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Site-Symmetry Restrictions on Thermal-Motion-Tensor Coefficients up to Rank 8

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Abstract

An extension of the tables for the site-symmetry restrictions on the thermal-motion-tensor coefficients to include tensors up to rank 6 (up to rank 8 for cubic, hexagonal, tetragonal and trigonal site symmetries) is presented. The dependence relationships of these symmetric polar tensors are calculated in their natural crystallographic lattice frames using a direct method.

Introduction

Recently there has been a growing interest in the study of anharmonicity in thermal motion; anharmonic parameters are essential, for example, in modelling the structures of fast ionic conductors or other disordered systems like ferroelectrics. These highly anharmonic systems very often need thermal parameters higher than fourth order to obtain a satisfactory description. Moreover, anisotropic modifications in a plane of hexagonal symmetry can be described only with sixth- (or higher) order terms. Nowadays the accuracy and precision of diffraction data are in general no longer an obstacle to a meaningful refinement of such high-order thermal parameters in a least-squares procedure, *e.g.* $CsPbCl_3$ (Hutton & Nelmes, 1981), Li_3N (Zucker & Schulz, 1982), Ag_3SI (Perenthaler & Schulz, 1981), PbF_2 (Schulz, Perenthaler & Zucker, 1982), $RbAg_4I_5$ (Kuhs, 1983). Crystallographic program systems like *PROMETHEUS* (Zucker, Perenthaler, Kuhs, Bachmann & Schulz, 1983) allow for the routine insertion and refinement of parameters up to sixth order. To facilitate a general application, a tabulation of the symmetry constraints for all crystallographic site symmetries is clearly needed.

Whilst the symmetry restrictions of, for example, the elastic coefficients based on orthogonal lattice frames are at least partially available up to twelfth order (*i.e.* sixth-order elastic constants) (Chung & Li, 1974; Brendel, 1979; Fumi & Ripamonti, 1983), a tabulation for general (even- and odd-rank) symmetric polar tensors based on the natural crystallographic lattice frames is available only for tensors up to fourth order (Johnson & Levy, 1974). This paper presents the extension of that tabulation.

Method

The method used to derive the dependence relations for symmetric polar tensor coefficients is based on the fundamental transformation law for tensors ('direct method'). A tensor coefficient remains unchanged when the transformation corresponds to the site symmetry:

$$C_T^{jklmnp\cdots} = T_{jq}T_{kr}T_{ls}T_{mt}T_{nu}T_{pv}\ldots C^{qrstuv\ldots}$$

with $C_T^{jklmnp\cdots} = C^{qrstuv\cdots}$ and $1 \le j, k, l, m, n, p, q, r, s, t, u, v \ldots \le 3$. The point-group generators **T** were taken from Johnson & Levy (1974). For site symmetries having several generators all of them have been treated simultaneously. The homogeneous system of equations obtained (one equation for each coefficient) was reduced using a Gaussian elimination procedure. The order of assignment of independency is with increasing indices of the coefficients, except for the unmixed coefficients C^{jjjjjj}, which have highest priority in every case.* The correctness of the remaining system of equations giving the dependence relationships was checked algebraically by inserting numerical values. In addition, the number of unrestricted parameters was checked by comparison with results obtained by group-theoretical calculations (Sirotin, 1960).

* This is the same ordering, as, for example, in the *PROMETHEUS* system (Zucker, Perenthaler, Kuhs, Bachmann & Schulz, 1983).

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Table 1. *Site-symmetry table giving key to tables 2A, B, for restrictions on the symmetry of various thermal-motion tensors (Hex denotes hexagonal axes)*

