

1.9. ATOMIC DISPLACEMENT PARAMETERS

Atomic displacement tensors may also be partially contracted or expanded; rules for these operations are found in Kuhs (1992).

1.9.3. Site-symmetry restrictions

Atoms (or molecules) situated on special positions of a space group exhibit (time–space averaged) probability distributions with a symmetry corresponding to the site symmetry. The p.d.f.'s describing these distributions contain the atomic displacement tensors. The displacement tensors enter into the structure-factor equation, which is the Fourier transform of the scattering density of the unit cell, *via* the atomic Debye–Waller factor, which is the Fourier transform of the atomic p.d.f. (see Chapter 1.2 of *IT B*). As discussed above, the tensor is fully symmetric with respect to the interchange of indices (*inner symmetry*). The site-symmetry restrictions (*outer symmetry*) of atomic displacement tensors of rank 2 are given in Chapter 8.3 of *IT C* (2004), where the tabulation of the constraints on the tensor coefficients are quoted for every Wyckoff position in each space group. Here the constraints for atomic displacement tensors of ranks 2, 3, 4, 5 and 6 for any crystallographic site symmetry are tabulated; some restrictions for tensors of rank 7 and 8 can be found in Kuhs (1984). To use these tables, first the site symmetry has to be identified. The site symmetries are given in *IT A* (2005) for the first equipoint of every Wyckoff position in each space group. The tabulated constraints may be introduced in least-squares refinements (some programs have the constraints of second-order displacement tensor components already imbedded). It should also be remembered that, due to arbitrary phase shifts in the structure-factor equation in a least-squares refinement of a noncentrosymmetric structure, for all odd-order tensors *one* coefficient corresponding to a nonzero entry for the corresponding acentric space group has to be kept fixed (in very much the same way as for positional parameters); *e.g.* the term b^{123} has to be kept fixed for *one* atom for all refinements in all space groups belonging to the point groups $43m$ or 23 , while all other terms b^{ijk} are allowed to vary freely for all atoms (Hazell & Willis, 1978). Even if this is strictly true only for the Edgeworth-series expansion, it also holds in practice for the Gram–Charlier case (Kuhs, 1992).

1.9.3.1. Calculation procedures

Levy (1956) and Peterse & Palm (1966) have given algorithms for determining the constraints on anisotropic displacement tensor coefficients, which are also applicable to higher-order tensors. The basic idea is that a tensor transformation according to the symmetry operation of the site symmetry under consideration (represented by the point-group generators) should leave the tensor unchanged. For symmetries higher than the identity 1, this only holds true if some of the tensor coefficients are either zero or interrelated. The constraints may be obtained explicitly from solving the homogeneous system of equations of tensor transformations (with one equation for each coefficient).

1.9.3.2. Key to tables

After identification of the site symmetry of the atomic site under consideration, the entry point (cross-reference) for the tabulation of the displacement tensors of a given rank (Tables 1.9.3.2–1.9.3.6) needs to be looked up in Table 1.9.3.1. The line entry corresponding to the cross-reference number in Tables 1.9.3.2–1.9.3.6 holds the information on the constraints imposed by the outer symmetry on the tensor coefficients. The order of assignment of independency of the coefficients is as for increasing indices of the coefficients (first 1, then 2, then 3, where 1, 2 and 3 refer to the three crystallographic axes), except for the unmixed coefficients, which have highest priority in every case; this order of priority is the same as the order in the tables reading from left to right. For better readability, each coefficient is assigned a letter (or 0 if the component is equal to zero by symmetry). Constraints

Table 1.9.3.2. Symmetry restrictions on coefficients in second-order tensors

Cross-reference	No. of independent variables	Symbols and coefficient indices					
		A	B	C	D	E	F
		(1) (1)	(2) (2)	(3) (3)	(1) (2)	(1) (3)	(2) (3)
B1	1	A	A	A	0	0	0
B2	2	A	A	C	0	0	0
B3	2	A	B	A	0	0	0
B4	2	A	B	B	0	0	0
B5	2	A	A	A	D	D	D
B6	2	A	A	A	D	–D	–D
B7	2	A	A	A	D	–D	D
B8	2	A	A	A	D	D	–D
B9	2	A	A	C	A/2	0	0
B10	3	A	B	C	0	0	0
B11	3	A	A	C	D	0	0
B12	3	A	B	A	0	E	0
B13	3	A	B	B	0	0	F
B14	3	A	B	C	B/2	0	0
B15	3	A	B	C	A/2	0	0
B16	4	A	B	C	D	0	0
B17	4	A	B	C	0	E	0
B18	4	A	B	C	0	0	F
B19	4	A	A	C	D	E	–E
B20	4	A	A	C	D	E	E
B21	4	A	B	A	D	E	–D
B22	4	A	B	A	D	E	D
B23	4	A	B	B	D	–D	F
B24	4	A	B	B	D	D	F
B25	4	A	B	C	B/2	E	2E
B26	4	A	B	C	A/2	0	F
B27	4	A	B	C	B/2	E	0
B28	4	A	B	C	A/2	E	E/2
B29	6	A	B	C	D	E	F

thus read as algebraic relations between letter variables. Some more complicated constraint relations are quoted as footnotes to the tables.

1.9.4. Graphical representation

Atomic displacement tensors (ADTs) described by their tensor coefficients may be represented graphically to clarify their physical meaning. Different graphical representations exist and will be discussed separately for second- and higher-order tensors in the following.

1.9.4.1. Representation surfaces of second-order ADTs

Numerous examples of graphical representations of thermal-motion tensors (or, more generally speaking, atomic displacement tensors) have appeared in the literature since the early days of the computer program *ORTEP* written by C. K. Johnson (1965), yet the equal-probability surface usually displayed is only one of the possible representations of a second-order atomic displacement tensor. Representation surfaces are usually calculated in a Cartesian coordinate system. Accordingly, one has to transform the second-order ADT \mathbf{b} into \mathbf{U}_C described in a Cartesian frame:

$$\mathbf{U}_C = (2\pi^2)^{-1} \mathbf{F}^T \mathbf{b} \mathbf{F}. \quad (1.9.4.1)$$

The transformation matrix depends on the choice of Cartesian axes \mathbf{e}_i with respect to the reciprocal-cell axes \mathbf{a}^i (or equally well with respect to the direct axes \mathbf{a}_i). Choosing \mathbf{e}_1 along \mathbf{a}^1 , \mathbf{e}_2 in the $\mathbf{a}^1 \mathbf{a}^2$ plane and \mathbf{e}_3 completing the right-handed set, one obtains for the transformation matrix \mathbf{F} (see also Willis & Pryor, 1975)

$$\mathbf{F} = \begin{pmatrix} 1/a^1 & a^2 \cos \gamma^* & a^3 \cos \beta^* \\ 0 & a^2 \sin \gamma^* & -a^3 \sin \beta^* \cos \alpha \\ 0 & 0 & 1/a_3 \end{pmatrix}. \quad (1.9.4.2)$$

Clearly, there is an infinite number of possible choices for relating a Cartesian frame to a crystallographic coordinate

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

Table 1.9.3.3. *Symmetry restrictions on coefficients in third-rank symmetric polar tensors*

