+l	
2n	2n	8(C+D)
2n	2n+1	-8(E+F)
2n+1	2n	-8(G+H)
2n+1	2n+1	-8(I+J)

No. 225: O_h^5 - Fm3m

h, k, l all even or all odd	32(C+D)

No. 226: O_h^6 - Fm3c

h, k, l all even	32(C+D)
h, k, l all odd	32(C-D)

No. 227: O_h^7 - Fd3m

h+k	k+l	l+h	
4n	4n	4n	32(C+D)
4n	4n+2	4n+2	-32(E+F)
4n+2	4n	4n+2	-32(G+H)
4n+2	4n+2	4n	-32(I+J)
4n	4n	4n+2	16(C-E-G+I+D-F-H+J)
4n	4n+2	4n	16(C-E+G-I+D-F+H-J)
4n+2	4n	4n	16(C+E-G-I+D+F-H-J)
4n+2	4n+2	4n+2	-16(C+E+G+I+D+F+H+J)

No. 228: O_h^8 - Fd3c

h+k	k+l	l+h	
4n	4n	4n	32(C+D)
4n	4n+2	4n+2	-32(E+F)
4n+2	4n	4n+2	-32(G+H)
4n+2	4n+2	4n	-32(I+J)
4n	4n	4n+2	-16(C-E+G-I-D+F-H+J)
4n	4n+2	4n	-16(C+E-G-I-D-F+H+J)
4n+2	4n	4n	-16(C-E-G+I-D+F+H-J)
4n+2	4n+2	4n+2	-16(C+E+G+I-D-F-H-J)

No. 229: O_h^9 - Im3m

h + k + l = 2n	16(C+D)

No. 230: O_h^{10} - Ia3d

h	k	l	h+k+l	
2n	2n	2n	4n	16(C+D)
2n	2n+1	2n+1	4n	-16(I+F)
2n+1	2n	2n+1	4n	-16(E+H)
2n+1	2n+1	2n	4n	-16(G+J)
2n	2n	2n	4n+2	16(C-D)
2n	2n+1	2n+1	4n+2	-16(I-F)
2n+1	2n	2n+1	4n+2	-16(E-H)
2n+1	2n+1	2n	4n+2	-16(G-J)

triple product are listed. For example, the derivative of C ($C = c_1 + c_2 + c_3$) with respect to x is equal to $2\pi(-hm_1 - lq_2 - ko_3)$.

The geometrical structure factors for each set of parity conditions on the indices for every cubic space group are presented in Table 3 in terms of the sums of triple products defined in Table 1. The presentation follows that of *International Tables for X-ray Crystallography* (1952); in cases where the *International Tables* give a choice of origins, the origin is taken at a center. Corrections in O^7 and O_h^7 have been made as directed by the errata sheet.

For our programs we have utilized similarities in the structure factor expressions for different space groups. For example, the structure factor expressions for T^1, T^2, and T^3 are identical except for a different multiplicity factor; the same applies for space groups T_h^1, T_h^3, and T_h^5, O^1, O^3, and O^5, T_d^1, T_d^2, and T_d^3, and O_h^1, O_h^5, and O_h^9. Some pairs of space groups whose similarities have been utilized are T^4 and T^5, T_h^2 and T_h^4, T_h^4 and O_h^7, O^6 and O^7, O^8 and T_d^6, T_d^6 and O_h^{10}, O_h^2 and O_h^4, and O_h^7 and O_h^8.

We give one example to illustrate the use of the tables. Consider reflections $h+k=2n+1$, $k+l=2n+1$ in space group T_h^2. For the atoms in one set of general 24-fold positions,

$$
\begin{aligned}
F_c &= -8I = -8(i_1+i_2+i_3) \\
\partial F_c/\partial x &= -8(2\pi)(hq_1+lm_2-kk_3) \\
&= -8(2\pi)[h\cos(2\pi hx)\cos(2\pi ky)\sin(2\pi lz) \\
&\qquad + l\sin(2\pi hy)\cos(2\pi kz)\cos(2\pi lx) \\
&\qquad - k\sin(2\pi hz)\sin(2\pi kx)\sin(2\pi ly)]\,.
\end{aligned}
$$

We get F_c from Table 3, I from Table 1, and the derivatives from Table 2.

I thank Drs Richard E. Marsh and Sten Samson for helpful discussions and encouragement.

References

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Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (D. W. Smits, Mathematisch Instituut, University of Groningen, Reitdiepskade 4, Groningen, The Netherlands). Publicat.on of an item in a particular issue cannot be guaranteed unless the draft is received 8 weeks before the date of publication.

International Union of Crystallography

Acta Crystallographica

The Executive Committee of the Union and the Commission on *Acta Crystallographica* regret to announce that pressure of other work has caused the resignation of Professor E. W. Hughes as Co-editor of *Acta Crystallographica*. Professor Hughes was appointed in 1956 when the increasing number of papers offered for publicaiton in the journal made the appointment of a second U.S.A. Co-editor desirable. The Union is greatly indebted to him for his work for *Acta Crystallographica*, and in this way for the community of crystallographers.

The Executive Committee has approved the appointment of Dr R. E. Marsh, of the California Institute of Technology, as successor to Professor Hughes.