Point symmetry at special position					Position	Cross-reference number for	
Symmetry axes		Point-group generators			x, y, z	$2A$	$2B$
$m3m$		4[0, 0, 1]	3[1, 1, 1]	$\bar{1}$	0, 0, 0	$E0$	$F1$
$\bar{4}3m$		$\bar{4}$[0, 0, 1]	3[1, 1, 1]		0, 0, 0	$E1$	$F1$
432		4[0, 0, 1]	3[1, 1, 1]		0, 0, 0	$E0$	$F1$
$m3$		3[1, 1, 1]	2[0, 0, 1]	$\bar{1}$	0, 0, 0	$E0$	$F2$
23		3[1, 1, 1]	2[0, 0, 1]		0, 0, 0	$E1$	$F2$
$6/mmm$	Hex	6[0, 0, 1]	2[1, 0, 0]	$\bar{1}$	0, 0, 0	$E0$	$F3$
$\bar{6}$m2	Hex	$\bar{6}$[0, 0, 1]	2[1, 0, 0]		0, 0, 0	$E5$	$F3$
$\bar{6}$m2	Hex	$\bar{6}$[0, 0, 1]	2[1, 2, 0]		0, 0, 0	$E6$	$F3$
$6mm$	Hex	6[0, 0, 1]	$\bar{2}$[1, 0, 0]		0, 0, z	$E17$	$F3$
622	Hex	6[0, 0, 1]	2[1, 0, 0]		0, 0, 0	$E0$	$F4$
$6/m$	Hex	6[0, 0, 1]	$\bar{1}$		0, 0, 0	$E0$	$F4$
$\bar{6}$	Hex	$\bar{6}$[0, 0, 1]			0, 0, 0	$E24$	$F4$
6	Hex	6[0, 0, 1]			0, 0, z	$E17$	$F4$
$4/mmm$		4[0, 0, 1]	2[1, 0, 0]	$\bar{1}$	0, 0, 0	$E0$	$F5$
$4/mmm$		4[0, 1, 0]	2[0, 0, 1]	$\bar{1}$	0, 0, 0	$E0$	$F6$
$4/mmm$		4[1, 0, 0]	2[0, 1, 0]	$\bar{1}$	0, 0, 0	$E0$	$F7$
$\bar{4}2m$		$\bar{4}$[0, 0, 1]	2[1, 0, 0]		0, 0, 0	$E7$	$F5$
$\bar{4}2m$		$\bar{4}$[0, 0, 1]	2[1, 1, 0]		0, 0, 0	$E8$	$F5$
$\bar{4}2m$		$\bar{4}$[0, 1, 0]	2[0, 0, 1]		0, 0, 0	$E9$	$F6$
$\bar{4}2m$		$\bar{4}$[0, 1, 0]	2[1, 0, 1]		0, 0, 0	$E10$	$F6$
$\bar{4}2m$		$\bar{4}$[1, 0, 0]	2[0, 1, 0]		0, 0, 0	$E11$	$F7$
$\bar{4}2m$		$\bar{4}$[1, 0, 0]	2[0, 1, 1]		0, 0, 0	$E12$	$F7$
$4mm$		4[0, 0, 1]	$\bar{2}$[1, 0, 0]		0, 0, z	$E25$	$F5$
$4mm$		4[0, 1, 0]	$\bar{2}$[0, 0, 1]		0, y, 0	$E26$	$F6$
$4mm$		4[1, 0, 0]	$\bar{2}$[0, 1, 0]		x, 0, 0	$E27$	$F7$
422		4[0, 0, 1]	2[1, 0, 0]		0, 0, 0	$E2$	$F5$
422		4[0, 1, 0]	2[0, 0, 1]		0, 0, 0	$E3$	$F6$
422		4[1, 0, 0]	2[0, 1, 0]		0, 0, 0	$E4$	$F7$
$4/m$		4[0, 0, 1]	$\bar{1}$		0, 0, 0	$E0$	$F14$
$4/m$		4[0, 1, 0]	$\bar{1}$		0, 0, 0	$E0$	$F15$
$4/m$		4[1, 0, 0]	$\bar{1}$		0, 0, 0	$E0$	$F16$
$\bar{4}$		$\bar{4}$[0, 0, 1]			0, 0, 0	$E28$	$F14$
$\bar{4}$		$\bar{4}$[0, 1, 0]			0, 0, 0	$E29$	$F15$
$\bar{4}$		$\bar{4}$[1, 0, 0]			0, 0, 0	$E30$	$F16$
4		4[0, 0, 1]			0, 0, z	$E31$	$F14$
4		4[0, 1, 0]			0, y, 0	$E32$	$F15$
4		4[1, 0, 0]			x, 0, 0	$E33$	$F16$
$\bar{3}m$		3[1, 1, 1]	2[1, $\bar{1}$, 0]	$\bar{1}$	0, 0, 0	$E0$	$F8$
$\bar{3}m$		3[1, 1, $\bar{1}$]	2[1, $\bar{1}$, 0]	$\bar{1}$	0, 0, 0	$E0$	$F9$
$\bar{3}m$		3[1, $\bar{1}$, 1]	2[1, 1, 0]	$\bar{1}$	0, 0, 0	$E0$	$F10$
$\bar{3}m$		3[$\bar{1}$, 1, 1]	2[1, 1, 0]	$\bar{1}$	0, 0, 0	$E0$	$F11$
$\bar{3}m$	Hex	3[0, 0, 1]	2[1, 0, 0]	$\bar{1}$	0, 0, 0	$E0$	$F12$
$\bar{3}m$	Hex	3[0, 0, 1]	2[1, 2, 0]	$\bar{1}$	0, 0, 0	$E0$	$F13$
$3m$		3[1, 1, 1]	$\bar{2}$[1, $\bar{1}$, 0]		x, x, x	$E34$	$F8$
$3m$		3[1, 1, $\bar{1}$]	$\bar{2}$[1, $\bar{1}$, 0]		$x, x, \bar{x}$	$E35$	$F9$
$3m$		3[1, $\bar{1}$, 1]	$\bar{2}$[1, 1, 0]		$x, \bar{x}, x$	$E36$	$F10$