Cross-reference	No. of independent variables	Symbols and coefficient indices									
		A	B	C	D	E	F	G	H	I	J
		(1)	(2)	(3)	(1)	(1)	(1)	(1)	(2)	(2)	(1)
		(1)	(2)	(3)	(1)	(2)	(1)	(3)	(2)	(3)	(2)
C0	0	0	0	0	0	0	0	0	0	0	0
C1	1	0	0	0	0	0	0	0	0	0	J
C2	1	0	0	0	0	0	F	0	-F	0	0
C3	1	0	0	0	D	0	0	0	0	-D	0
C4	1	0	0	0	0	E	0	-E	0	0	0
C5	1	0	0	0	D	-D	-D	D	D	-D	0
C6	1	0	0	0	D	-D	D	D	-D	-D	0
C7	1	0	0	0	D	D	D	-D	-D	-D	0
C8	1	0	0	0	D	D	-D	-D	D	-D	0
C9	1	0	0	0	D	D	0	0	0	0	0
C10	1	A	-A	0	A/2	-A/2	0	0	0	0	0
C11	1	0	0	0	0	0	F	0	0	0	F
C12	1	0	0	0	0	0	0	0	H	0	H
C13	2	0	0	C	0	0	F	0	F	0	0
C14	2	0	B	0	D	0	0	0	0	D	0
C15	2	A	0	0	0	E	0	E	0	0	0
C16	2	0	0	0	0	0	F	0	-F	0	J
C17	2	0	0	0	D	0	0	0	0	-D	J
C18	2	0	0	0	0	E	0	-E	0	0	J
C19	2	0	0	C	0	0	F	0	F	0	F/2
C20	2	A	-A	0	D	D - A	0	0	0	0	0
C21	3	0	0	C	0	0	F	0	H	0	0
C22	3	0	0	C	0	0	F	0	F	0	J
C23	3	0	B	0	D	0	0	0	0	I	0
C24	3	0	B	0	D	0	0	0	0	D	J
C25	3	A	0	0	0	E	0	G	0	0	0
C26	3	A	0	0	0	E	0	E	0	0	J
C27	3	A	A	0	D	D	0	G	0	G	0
C28	3	A	-A	0	D	-D	0	G	0	-G	0
C29	3	A	0	A	0	E	F	F	E	0	0
C30	3	A	0	-A	0	E	F	-F	-E	0	0
C31	3	0	B	B	D	0	D	0	H	H	0
C32	3	0	B	-B	D	0	-D	0	H	-H	0
C33	3	A	A	A	D	D	D	D	D	D	J
C34	3	A	A	-A	D	D	-D	D	-D	D	J
C35	3	A	-A	A	D	-D	-D	-D	-D	D	J
C36	3	A	-A	-A	D	-D	D	-D	D	D	J
C37	3	A	-A	C	A/2	-A/2	F	0	F	0	F/2
C38	3	0	0	C	D	D	F	0	F	0	F/2
C39	3	0	0	C	0	0	F	0	H	0	F/2
C40	3	0	0	C	0	0	F	0	H	0	H/2
C41	3	A	0	0	D	D	0	G	0	0	0
C42	3	A	B	0	A/2	A/6 + 2B/3	0	G	0	G/2	0
C43	3	A	B	0	B/6 + 2A/3	B/2	0	G	0	2G	0
C44	3	0	B	0	D	D	0	0	0	I	0
C45	4	0	0	C	0	0	F	0	H	0	J
C46	4	0	B	0	D	0	0	0	0	I	J
C47	4	A	0	0	0	E	0	G	0	0	J
C48	4	A	A	0	D	D	F	G	-F	G	0
C49	4	A	-A	0	D	-D	F	G	-F	-G	0
C50	4	A	0	A	D	E	F	F	E	-D	0
C51	4	A	0	-A	D	E	F	-F	-E	-D	0
C52	4	0	B	-B	D	E	D	-E	H	H	0
C53	4	0	B	-B	D	E	-D	-E	H	-H	0
C54	4	A	A	A	D	E	E	D	D	E	J
C55	4	A	A	-A	D	E	-E	D	-D	E	J
C56	4	A	-A	A	D	E	E	-D	-D	-E	J
C57	4	A	-A	-A	D	E	-E	-D	D	-E	J
C58	4	A	-A	C	D	D - A	F	0	F	0	F/2
C59	4	A	0	0	D	D	F	G	0	0	F
C60	4	A	B	0	A/2	A/6 + 2B/3	0	G	H	G/2	H
C61	4	A	B	0	B/6 + 2A/3	B/2	F	G	0	2G	F
C62	4	0	B	0	D	D	0	0	H	I	H
C63	6	A	B	0	D	E	0	G	0	I	0
C64	6	A	0	C	0	0	F	G	H	0	0
C65	6	0	B	C	D	0	F	0	H	I	0
C66	6	A	-A	C	D	-D	F	G	F	-G	J
C67	6	A	A	C	D	D	F	G	F	G	J
C68	6	A	B	-A	D	E	F	-F	-E	D	J
C69	6	A	B	A	D	E	F	F	E	D	J
C70	6	A	B	-B	D	E	-D	E	H	-H	J
C71	6	A	B	B	D	E	D	E	H	H	J
C72	6	A	B	C	B/6 + 2A/3	B/2	F	G	H	2G	H/2
C73	6	0	B	C	D	D	F	0	H	I	F/2
C74	6	A	0	C	D	D	F	G	H	0	H/2
C75	6	A	B	C	A/2	A/6 + 2B/3	F	G	H	G/2	F/2
C76	10	A	B	C	D	E	F	G	H	I	J

1.9. ATOMIC DISPLACEMENT PARAMETERS

Table 1.9.3.4. Symmetry restrictions on coefficients in fourth-rank symmetric polar tensors

(a) A-H.

Cross-reference	No. of independent variables	Symbols and coefficient indices							
		A	B	C	D	E	F	G	H
		(1)	(2)	(3)	(1)	(1)	(1)	(1)	(1)
		(1)	(2)	(3)	(1)	(1)	(1)	(1)	(1)
		(1)	(2)	(3)	(2)	(3)	(2)	(3)	
D1	2	A	A	A	0	0	F	0	F
D2	3	A	A	C	A/2	0	A/2	0	H
D3	4	A	A	C	0	0	F	0	H
D4	4	A	B	A	0	0	F	0	H
D5	4	A	B	B	0	0	F	0	F
D6	4	A	A	A	D	D	F	G	F
D7	4	A	A	A	D	-D	F	G	F
D8	4	A	A	A	D	-D	F	G	F
D9	4	A	A	A	D	D	F	G	F
D10	4	A	A	C	A/2	E	A/2	E/2	H
D11	4	A	A	C	A/2	0	A/2	G	H
D12	5	A	A	C	D	0	F	0	H
D13	5	A	B	A	0	E	F	0	H
D14	5	A	B	B	0	0	F	0	F
D15	5	A	A	A	D	E	F	G	F
D16	5	A	A	A	D	E	F	G	F
D17	5	A	A	A	D	E	F	G	F
D18	5	A	A	A	D	E	F	G	F
D19	5	A	A	C	A/2	E	A/2	G	H
D20	6	A	B	C	0	0	F	0	H
D21	6	A	A	C	D	0	F	0	H
D22	6	A	B	A	0	E	F	0	H
D23	6	A	B	B	0	0	F	G	F
D24	6	A	B	C	D	0	B/6 + 2D/3	0	H
D25	6	A	B	C	A/2	0	F	0	H
D26	9	A	B	C	D	0	F	0	H
D27	9	A	B	C	0	E	F	0	H
D28	9	A	B	C	0	0	F	G	H
D29	9	A	A	C	D	E	F	G	H
D30	9	A	A	C	D	E	F	G	H
D31	9	A	B	A	D	E	F	G	H
D32	9	A	B	A	D	E	F	G	H
D33	9	A	B	B	D	-D	F	G	F
D34	9	A	B	B	D	D	F	G	F
D35	9	A	B	C	D	E	B/6 + 2D/3	G	H
D36	9	A	B	C	A/2	0	F	G	H
D37	9	A	B	C	D	E	B/6 + 2D/3	G	H
D38	9	A	B	C	A/2	E	F	E/2	H
D39	15	A	B	C	D	E	F	G	H

(b) I-P.

Cross-reference	No. of independent variables	Symbols and coefficient indices						
		I	J	K	L	M	N	P
		(1)	(1)	(1)	(1)	(2)	(2)	(2)
		(2)	(2)	(2)	(3)	(2)	(2)	(3)
		(2)	(3)	(3)	(3)	(3)	(3)	
D1	2	0	0	0	0	0	F	0
D2	3	A/2	0	H/2	0	0	H	0
D3	4	0	0	0	0	0	H	0
D4	4	0	0	0	0	0	F	0
D5	4	0	0	0	0	0	N	0
D6	4	D	G	G	D	D	F	D
D7	4	D	G	-G	-D	-D	F	-D
D8	4	D	-G	G	-D	D	F	D
D9	4	D	-G	-G	D	-D	F	-D
D10	4	A/2	-E/2	H/2	0	-E	H	0
D11	4	A/2	G	H/2	0	0	H	0
D12	5	-D	0	0	0	0	H	0
D13	5	0	0	0	-E	0	F	0
D14	5	0	0	0	0	M	N	-M
D15	5	E	G	G	D	D	F	E
D16	5	-E	G	-G	-D	-D	F	-E
D17	5	-E	-G	G	-D	D	F	E
D18	5	E	-G	-G	D	-D	F	-E
D19	5	A/2	G - E	H/2	0	-E	H	0
D20	6	0	0	0	0	0	N	0
D21	6	D	0	K	0	0	H	0
D22	6	0	J	0	E	0	F	0
D23	6	0	0	0	0	M	N	M
D24	6	B/2	0	K	0	0	2K	0

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

Table 1.9.3.4 (cont.)

Cross-reference	No. of independent variables	Symbols and coefficient indices							
		I (1) (2) (2) (2)	J (1) (2) (2) (3)	K (1) (2) (3) (3)	L (1) (3) (3) (3)	M (2) (2) (2) (3)	N (2) (2) (3) (3)	P (2) (3) (3) (3)	
D25	6	$-A/4 + 3F/2$	0	H/2	0	0	N	0	
D26	9	I	0	K	0	0	N	0	
D27	9	0	J	0	L	0	N	0	
D28	9	0	0	0	0	M	N	P	
D29	9	D	$-G$	K	L	$-E$	H	$-L$	
D30	9	D	G	K	L	E	H	L	
D31	9	I	J	$-G$	E	$-I$	F	$-D$	
D32	9	I	J	G	E	I	F	D	
D33	9	I	J	$-J$	$-I$	M	N	M	
D34	9	I	J	J	I	M	N	M	
D35	9	B/2	$-E/8 + 3G$	K	L	$-E/4 + 6G$	2K	2L	
D36	9	$-A/4 + 3F/2$	G	H/2	0	M	N	P	
D37	9	B/2	G	K	L	0	2K	0	
D38	9	$-A/4 + 3F/2$	J	H/2	L	$-E/4 + 3J/2$	N	L/2	
D39	15	I	J	K	L	M	N	P	

Table 1.9.3.5. Symmetry restrictions on coefficients in fifth-rank symmetric polar tensors

(a) A-K.

Cross-reference	No. of independent coefficients	Symbols and coefficient indices										
		A	B	C	D	E	F	G	H	I	J	K
E0	0	0	0	0	0	0	0	0	0	0	0	0
E1	1	0	0	0	0	0	G	0	0	0	0	0
E2	1	0	0	0	0	0	G	0	0	0	0	0
E3	1	0	0	0	0	0	G	0	0	0	0	0
E4	1	0	0	0	0	0	0	0	0	0	0	0
E5	2	0	0	0	D	0	D	0	D	0	K	0
E6	2	A	$-A$	0	A/2	0	A/10	0	H	$-A/10$	0	H/2
E7	2	0	0	0	0	0	G	0	0	0	0	0
E8	2	0	0	0	0	E	0	0	0	0	0	0
E9	2	0	0	0	0	0	G	0	0	0	0	0
E10	2	0	0	0	D	0	0	0	I	0	0	0
E11	2	0	0	0	0	0	G	0	0	0	0	0
E12	2	0	0	0	0	F	0	$-F$	0	0	0	0
E13	2	0	0	0	D	$-D$	F	0	$-F$	$-F$	0	0
E14	2	0	0	0	D	D	F	0	$-F$	$-F$	0	0
E15	2	0	0	0	D	D	F	0	$-F$	F	0	0
E16	2	0	0	0	D	$-D$	F	0	$-F$	F	0	0
E17	3	0	0	C	0	E	0	E/2	0	0	E/2	0
E18	3	0	0	0	0	0	G	0	0	0	0	0
E19	3	0	0	0	0	E	0	G	0	0	0	0
E20	3	0	0	0	D	0	0	G	0	I	0	0
E21	3	0	0	0	0	0	F	0	$-F$	0	0	0
E22	3	0	0	0	0	0	G	0	0	2G	0	0
E23	3	0	0	0	0	0	G	0	0	G	0	0
E24	4	A	$-A$	0	D	0	(1)†	0	H	(3)†	0	K
E25	4	0	0	C	0	E	0	0	0	0	J	0
E26	4	0	B	0	D	0	0	0	0	I	0	K
E27	4	A	0	0	0	0	F	0	F	0	0	0
E28	4	0	0	0	0	E	0	G	0	0	0	0
E29	4	0	0	0	D	0	0	G	0	I	0	0
E30	4	0	0	0	0	0	F	G	$-F$	0	0	0
E31	5	0	0	C	0	E	0	G	0	0	J	0
E32	5	0	B	0	D	0	0	G	0	I	0	K
E33	5	A	0	0	0	0	F	0	F	0	0	0
E34	5	A	A	A	D	D	F	G	F	F	J	J
E35	5	A	A	$-A$	D	$-D$	F	G	F	F	J	$-J$
E36	5	A	$-A$	A	D	$-D$	F	G	F	$-F$	J	$-J$
E37	5	A	$-A$	$-A$	D	D	F	G	F	$-F$	J	J
E38	5	A	$-A$	C	A/2	E	A/10	E/2	H	$-A/10$	E/2	H/2
E39	5	0	0	C	D	E	D	E/2	0	D	E/2	K
E40	6	0	0	C	0	E	0	0	0	0	J	0
E41	6	0	0	C	0	E	0	G	0	0	J	0
E42	6	0	B	0	D	0	0	0	0	I	0	K
E43	6	0	B	0	D	0	0	0	0	I	0	K
E44	6	A	0	0	0	0	F	0	H	0	0	0
E45	6	A	0	0	0	0	F	G	H	0	0	0
E46	6	A	$-A$	0	D	0	F	0	H	F	0	K

1.9. ATOMIC DISPLACEMENT PARAMETERS

Table 1.9.3.5 (cont.)