$3m$		3[$\bar{1}$, 1, 1]	$\bar{2}$[1, 1, 0]		$\bar{x}, x, x$	$E37$	$F11$
$3m$	Hex	3[0, 0, 1]	$\bar{2}$[1, 0, 0]		0, 0, z	$E38$	$F12$
$3m$	Hex	3[0, 0, 1]	$\bar{2}$[1, 2, 0]		0, 0, z	$E39$	$F13$
32		3[1, 1, 1]	2[1, $\bar{1}$, 0]		0, 0, 0	$E13$	$F8$
32		3[1, 1, $\bar{1}$]	2[1, $\bar{1}$, 0]		0, 0, 0	$E14$	$F9$
32		3[1, $\bar{1}$, 1]	2[1, 1, 0]		0, 0, 0	$E15$	$F10$
32		3[$\bar{1}$, 1, 1]	2[1, 1, 0]		0, 0, 0	$E16$	$F11$
32	Hex	3[0, 0, 1]	2[1, 0, 0]		0, 0, 0	$E5$	$F12$
32	Hex	3[0, 0, 1]	2[1, 2, 0]		0, 0, 0	$E6$	$F13$
$\bar{3}$		$\bar{3}$[1, 1, 1]			0, 0, 0	$E0$	$F17$
$\bar{3}$		$\bar{3}$[1, 1, $\bar{1}$]			0, 0, 0	$E0$	$F18$
$\bar{3}$		$\bar{3}$[1, $\bar{1}$, 1]			0, 0, 0	$E0$	$F19$
$\bar{3}$		$\bar{3}$[$\bar{1}$, 1, 1]			0, 0, 0	$E0$	$F20$
$\bar{3}$	Hex	$\bar{3}$[0, 0, 1]			0, 0, 0	$E0$	$F21$
3		3[1, 1, 1]			x, x, x	$E58$	$F17$
3		3[1, 1, $\bar{1}$]			$x, x, \bar{x}$	$E59$	$F18$
3		3[1, $\bar{1}$, 1]			$x, \bar{x}, x$	$E60$	$F19$
3		3[$\bar{1}$, 1, 1]			$\bar{x}, x, x$	$E61$	$F20$
3	Hex	3[0, 0, 1]			0, 0, z	$E62$	$F21$
mmm		2[0, 0, 1]	2[1, 0, 0]	$\bar{1}$	0, 0, 0	$E0$	$F22$
mmm		2[0, 0, 1]	2[1, 1, 0]	$\bar{1}$	0, 0, 0	$E0$	$F23$
mmm		2[0, 1, 0]	2[1, 0, 1]	$\bar{1}$	0, 0, 0	$E0$	$F24$
mmm		2[1, 0, 0]	2[0, 1, 1]	$\bar{1}$	0, 0, 0	$E0$	$F25$
mmm	Hex	2[0, 0, 1]	2[1, 0, 0]	$\bar{1}$	0, 0, 0	$E0$	$F26$
mmm	Hex	2[0, 0, 1]	2[1, 1, 0]	$\bar{1}$	0, 0, 0	$E0$	$F23$
mmm	Hex	2[0, 0, 1]	2[0, 1, 0]	$\bar{1}$	0, 0, 0	$E0$	$F27$
mm		2[0, 0, 1]	$\bar{2}$[1, 0, 0]		0, 0, z	$E40$	$F22$
mm		2[0, 0, 1]	$\bar{2}$[1, 1, 0]		0, 0, z	$E41$	$F23$
mm		2[0, 1, 0]	$\bar{2}$[0, 0, 1]		0, y, 0	$E42$	$F22$
mm		2[0, 1, 0]	$\bar{2}$[1, 0, 1]		0, y, 0	$E43$	$F24$
mm		2[1, 0, 0]	$\bar{2}$[0, 0, 1]		x, 0, 0	$E44$	$F22$
mm		2[1, 0, 0]	$\bar{2}$[0, 1, 1]		x, 0, 0	$E45$	$F25$
mm		2[1, 1, 0]	$\bar{2}$[0, 0, 1]		x, x, 0	$E46$	$F23$
mm		2[1, $\bar{1}$, 0]	$\bar{2}$[0, 0, 1]		$x, \bar{x}$, 0	$E47$	$F23$
mm		2[1, 0, 1]	$\bar{2}$[0, 1, 0]		x, 0, x	$E48$	$F24$
mm		2[1, 0, $\bar{1}$]	$\bar{2}$[0, 1, 0]		x, 0, $\bar{x}$	$E49$	$F24$
mm		2[0, 1, 1]	$\bar{2}$[1, 0, 0]		0, y, y	$E50$	$F25$
mm		2[0, 1, $\bar{1}$]	$\bar{2}$[1, 0, 0]		0, $y, \bar{y}$	$E51$	$F25$
mm	Hex	2[0, 0, 1]	$\bar{2}$[1, 0, 0]		0, 0, z	$E52$	$F26$
mn	Hex	2[0, 0, 1]	$\bar{2}$[1, 1, 0]		0, 0, z	$E41$	$F23$
mm	Hex	2[0, 0, 1]	$\bar{2}$[0, 1, 0]		0, 0, z	$E53$	$F27$
mm	Hex	2[1, 0, 0]	$\bar{2}$[0, 0, 1]		x, 0, 0	$E54$	$F26$
mm	Hex	2[2, 1, 0]	$\bar{2}$[0, 0, 1]		2x, x, 0	$E55$	$F27$
mm	Hex	2[1, 1, 0]	$\bar{2}$[0, 0, 1]		x, x, 0	$E46$	$F23$
mm	Hex	2[1, 2, 0]	$\bar{2}$[0, 0, 1]		x, 2x, 0	$E56$	$F26$
mm	Hex	2[0, 1, 0]	$\bar{2}$[0, 0, 1]		0, y, 0	$E57$	$F27$
mm	Hex	2[1, $\bar{1}$, 0]	$\bar{2}$[0, 0, 1]		$x, \bar{x}$, 0	$E47$	$F23$
222		2[0, 0, 1]	2[1, 0, 0]		0, 0, 0	$E18$	$F22$