Cross-reference	No. of independent coefficients	Symbols and coefficient indices										
		A	B	C	D	E	F	G	H	I	J	K
		1	2	3	1	1	1	1	1	1	1	1
		1	2	3	1	1	1	1	1	1	1	1
		1	2	3	1	1	1	1	1	1	1	1
		1	2	3	1	1	1	1	1	2	2	2
		1	2	3	1	1	2	2	3	2	2	3
		1	2	3	2	3	2	3	3	2	3	3
E47	6	A	-A	0	D	0	F	0	H	-F	0	K
E48	6	A	0	A	0	E	F	0	H	0	J	0
E49	6	A	0	-A	0	E	F	0	H	0	G	0
E50	6	0	B	B	D	D	0	0	0	I	J	J
E51	6	0	B	-B	D	-D	0	0	0	I	J	-J
E52	6	0	0	C	0	E	0	G	0	0	J	0
E53	6	0	0	C	0	E	0	E/2	0	0	J	0
E54	6	A	0	0	D	0	F	0	H	(4)†	0	K
E55	6	A	B	0	A/2	0	F	0	H	(5)†	0	H/2
E56	6	A	B	0	D	0	(2)†	0	H	(6)†	0	K
E57	6	0	B	0	D	0	D	0	0	I	0	K
E58	7	A	A	A	D	E	F	G	H	H	J	J
E59	7	A	A	-A	D	E	F	G	H	H	J	-J
E60	7	A	-A	A	D	E	F	G	H	-H	J	-J
E61	7	A	-A	-A	D	E	F	G	H	-H	J	J
E62	7	A	-A	C	D	E	(1)†	E/2	H	(3)†	E/2	K
E63	9	0	0	C	0	E	0	G	0	0	J	0
E64	9	0	B	0	D	0	0	G	0	I	0	K
E65	9	A	0	0	0	0	F	G	H	0	0	0
E66	9	A	A	0	D	E	F	G	H	F	0	K
E67	9	A	-A	0	D	E	F	G	H	-F	0	K
E68	9	A	0	A	D	E	F	G	H	I	J	0
E69	9	A	0	-A	D	E	F	G	H	I	J	0
E70	9	0	B	B	D	D	F	0	-F	I	J	J
E71	9	0	B	-B	D	-D	F	0	-F	I	J	-J
E72	9	A	0	0	D	E	F	G	H	(4)†	2G	K
E73	9	A	B	0	A/2	0	F	G	H	(5)†	G	H/2
E74	9	A	B	0	D	E	(2)†	G	H	(6)†	2G	K
E75	9	0	B	0	D	0	D	G	0	I	G	K
E76	12	A	B	0	D	0	F	0	H	I	0	K
E77	12	A	0	C	0	E	F	0	H	0	J	0
E78	12	0	B	C	D	E	0	0	0	I	J	K
E79	12	A	-A	C	D	E	F	G	H	-F	J	K
E80	12	A	A	C	D	E	F	G	H	F	J	K
E81	12	A	B	-A	D	E	F	G	H	I	J	K
E82	12	A	B	A	D	E	F	G	H	I	J	K
E83	12	A	B	-B	D	-D	F	G	F	I	J	-J
E84	12	A	B	B	D	D	F	G	F	I	J	J
E85	12	A	B	C	D	E	(2)†	G	H	(6)†	J	K
E86	12	0	B	C	D	E	D	E/2	0	I	J	K
E87	12	A	0	C	D	E	F	G	H	(4)†	J	K
E88	12	A	B	C	A/2	E	F	E/2	H	(5)†	J	H/2
E89	21	A	B	C	D	E	F	G	H	I	J	K

(b) L-V.

Cross-reference	No. of independent coefficients	Symbols and coefficient indices									
		L	M	N	P	Q	R	S	T	U	V
		1	1	1	1	1	1	1	2	2	2
		1	2	2	2	2	3	2	2	2	3
		3	2	2	2	3	3	2	2	3	3
		3	2	2	3	3	3	2	3	3	3
		3	2	3	3	3	3	3	3	3	3
E0	0	0	0	0	0	0	0	0	0	0	0
E1	1	0	0	G	0	G	0	0	0	0	0
E2	1	0	0	-G	0	0	0	0	0	0	0
E3	1	0	0	0	0	-G	0	0	0	0	0
E4	1	0	0	N	0	-N	0	0	0	0	0
E5	2	0	D	0	K	0	0	0	0	0	0
E6	2	0	-A/2	0	-H/2	0	0	0	0	-H	0
E7	2	0	0	G	0	Q	0	0	0	0	0
E8	2	L	0	0	0	0	0	-E	0	-L	0
E9	2	0	0	N	0	G	0	0	0	0	0
E10	2	0	0	0	0	0	0	0	-I	0	-D
E11	2	0	0	N	0	N	0	0	0	0	0
E12	2	0	M	0	0	0	-M	0	0	0	0
E13	2	F	-D	0	0	0	D	D	F	-F	-D
E14	2	-F	-D	0	0	0	D	-D	F	F	-D
E15	2	F	D	0	0	0	-D	-D	-F	-F	-D
E16	2	-F	D	0	0	0	-D	D	-F	F	-D
E17	3	L	0	E/2	0	L/2	0	E	0	L	0
E18	3	0	0	N	0	Q	0	0	0	0	0
E19	3	L	0	-G	0	0	0	-E	0	-L	0

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

Table 1.9.3.5 (cont.)

Cross-reference	No. of independent coefficients	Symbols and coefficient indices									
		L	M	N	P	Q	R	S	T	U	V
		1	1	1	1	1	1	2	2	2	2
		1	2	2	2	2	3	2	2	2	3
		3	2	2	2	3	3	2	2	3	3
		3	2	2	3	3	3	2	3	3	3
		3	2	3	3	3	3	3	3	3	3
E20	3	0	0	0	0	-G	0	0	-I	0	-D
E21	3	0	M	N	0	-N	-M	0	0	0	0
E22	3	L	0	2G	0	L	0	S	0	0	0
E23	3	0	0	N	0	Q	0	(14)†	0	Q	0
E24	4	0	(7)†	0	(13)†	0	0	0	-H	0	0
E25	4	L	0	0	0	0	0	E	0	L	0
E26	4	0	0	0	0	0	0	0	I	0	D
E27	4	0	M	0	P	0	M	0	0	0	0
E28	4	L	0	G	0	Q	0	-E	0	-L	0
E29	4	0	0	N	0	G	0	0	-I	0	-D
E30	4	0	M	N	0	N	-M	0	0	0	0
E31	5	L	0	-G	0	0	0	E	0	L	0
E32	5	0	0	0	0	-G	0	0	I	0	D
E33	5	0	M	N	P	-N	M	0	0	0	0
E34	5	F	D	G	J	G	D	D	F	F	D
E35	5	-F	D	G	-J	G	D	-D	F	-F	D
E36	5	F	-D	G	J	G	-D	-D	--F	F	D
E37	5	-F	-D	G	-J	G	-D	D	-F	-F	D
E38	5	L	-A/2	E/2	-H/2	L/2	0	E	-H	L	0
E39	5	L	D	E/2	K	L/2	0	E	0	L	0
E40	6	L	0	0	0	0	0	S	0	U	0
E41	6	L	0	G	0	Q	0	E	0	L	0
E42	6	0	0	0	0	0	0	0	T	0	V
E43	6	0	0	N	0	G	0	0	I	0	D
E44	6	0	M	0	P	0	R	0	0	0	0
E45	6	0	M	N	P	N	M	0	0	0	0
E46	6	0	D	0	K	0	R	0	H	0	R
E47	6	0	-D	0	-K	0	R	0	-H	0	-R
E48	6	H	M	0	J	0	E	M	0	F	0
E49	6	-H	M	0	-J	0	-E	-M	0	-F	0
E50	6	I	0	0	0	0	0	S	T	T	S
E51	6	-I	0	0	0	0	0	S	T	-T	-S
E52	6	L	0	(10)†	0	Q	0	(15)†	0	2Q	0
E53	6	L	0	(11)†	0	L/2	0	S	0	U	0
E54	6	0	(4)†	0	K	0	R	0	0	0	0
E55	6	0	(8)†	0	P	0	R	0	(16)†	0	R/2
E56	6	0	B/2	0	(12)†	0	R	0	(17)†	0	2R
E57	6	0	(9)†	0	K	0	0	0	T	0	V
E58	7	F	E	G	J	G	D	D	F	H	E
E59	7	-F	-E	G	-J	G	D	-D	F	-H	-E
E60	7	F	E	G	J	G	-D	-D	-F	H	-E
E61	7	-F	-E	G	-J	G	-D	D	-F	-H	E
E62	7	L	(7)†	E/2	(13)†	L/2	0	E	-H	L	0
E63	9	L	0	N	0	Q	0	S	0	U	0
E64	9	0	0	N	0	Q	0	0	T	0	V
E65	9	0	M	N	P	Q	R	0	0	0	0
E66	9	L	D	-G	K	0	R	-E	H	-L	R
E67	9	L	-D	-G	-K	0	R	-E	-H	-L	-R
E68	9	H	M	0	J	-G	E	M	-I	F	-D
E69	9	-H	M	0	-J	-G	-E	-M	-I	-F	-D
E70	9	I	M	N	0	-N	-M	S	T	T	S
E71	9	-I	M	N	0	-N	-M	S	T	-T	-S
E72	9	L	(4)†	2G	K	L	R	0	0	0	0
E73	9	0	(8)†	N	P	Q	R	(14)†	(16)†	Q	R/2
E74	9	L	B/2	2G	(12)†	L	R	0	(17)†	0	2R
E75	9	0	(9)†	N	K	Q	0	(14)†	T	Q	V
E76	12	0	M	0	P	0	R	0	T	0	V
E77	12	L	M	0	P	0	R	S	0	U	0
E78	12	L	0	0	0	0	0	S	T	U	V
E79	12	L	-D	G	-K	Q	R	E	-H	L	-R
E80	12	L	D	G	J	Q	R	E	H	L	R
E81	12	-H	M	N	-J	G	-E	-M	I	-F	D
E82	12	H	M	N	J	G	E	M	I	F	D
E83	12	-I	M	N	P	N	M	S	T	-T	-S
E84	12	I	M	N	P	N	M	S	T	T	S
E85	12	L	B/2	(10)†	(12)†	N	M	(15)†	(17)†	2N	2M
E86	12	L	2I	(11)†	K	L/2	0	S	T	U	V
E87	12	L	(4)†	(10)†	K	N	M	(15)†	0	2N	0
E88	12	L	(8)†	(11)†	P	L/2	R	S	(16)†	U	U/2
E89	21	L	M	N	P	Q	R	S	T	U	V

† (1) $-2A/5 + D$; (2) $-3A/5 + B/10 + 3D/2$; (3) $-3A/5 + D$; (4) $-D + 2F$; (5) $-A/4 + 3F/2$; (6) $-2A/5 + B/5 + D$; (7) $-A + D$; (8) $-A/5 + 2B/5 + F$; (9) $-D + 2I$; (10) $-2G + 3J$; (11) $-E/4 + 3J/2$; (12) $-2H + 3K$; (13) $-H + K$; (14) $-G + 2N$; (15) $-4G + 6J$; (16) $-H/4 + 3P/2$; (17) $-4H + 6K$.

1.9. ATOMIC DISPLACEMENT PARAMETERS

Table 1.9.3.6. Symmetry restrictions on coefficients in sixth-rank symmetric polar tensors

(a) A-N.

Cross-reference	No. of independent parameters	Symbols and coefficient indices													
		A	B	C	D	E	F	G	H	I	J	K	L	M	N
		1	2	3	1	1	1	1	1	1	1	1	1	1	1
		1	2	3	1	1	1	1	1	1	1	1	1	1	
		1	2	3	1	1	1	1	1	1	1	1	1	1	
		1	2	3	1	1	1	1	1	1	1	1	2	2	
		1	2	3	1	1	1	1	2	2	2	3	2	2	
		1	2	3	1	1	2	2	3	2	2	3	2	2	
		1	2	3	2 <th>3</th> <th>2</th> <th>3</th> <th>3</th> <th>2</th> <th>3</th> <th>3</th> <th>2</th> <th>3</th>	3	2	3	3	2	3	3	2	3	
F1	3	A	A	A	0	0	F	0	F	0	0	0	F	0	
F2	4	A	A	A	0	0	F	0	H	0	0	0	H	0	
F3	5	A	A	C	A/2	0	F	0	H	(1)†	0	H/2	0	F	
F4	6	A	A	C	D	0	F	0	H	(2)†	0	H/2	0	(5)†	
F5	6	A	A	C	0	0	F	0	H	0	0	0	F	0	
F6	6	A	B	A	0	0	F	0	H	0	0	0	M	0	
F7	6	A	B	B	0	0	F	0	F	0	0	0	M	0	
F8	7	A	A	A	D	D	F	G	F	I	J	J	I	F	
F9	7	A	A	A	D	-D	F	G	F	I	J	-J	-I	F	
F10	7	A	A	A	D	-D	F	G	F	I	J	-J	-I	F	
F11	7	A	A	A	D	D	F	G	F	I	J	J	I	F	
F12	7	A	A	C	A/2	E	F	E/2	H	(1)†	E/10	H/2	I	F	
F13	7	A	A	C	A/2	0	F	G	H	(1)†	G	H/2	0	F	
F14	8	A	A	C	D	0	F	0	H	0	0	K	0	F	
F15	8	A	B	A	0	E	F	0	H	0	J	0	0	M	
F16	8	A	B	B	0	0	F	0	H	0	0	0	0	M	
F17	10	A	A	A	D	E	F	G	H	I	J	K	I	H	
F18	10	A	A	A	D	E	F	G	H	I	J	K	-I	H	
F19	10	A	A	A	D	E	F	G	H	I	J	K	-I	H	
F20	10	A	A	A	D	E	F	G	H	I	J	K	I	H	
F21	10	A	A	C	D	E	F	G	H	(2)†	(4)†	H/2	L	(5)†	
F22	10	A	B	C	0	0	F	0	H	0	0	0	0	M	
F23	10	A	A	C	D	0	F	0	H	I	0	K	0	F	
F24	10	A	B	A	0	E	F	0	H	0	J	0	L	M	
F25	10	A	B	B	0	0	F	G	F	0	0	0	0	M	
F26	10	A	B	C	D	0	F	0	H	(3)†	0	K	0	(6)†	
F27	10	A	B	C	A/2	0	F	0	H	(1)†	0	H/2	0	M	
F28	16	A	B	C	D	0	F	0	H	I	0	K	0	M	
F29	16	A	B	C	0	E	F	0	H	0	J	0	L	M	
F30	16	A	B	C	0	0	F	G	H	0	0	0	0	M	
F31	16	A	A	C	D	E	F	G	H	I	J	K	L	F	
F32	16	A	A	C	D	E	F	G	H	I	J	K	L	F	
F33	16	A	B	A	D	E	F	G	H	I	J	K	L	M	
F34	16	A	B	A	D	E	F	G	H	I	J	K	L	M	
F35	16	A	B	B	D	-D	F	G	F	I	J	-J	-I	M	
F36	16	A	B	B	D	D	F	G	F	I	J	J	I	M	
F37	16	A	B	C	D	E	F	G	H	(3)†	J	K	L	(6)†	
F38	16	A	B	C	A/2	0	F	G	H	(1)†	G	H/2	0	M	
F39	16	A	B	C	D	E	F	G	H	(3)†	J	K	L	(6)†	
F40	16	A	B	C	A/2	E	F	E/2	H	(1)†	J	H/2	L	M	
F41	28	A	B	C	D	E	F	G	H	I	J	K	L	M	