222		2[0, 0, 1]	2[1, 1, 0]		0, 0, 0	$E19$	$F23$
222		2[0, 1, 0]	2[1, 0, 1]		0, 0, 0	$E20$	$F24$
222		2[1, 0, 0]	2[0, 1, 1]		0, 0, 0	$E21$	$F25$
222	Hex	2[0, 0, 1]	2[1, 0, 0]		0, 0, 0	$E22$	$F26$
222	Hex	2[0, 0, 1]	2[1, 1, 0]		0, 0, 0	$E19$	$F23$
222	Hex	2[0, 0, 1]	2[0, 1, 0]		0, 0, 0	$E23$	$F27$
$2/m$		2[0, 0, 1]	$\bar{1}$		0, 0, 0	$E0$	$F28$
$2/m$		2[0, 1, 0]	$\bar{1}$		0, 0, 0	$E0$	$F29$
$2/m$		2[1, 0, 0]	$\bar{1}$		0, 0, 0	$E0$	$F30$
$2/m$		2[1, 1, 0]	$\bar{1}$		0, 0, 0	$E0$	$F31$
$2/m$		2[1, $\bar{1}$, 0]	$\bar{1}$		0, 0, 0	$E0$	$F32$
$2/m$		2[1, 0, 1]	$\bar{1}$		0, 0, 0	$E0$	$F33$
$2/m$		2[1, 0, $\bar{1}$]	$\bar{1}$		0, 0, 0	$E0$	$F34$
$2/m$		2[0, 1, 1]	$\bar{1}$		0, 0, 0	$E0$	$F35$
$2/m$		2[0, 1, $\bar{1}$]	$\bar{1}$		0, 0, 0	$E0$	$F36$
$2/m$	Hex	2[0, 0, 1]	$\bar{1}$		0, 0, 0	$E0$	$F28$
$2/m$	Hex	2[1, 0, 0]	$\bar{1}$		0, 0, 0	$E0$	$F37$
$2/m$	Hex	2[2, 1, 0]	$\bar{1}$		0, 0, 0	$E0$	$F38$
$2/m$	Hex	2[1, 1, 0]	$\bar{1}$		0, 0, 0	$E0$	$F31$
$2/m$	Hex	2[1, 2, 0]	$\bar{1}$		0, 0, 0	$E0$	$F39$
$2/m$	Hex	2[0, 1, 0]	$\bar{1}$		0, 0, 0	$E0$	$F40$
$2/m$	Hex	2[1, $\bar{1}$, 0]	$\bar{1}$		0, 0, 0	E0	F32
m		$\bar{2}$[0, 0, 1]			x, y, 0	$E76$	$F28$
m		$\bar{2}$[0, 1, 0]			x, 0, z	$E77$	$F29$
m		$\bar{2}$[1, 0, 0]			0, y, z	$E78$	$F30$
m		$\bar{2}$[1, 1, 0]			$x, \bar{x}$, z	$E79$	$F31$
m		$\bar{2}$[1, $\bar{1}$, 0]			x, x, z	$E80$	$F32$
m		$\bar{2}$[1, 0, 1]			$x, y, \bar{x}$	$E81$	$F33$
m		$\bar{2}$[1, 0, $\bar{1}$]			x, y, x	$E82$	$F34$
m		$\bar{2}$[0, 1, 1]			$x, y, \bar{y}$	$E83$	$F35$
m		$\bar{2}$[0, 1, $\bar{1}$]			x, y, y	$E84$	$F36$
m	Hex	$\bar{2}$[0, 0, 1]			x, y, 0	$E76$	$F28$
m	Hex	$\bar{2}$[1, 0, 0]			x, 2x, z	$E85$	$F37$
m	Hex	$\bar{2}$[2, 1, 0]			0, y, z	$E86$	$F38$
m	Hex	$\bar{2}$[1, 1, 0]			$x, \bar{x}$, z	$E79$	$F31$
m	Hex	$\bar{2}$[1, 2, 0]			x, 0, z	$E87$	$F39$
m	Hex	$\bar{2}$[0, 1, 0]			2x, x, z	$E88$	$F40$
m	Hex	$\bar{2}$[1, $\bar{1}$, 0]			x, x, z	$E80$	$F32$
2		2[0, 0, 1]			0, 0, z	$E63$	$F28$
2		2[0, 1, 0]			0, y, 0	$E64$	$F29$
2		2[1, 0, 0]			x, 0, 0	$E65$	$F30$
2		2[1, 1, 0]			x, x, 0	$E66$	$F31$
2		2[1, $\bar{1}$, 0]			$x, \bar{x}$, 0	$E67$	$F32$
2		2[1, 0, 1]			x, 0, x	$E68$	$F33$
2		2[1, 0, $\bar{1}$]			x, 0, $\bar{x}$	$E69$	$F34$
2		2[0, 1, 1]			0, y, y	$E70$	$F35$
2		2[0, 1, $\bar{1}$]			0, $y, \bar{y}$	$E71$	$F36$
2	Hex	2[0, 0, 1]			0, 0, z	$E63$	$F28$
2	Hex	2[1, 0, 0]			x, 0, 0	$E72$	$F37$
2	Hex	2[2, 1, 0]			2x, x, 0	$E73$	$F38$
2	Hex	2[1, 1, 0]			x, x, 0	$E66$	$F31$
2	Hex	2[1, 2, 0]			x, 2x, 0	$E74$	$F39$
2	Hex	2[0, 1, 0]			0, y, 0	$E75$	$F40$
2	Hex	2[1, $\bar{1}$, 0]			$x, \bar{x}$, 0	$E67$	$F32$
$\bar{1}$		$\bar{1}$			0, 0, 0	$E0$	$F41$
$\bar{1}$	Hex	$\bar{1}$			0, 0, 0	$E0$	$F41$
1		1			x, y, z	$E89$	$F41$
1	Hex	1			x, y, z	$E89$	$F41$