(b) P-c.

Cross-reference	No. of independent parameters	Symbols and coefficient indices													
		P	Q	R	S	T	U	V	W	X	Y	Z	a	b	c
		1	1	1	1	1	1	1	1	1	2	2	2	2	2
		1	1	1	2	2	2	2	2	3	2	2	2	2	
		2	2	3	2	2	2	2	3	3	2	2	2	3	
		2	3	3	2	2	2	3	3	3	2	2	3	3	
		3	3	3	2	2	3	3	3	3	2	3	3	3	
		3	3	3	2	3	3	3	3	3	3	3	3	3	
F1	3	P	0	F	0	0	0	0	0	0	0	F	0	F	
F2	4	P	0	F	0	0	0	0	0	0	0	F	0	H	
F3	5	H/2	0	R	A/2	0	H/2	0	R/2	0	0	H	0	R	
F4	6	H/2	0	R	(11)†	0	H/2	0	R/2	0	0	H	0	R	
F5	6	P	0	R	0	0	0	0	0	0	0	H	0	R	
F6	6	P	0	H	0	0	0	0	0	0	0	M	0	F	
F7	6	P	0	M	0	0	0	0	0	0	0	Z	0	Z	
F8	7	P	J	F	D	G	J	J	G	D	D	F	I	F	
F9	7	P	J	F	D	G	-J	J	-G	-D	-D	F	-I	F	
F10	7	P	-J	F	D	-G	-J	-J	G	-D	D	F	I	F	
F11	7	P	-J	F	D	-G	J	-J	-G	D	-D	F	-I	F	
F12	7	H/2	I/2	R	A/2	-E/2	H/2	-I/2	R/2	0	-E	H	-I	R	
F13	7	H/2	Q	R	A/2	G	H/2	Q	R/2	0	0	H	0	R	
F14	8	P	0	R	-D	0	-K	0	0	0	0	H	0	R	
F15	8	P	0	H	0	0	0	-J	0	-E	0	M	0	F	
F16	8	P	-N	M	0	0	0	0	0	0	Y	Z	0	Z	
F17	10	P	J	F	E	G	J	K	G	D	D	F	I	H	
F18	10	P	J	F	-E	G	-J	-K	-G	-D	-D	F	-I	H	

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

Table 1.9.3.6 (cont.)

Cross-reference	No. of independent parameters	Symbols and coefficient indices													
		P	Q	R	S	T	U	V	W	X	Y	Z	a	b	c
		1	1	1	1	1	1	1	1	1	2	2	2	2	2
		1	1	1	2	2	2	2	3	3	2	2	2	2	3
		2	2	3	2	2	2	2	3	3	2	2	2	3	3
		2	3	3	2	2	2	3	3	3	2	2	3	3	3
		3	3	3	2	2	3	3	3	3	2	3	3	3	3
		3	3	3	2	3	3	3	3	3	3	3	3	3	3
F19	10	P	-J	F	-E	-G	-J	-K	G	-D	D	F	I	H	-E
F20	10	P	-J	F	E	-G	J	K	-G	D	-D	F	-I	H	-E
F21	10	H/2	Q	R	(11)†	(13)†	H/2	(18)†	R/2	0	-E	H	-L	R	0
F22	10	P	0	R	0	0	0	0	0	0	0	Z	0	b	0
F23	10	P	0	R	D	0	K	0	W	0	0	H	0	R	0
F24	10	P	0	H	0	T	0	J	0	E	0	M	0	F	0
F25	10	P	N	M	0	0	0	0	0	0	Y	Z	a	Z	Y
F26	10	P	0	R	B/2	0	(16)†	0	W	0	0	(22)†	0	2W	0
F27	10	P	0	R	(12)†	0	(17)†	0	R/2	0	0	Z	0	b	0
F28	16	P	0	R	S	0	U	0	W	0	0	Z	0	b	0
F29	16	P	0	R	0	T	0	V	0	X	0	Z	0	b	0
F30	16	P	Q	R	0	0	0	0	0	0	Y	Z	a	b	c
F31	16	P	Q	R	D	-G	K	-Q	W	X	-E	H	-L	R	-X
F32	16	P	Q	R	D	G	K	Q	W	X	E	H	L	R	X
F33	16	P	-K	H	S	T	-N	J	-G	E	-S	M	-I	F	-D
F34	16	P	K	H	S	T	N	J	G	E	S	M	I	F	D
F35	16	P	N	M	S	T	U	-U	-T	-S	Y	Z	a	Z	Y
F36	16	P	N	M	S	T	U	U	T	S	Y	Z	a	Z	Y
F37	16	P	Q	R	B/2	(14)†	(16)†	(19)†	W	X	(20)†	(22)†	(23)†	2W	2X
F38	16	P	Q	R	(12)†	(15)†	(17)†	Q	R/2	0	Y	Z	a	b	c
F39	16	P	Q	R	B/2	(9)†	(16)†	Q	W	X	0	(22)†	0	2W	0
F40	16	P	L/2	R	(12)†	T	(17)†	V	R/2	X	(21)†	Z	(24)†	b	X/2
F41	28	P	Q	R	S	T	U	V	W	X	Y	Z	a	b	c

† (1) $-A/4 + F/2$; (2) $A/2 - 3D/2 + 3F/2$; (3) $B/20 - 3D/5 + 3F/2$; (4) $-2E/5 + G$; (5) $A - 2D + F$; (6) $B/5 - 2D/5 + F$; (7) $-3E/5 + G$; (8) $2E - 5G + 4J$; (9) $-G + 2J$; (10) $-E/4 + 3J/2$; (11) $A - D$; (12) $A/2 - 5F/2 + 5M/2$; (13) $-E + G$; (14) $6E - 15G + 10J$; (15) $-G + 2N$; (16) $-2K + 3P$; (17) $-H/4 + 3P/2$; (18) $-L + Q$; (19) $-2L + 3Q$; (20) $12E - 30G + 20J$; (21) $E/2 - 5J/2 + 5T/2$; (22) $-4K + 6P$; (23) $-4L + 6Q$; (24) $-L/4 + 3V/2$.