Table 2*A*. *Symmetry restrictions on coefficients in fifth-rank symmetric polar tensors*

Cross reference	Number of independent coefficients	*A*	*B*	*C*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	*L*	*M*	*N*	*P*	*Q*	*R*	*S*	*T*	*U*	*V*
		1	2	3	1	1	1	1	1	1	1	1	1	1	1	1	1	1	2	2	2	2
	Number of	1	2	3	1	1	1	1	1	1	1	1	1	2	2	2	2	3	2	2	2	3
		1	2	3	1	1	1	1	1	2	2	2	3	2	2	2	3	3	2	2	3	3
		1	2	3	1	1	2	2	3	2	2	3	3	2	2	3	3	3	2	3	3	3
		1	2	3	2	3	2	3	3	2	3	3	3	2	3	3	3	3	3	3	3	3
*E*0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
*E*1	1	0	0	0	0	0	0	*G*	0	0	0	0	0	0	*G*	0	*G*	0	0	0	0	0
*E*2	1	0	0	0	0	0	0	*G*	0	0	0	0	0	0	$-G$	0	0	0	0	0	0	0
*E*3	1	0	0	0	0	0	0	*G*	0	0	0	0	0	0	0	0	$-G$	0	0	0	0	0
*E*4	1	0	0	0	0	0	0	0	0	0	0	0	0	0	*N*	0	$-N$	0	0	0	0	0
*E*5	2	0	0	0	*D*	0	*D*	0	0	*D*	0	*K*	0	*D*	0	*K*	0	0	0	0	0	0
*E*6	2	*A*	$-A$	0	$A/2$	0	$A/10$	0	*H*	$-A/10$	0	$H/2$	0	$-A/2$	0	$-H/2$	0	0	0	0	$-H$	0
*E*7	2	0	0	0	0	0	0	*G*	0	0	0	0	0	0	*G*	0	*Q*	0	0	0	0	0
*E*8	2	0	0	0	0	*E*	0	0	0	0	0	0	*L*	0	0	0	0	0	$-E$	0	$-L$	0
*E*9	2	0	0	0	0	0	0	*G*	0	0	0	0	0	0	*N*	0	*G*	0	0	0	0	0
*E*10	2	0	0	0	*D*	0	0	0	0	*I*	0	0	0	0	0	0	0	0	0	$-I$	0	$-D$
*E*11	2	0	0	0	0	0	0	*G*	0	0	0	0	0	0	*N*	0	*N*	0	0	0	0	0
*E*12	2	0	0	0	0	0	*F*	0	$-F$	0	0	0	0	*M*	0	0	0	$-M$	0	0	0	0
*E*13	2	0	0	0	*D*	$-D$	*F*	0	$-F$	$-F$	0	0	*F*	$-D$	0	0	0	*D*	*D*	*F*	$-F$	$-D$
*E*14	2	0	0	0	*D*	*D*	*F*	0	$-F$	$-F$	0	0	$-F$	$-D$	0	0	0	*D*	$-D$	*F*	*F*	$-D$
*E*15	2	0	0	0	*D*	*D*	*F*	0	$-F$	*F*	0	0	*F*	*D*	0	0	0	$-D$	$-D$	$-F$	$-F$	$-D$
*E*16	2	0	0	0	*D*	$-D$	*F*	0	$-F$	*F*	0	0	$-F$	*D*	0	0	0	$-D$	*D*	$-F$	*F*	$-D$
*E*17	3	0	0	*C*	0	*E*	0	$E/2$	0	0	$E/2$	0	*L*	0	$E/2$	0	$L/2$	0	*E*	0	*L*	0
*E*18	3	0	0	0	0	0	0	*G*	0	0	0	0	0	0	*N*	0	*Q*	0	0	0	0	0
*E*19	3	0	0	0	0	*E*	0	*G*	0	0	0	0	*L*	0	$-G$	0	0	0	$-E$	0	$-L$	0
*E*20	3	0	0	0	*D*	0	0	*G*	0	*I*	0	0	0	0	0	0	$-G$	0	0	$-I$	0	$-D$
*E*21	3	0	0	0	0	0	*F*	0	$-F$	0	0	0	0	*M*	*N*	0	$-N$	$-M$	0	0	0	0
*E*22	3	0	0	0	0	0	0	*G*	0	0	$2G$	0	*L*	0	$2G$	0	*L*	0	*S*	0	0	0
*E*23	3	0	0	0	0	0	0	*G*	0	0	*G*	0	0	0	*N*	0	*Q*	0	14*	0	*Q*	0
*E*24	4	*A*	$-A$	0	*D*	0	1*	0	*H*	3*	0	*K*	0	7*	0	13*	0	0	0	$-H$	0	0
*E*25	4	0	0	*C*	0	*E*	0	0	0	0	*J*	0	*L*	0	0	0	0	0	*E*	0	*L*	0
*E*26	4	0	*B*	0	*D*	0	0	0	0	*I*	0	*K*	0	0	0	0	0	0	0	*I*	0	*D*