system with correspondingly different transformation matrices \mathbf{F} (see e.g. Chapter 1.1 of *IT B*). The most useful representation surface of the second-order atomic displacement tensor \mathbf{U}_C is the representation quadric defined by the tensor invariant

$${}^2I_0 = \mathbf{u}^T \mathbf{U}_C^{-1} \mathbf{u} \quad (1.9.4.3)$$

where \mathbf{u} is a displacement vector; \mathbf{U}^{-1} is often called the *variance-covariance matrix* and has (in a general axes frame) covariant components. Under the conditions of *positive definiteness*,

$$\left. \begin{array}{l} \text{Det}(\mathbf{U}_C) \\ \mathbf{U}_C^{ij} \end{array} \right\} \text{all positive,} \quad (1.9.4.4)$$

$$\mathbf{U}_C^{ii} \mathbf{U}_C^{jj} - \mathbf{U}_C^{ij} \mathbf{U}_C^{ji} \text{ (no summation)}$$

the surface of the representation quadric is an ellipsoid whose semi-major axes (for ${}^2I_0 = 0$) are of lengths equal to the root-mean-square displacements (r.m.s.d.'s) along the axes directions. The *thermal vibration ellipsoids* calculated in *ORTEP* are related to this surface; considering the discussion in Section 1.9.1, they should more appropriately be called *atomic displacement ellipsoids* or simply *ORTEP ellipsoids*. One notes that the Fourier transform of the atomic DWF, the atomic probability density function $P(\mathbf{u})$, is given in the case of a second-order tensor as a trivariate Gaussian distribution,

$$P(\mathbf{u}) = \frac{[\text{Det}(\mathbf{U}_C^{-1})]^{1/2}}{(2\pi)^{3/2}} \exp\left\{-\frac{1}{2}\mathbf{u}^T \mathbf{U}_C^{-1} \mathbf{u}\right\}. \quad (1.9.4.5)$$

On comparing (1.9.4.3) and (1.9.4.5), it is evident that (1.9.4.3) defines a surface of constant probability of finding a (displaced) atom. The integral of (1.9.4.5) over the volume inside the ellipsoid is a constant. For ${}^2I_0 = C^2$ with the integration limit $C = 1.5382$ (2.5003), the integral is equal to one half (nine tenths), and the ellipsoid is then called a 50 (90) per cent probability ellipsoid.

Other representation surfaces can be defined and are useful for special considerations. The quantities of interest are either the r.m.s.d.'s or the mean-square displacements (m.s.d.'s) defined in direct space. Here a distinction has to be made between the averaged squared displacement along a certain direction and the average for all squared displacements of an atom projected onto a given direction. Representation surfaces may also be calculated in reciprocal space, related to surfaces in direct space by Fourier transformation. For further details, see Nelmes (1969) and Hummel *et al.* (1990).

1.9.4.2. Higher-order representations

Representation surfaces of higher-order tensors may be calculated from their invariants. While for second-order tensors surfaces can be found that fully describe the directional aspects of the tensor involved, higher-order tensors need several different surfaces for a full description (see e.g. Wondratschek, 1958; Sirotnin, 1961). This makes the graphical representation of the displacements somewhat cumbersome and it is therefore rarely used. Instead, the probability density functions [given in equations (6.1.1.46), (6.1.1.48) or (6.1.1.49) of *IT C*] are calculated from the tensor coefficients and displayed in sections or as three-dimensional surfaces. If the higher-order terms are small, it is more appropriate to display only the difference between the total p.d.f. and the related Gaussian p.d.f., which may be calculated from the second-order displacement tensor using equation (1.9.4.5). Here, the second-order terms that were refined together with the higher-order terms are usually used (not the best-fitting second-order terms of a fit in the harmonic approximation):

$$P_{\text{deformation}}(\mathbf{u}) = P_{\text{general}}(\mathbf{u}) - P_{\text{Gaussian}}(\mathbf{u}). \quad (1.9.4.6)$$

The resulting *anharmonic deformation densities* (or *disorder deformation densities* in the case of static disorder) $P_{\text{deformation}}(\mathbf{u})$ may be displayed in a similar way to the total p.d.f.'s $P_{\text{general}}(\mathbf{u})$. The graphical representations appropriate for displaying those densities are similar to those used for electronic deformation