*E*27	4	*A*	0	0	0	0	*F*	0	*F*	0	0	0	0	*M*	0	*P*	0	*M*	0	0	0	0
*E*28	4	0	0	0	0	*E*	0	*G*	0	0	0	0	*L*	0	*G*	0	*Q*	0	$-E$	0	$-L$	0
*E*29	4	0	0	0	*D*	0	0	*G*	0	*I*	0	0	0	0	*N*	0	*G*	0	0	$-I$	0	$-D$
*E*30	4	0	0	0	0	0	*F*	*G*	$-F$	0	0	0	0	*M*	*N*	0	*N*	$-M$	0	0	0	0
*E*31	5	0	0	*C*	0	*E*	0	*G*	0	0	*J*	0	*L*	0	$-G$	0	0	0	*E*	0	*L*	0
*E*32	5	0	*B*	0	*D*	0	0	*G*	0	*I*	0	*K*	0	0	0	0	$-G$	0	0	*I*	0	*D*
*E*33	5	*A*	0	0	0	0	*F*	0	*F*	0	0	0	0	*M*	*N*	*P*	$-N$	*M*	0	0	0	0
*E*34	5	*A*	*A*	*A*	*D*	*D*	*F*	*G*	*F*	*F*	*J*	*J*	*F*	*D*	*G*	*J*	*G*	*D*	*D*	*F*	*F*	*D*
*E*35	5	*A*	*A*	$-A$	*D*	$-D$	*F*	*G*	*F*	*F*	*J*	$-J$	$-F$	*D*	*G*	$-J$	*G*	*D*	$-D$	*F*	$-F$	*D*
*E*36	5	*A*	$-A$	*A*	*D*	$-D$	*F*	*G*	*F*	$-F$	*J*	$-J$	*F*	$-D$	*G*	*J*	*G*	$-D$	$-D$	$-F$	*F*	*D*
*E*37	5	*A*	$-A$	$-A$	*D*	*D*	*F*	*G*	*F*	$-F$	*J*	*J*	$-F$	$-D$	*G*	$-J$	*G*	$-D$	*D*	$-F$	$-F$	*D*
*E*38	5	*A*	$-A$	*C*	$A/2$	*E*	$A/10$	$E/2$	*H*	$-A/10$	$E/2$	$H/2$	*L*	$-A/2$	$E/2$	$-H/2$	$L/2$	0	*E*	$-H$	*L*	0
*E*39	5	0	0	*C*	*D*	*E*	*D*	$E/2$	0	*D*	$E/2$	*K*	*L*	*D*	$E/2$	*K*	$L/2$	0	*E*	0	*L*	0
*E*40	6	0	0	*C*	0	*E*	0	0	0	0	*J*	0	*L*	0	0	0	0	0	*S*	0	*U*	0
*E*41	6	0	0	*C*	0	*E*	0	*G*	0	0	*J*	0	*L*	0	*G*	0	*Q*	0	*E*	0	*L*	0
*E*42	6	0	*B*	0	*D*	0	0	0	0	*I*	0	*K*	0	0	0	0	0	0	0	*T*	0	*V*
*E*43	6	0	*B*	0	*D*	0	0	*G*	0	*I*	0	*K*	0	0	*N*	0	*G*	0	0	*I*	0	*D*
*E*44	6	*A*	0	0	0	0	*F*	0	*H*	0	0	0	0	*M*	0	*P*	0	*R*	0	0	0	0
*E*45	6	*A*	0	0	0	0	*F*	*G*	*H*	0	0	0	0	*M*	*N*	*P*	*N*	*M*	0	0	0	0
*E*46	6	*A*	$-A$	0	*D*	0	*F*	0	*H*	*F*	0	*K*	0	*D*	0	*K*	0	*R*	0	*H*	0	*R*
*E*47	6	*A*	$-A$	0	*D*	0	*F*	0	*H*	$-F$	0	*K*	0	$-D$	0	$-K$	0	*R*	0	$-H$	0	$-R$
*E*48	6	*A*	0	*A*	0	*E*	*F*	0	*H*	0	*J*	0	*H*	*M*	0	*J*	0	*E*	*M*	0	*F*	0
*E*49	6	*A*	0	$-A$	0	*E*	*F*	0	*H*	0	*G*	0	$-H$	*M*	0	$-J$	0	$-E$	$-M$	0	$-F$	0
*E*50	6	0	*B*	*B*	*D*	*D*	0	0	0	*I*	*J*	*J*	*I*	0	0	0	0	0	*S*	*T*	*T*	*S*
*E*51	6	0	*B*	$-B$	*D*	$-D$	0	0	0	*I*	*J*	$-J$	$-I$	0	0	0	0	0	*S*	*T*	$-T$	$-S$
*E*52	6	0	0	*C*	0	*E*	0	*G*	0	0	*J*	0	*L*	0	10*	0	*Q*	0	15*	0	$2Q$	0
*E*53	6	0	0	*C*	0	*E*	0	$E/2$	0	0	*J*	0	*L*	0	11*	0	$L/2$	0	*S*	0	*U*	0
*E*54	6	*A*	0	0	*D*	0	*F*	0	*H*	4*	0	*K*	0	4*	0	*K*	0	*R*	0	0	0	0
*E*55	6	*A*	*B*	0	$A/2$	0	*F*	0	*H*	5*	0	$H/2$	0	8*	0	*P*	0	*R*	0	16*	0	$R/2$
*E*56	6	*A*	*B*	0	*D*	0	2*	0	*H*	6*	0	*K*	0	$B/2$	0	12*	0	*R*	0	17*	0	$2R$
*E*57	6	0	*B*	0	*D*	0	*D*	0	0	*I*	0	*K*	0	9*	0	*K*	0	0	0	*T*	0	*V*
*E*58	7	*A*	*A*	*A*	*D*	*E*	*F*	*G*	*H*	*H*	*J*	*J*	*F*	*E*	*G*	*J*	*G*	*D*	*D*	*F*	*H*	*E*
*E*59	7	*A*	*A*	$-A$	*D*	*E*	*F*	*G*	*H*	*H*	*J*	$-J$	$-F$	$-E$	*G*	$-J$	*G*	*D*	$-D$	*F*	$-H$	$-E$
*E*60	7	*A*	$-A$	*A*	*D*	*E*	*F*	*G*	*H*	$-H$	*J*	$-J$	*F*	*E*	*G*	*J*	*G*	$-D$	$-D$	$-F$	*H*	$-E$
*E*61	7	*A*	$-A$	$-A$	*D*	*E*	*F*	*G*	*H*	$-H$	*J*	*J*	$-F$	$-E$	*G*	$-J$	*G*	$-D$	*D*	$-F$	$-H$	*E*
*E*62	7	*A*	$-A$	*C*	*D*	*E*	1*	$E/2$	*H*	3*	$E/2$	*K*	*L*	7*	$E/2$	13*	$L/2$	0	*E*	$-H$	*L*	0
*E*63	9	0	0	*C*	0	*E*	0	*G*	0	0	*J*	0	*L*	0	*N*	0	*Q*	0	*S*	0	*U*	0
*E*64	9	0	*B*	0	*D*	0	0	*G*	0	*I*	0	*K*	0	0	*N*	0	*Q*	0	0	*T*	0	*V*
*E*65	9	*A*	0	0	0	0	*F*	*G*	*H*	0	0	0	0	*M*	*N*	*P*	*Q*	*R*	0	0	0	0
*E*66	9	*A*	*A*	0	*D*	*E*	*F*	*G*	*H*	*F*	0	*K*	*L*	*D*	$-G$	*K*	0	*R*	$-E$	*H*	$-L$	*R*
*E*67	9	*A*	$-A$	0	*D*	*E*	*F*	*G*	*H*	$-F$	0	*K*	*L*	$-D$	$-G$	$-K$	0	*R*	$-E$	$-H$	$-L$	$-R$
*E*68	9	*A*	0	*A*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	0	*H*	*M*	0	*J*	$-G$	*E*	*M*	$-I$	*F*	$-D$
*E*69	9	*A*	0	$-A$	*D*	*E*	*F*	*G*	*H*	*I*	*J*	0	$-H$	*M*	0	$-J$	$-G$	$-E$	$-M$	$-I$	$-F$	$-D$
*E*70	9	0	*B*	*B*	*D*	*D*	*F*	0	$-F$	*I*	*J*	*J*	*I*	*M*	*N*	0	$-N$	$-M$	*S*	*T*	*T*	*S*
*E*71	9	0	*B*	$-B$	*D*	$-D$	*F*	0	$-F$	*I*	*J*	$-J$	$-I$	*M*	*N*	0	$-N$	$-M$	*S*	*T*	$-T$	$-S$
*E*72	9	*A*	0	0	*D*	*E*	*F*	*G*	*H*	4*	$2G$	*K*	*L*	4*	$2G$	*K*	*L*	*R*	0	0	0	0
*E*73	9	*A*	*B*	0	$A/2$	0	*F*	*G*	*H*	5*	*G*	$H/2$	0	8*	*N*	*P*	*Q*	*R*	14*	16*	*Q*	$R/2$
*E*74	9	*A*	*B*	0	*D*	*E*	2*	*G*	*H*	6*	$2G$	*K*	*L*	$B/2$	$2G$	12*	*L*	*R*	0	17*	0	$2R$
*E*75	9	0	*B*	0	*D*	0	*D*	*G*	0	*I*	*G*	*K*	0	9*	*N*	*K*	*Q*	0	14*	*T*	*Q*	*V*
*E*76	12	*A*	*B*	0	*D*	0	*F*	0	*H*	*I*	0	*K*	0	*M*	0	*P*	0	*R*	0	*T*	0	*V*
*E*77	12	*A*	0	*C*	0	*E*	*F*	0	*H*	0	*J*	0	*L*	*M*	0	*P*	0	*R*	*S*	0	*U*	0
*E*78	12	0	*B*	*C*	*D*	*E*	0	0	0	*I*	*J*	*K*	*L*	0	0	0	0	0	*S*	*T*	*U*	*V*
*E*79	12	*A*	$-A$	*C*	*D*	*E*	*F*	*G*	*H*	$-F$	*J*	*K*	*L*	$-D$	*G*	$-K$	*Q*	*R*	*E*	$-H$	*L*	$-R$
*E*80	12	*A*	*A*	*C*	*D*	*E*	*F*	*G*	*H*	*F*	*J*	*K*	*L*	*D*	*G*	*J*	*Q*	*R*	*E*	*H*	*L*	*R*