1.9. ATOMIC DISPLACEMENT PARAMETERS

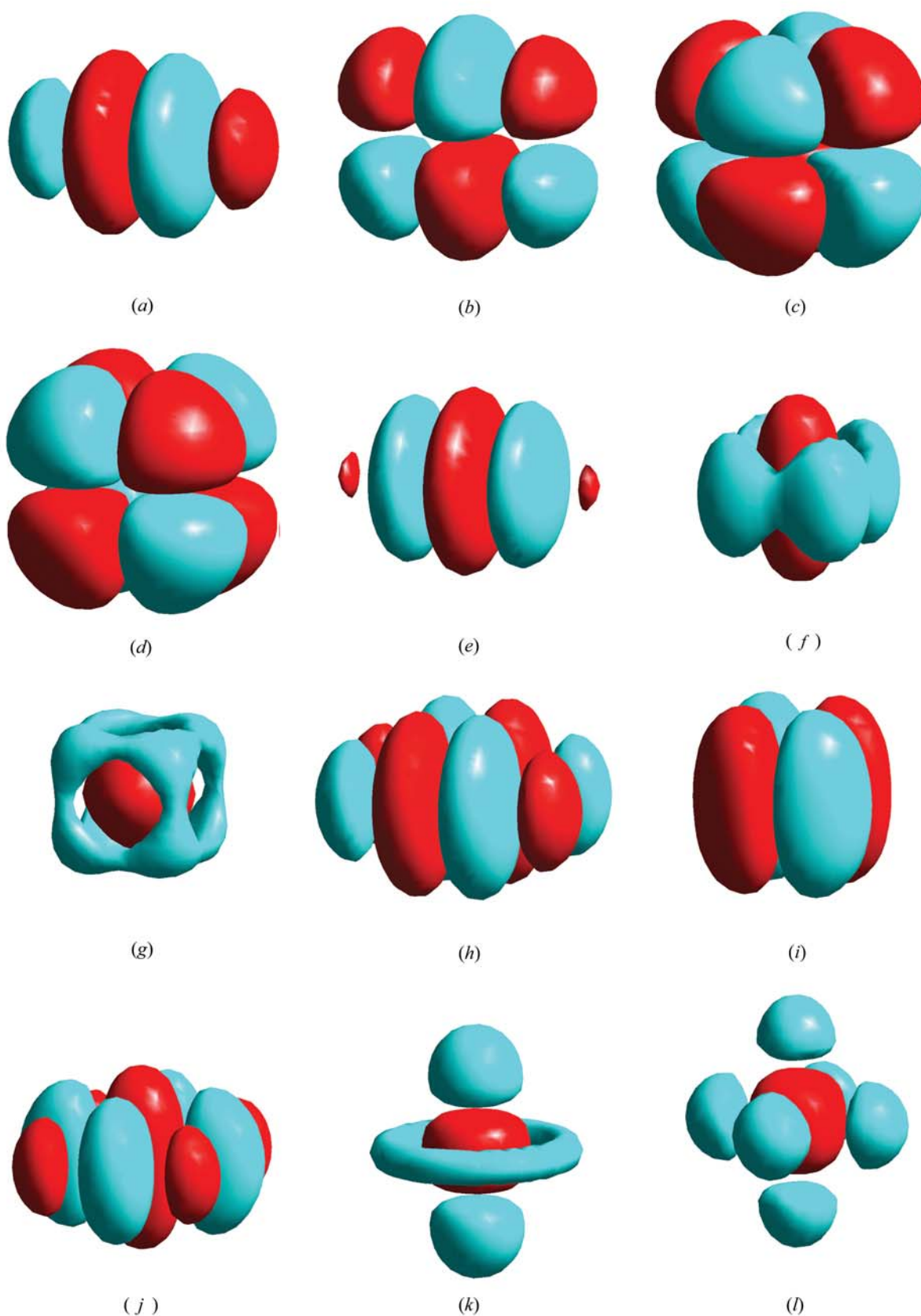


Fig. 1.9.4.1. A selection of graphical representations of density modulations due to higher-order terms in the Gram-Charlier series expansion of a Gaussian atomic probability density function. All figures are drawn on a common scale and have a common orientation. All terms within any given order of expansion are numerically identical and refer to the same underlying isotropic second-order term; the higher-order terms of different order of expansion differ by one order of magnitude, but refer again to the same underlying isotropic second-order term. The orthonormal crystallographic axes are oriented as follows: x oblique out of the plane of the paper towards the observer, y in the plane of the paper and to the right, and z in the plane of the paper and upwards. All surfaces are scaled to 1% of the absolute value of the maximum modulation within each density distribution. Positive modulations (*i.e.* an increase of density) are shown in red, negative modulations are shown in blue. The source of illumination is located approximately on the $[111]$ axis. The following graphs are shown (with typical point groups for specific cases given in parentheses). Third-order terms: (a) b^{222} ; (b) b^{223} ; (c) $b^{113} = -b^{223}$ (point group $\bar{4}$); (d) b^{123} (point group $43m$). Fourth-order terms: (e) b^{2222} ; (f) $b^{1111} = b^{2222}$; (g) $b^{1111} = b^{2222} = b^{3333}$ (point group $m\bar{3}m$); (h) b^{1222} ; (i) $b^{1112} = b^{1222}$; (j) b^{1122} ; (k) $b^{1153} = b^{2253}$; (l) $b^{1122} = b^{1153} = b^{2253}$ (point group $m\bar{3}m$).

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

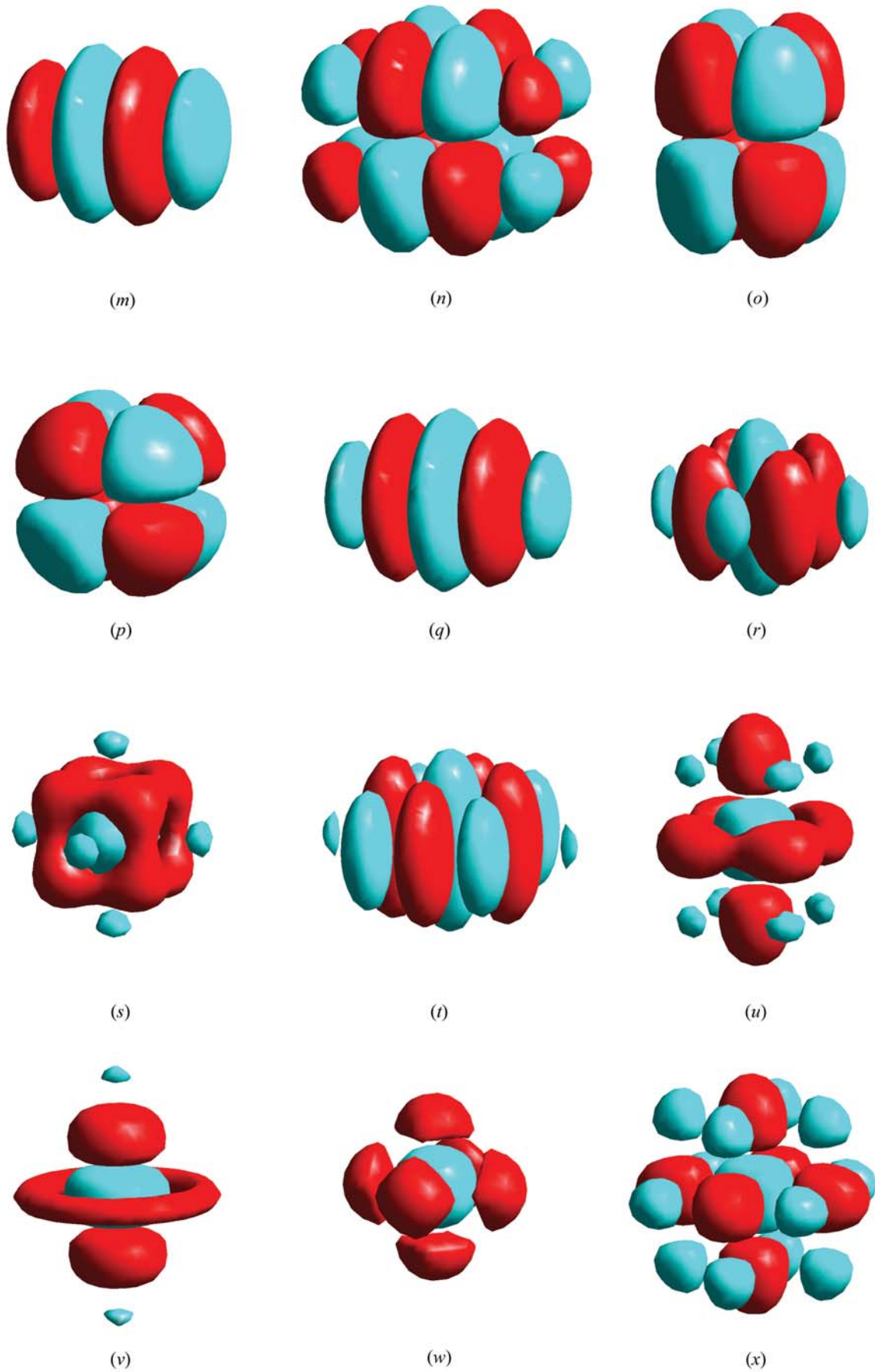


Fig. 1.9.4.1 (cont.). Fifth-order terms: (m) b^{22222} ; (n) b^{12223} ; (o) $b^{11123} = b^{12223}$; (p) $b^{11123} = b^{12223} = b^{12333}$ (point group $\bar{4}3m$). Sixth-order terms: (q) b^{222222} ; (r) $b^{111111} = b^{222222} = b^{333333}$ (point group $m\bar{3}m$); (t) b^{112222} ; (u) $b^{111133} = b^{222233}$; (v) $b^{113333} = b^{223333}$; (w) $b^{111122} = b^{112222} = b^{111133} = b^{113333} = b^{222233} = b^{223333}$ (point group $m\bar{3}m$); (x) b^{112233} (point group $m\bar{3}m$).

1.9. ATOMIC DISPLACEMENT PARAMETERS

densities (see *e.g.* Smith *et al.*, 1977). A number of examples of displacement deformation densities of high symmetry are shown in Fig. 1.9.4.1 as three-dimensional contour maps.

1.9.5. Glossary

$b^{ijk\dots}$	atomic displacement tensor
β^{ij} , $U^{ijk\dots}$	atomic displacement parameter
g_{ij}	metric tensor
S_α	atomic static Debye–Waller factor
T_α	atomic thermal Debye–Waller factor
\mathbf{Q}	scattering vector
u^i	atomic displacement

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