Table 2*A* (*cont.*)

		A	*B*	*C*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	*L*	*M*	*N*	*P*	*Q*	*R*	*S*	*T*	*U*	*V*
		1	2	3	1	1	1	1	1	1	1	1	1	1	1	1	1	1	2	2	2	2
	Number	1	2	3	1	1	1	1	1	1	1	1	1	2	2	2	2	3	2	2	2	3
	of	1	2	3	1	1	1	1	1	2	2	2	3	2	2	2	3	3	2	2	3	3
Cross	independent	1	2	3	1	1	2	2	3	2	2	3	3	2	2	3	3	3	2	3	3	3
reference	coefficients	1	2	3	2	3	2	3	3	2	3	3	3	2	3	3	3	3	3	3	3	3
*E*81	12	*A*	*B*	$-A$	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	$-H$	*M*	*N*	$-J$	*G*	$-E$	$-M$	*I*	$-F$	*D*
*E*82	12	*A*	*B*	*A*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	*H*	*M*	*N*	*J*	*G*	*E*	*M*	*I*	*F*	*D*
*E*83	12	*A*	*B*	$-B$	*D*	$-D$	*F*	*G*	*F*	*I*	*J*	$-J$	$-I$	*M*	*N*	*P*	*N*	*M*	*S*	*T*	$-T$	$-S$
*E*84	12	*A*	*B*	*B*	*D*	*D*	*F*	*G*	*F*	*I*	*J*	*J*	*I*	*M*	*N*	*P*	*N*	*M*	*S*	*T*	*T*	*S*
*E*85	12	*A*	*B*	*C*	*D*	*E*	2*	*G*	*H*	6*	*J*	*K*	*L*	*B*/2	10*	12*	*N*	*M*	15*	17*	2*N*	2*M*
*E*86	12	0	*B*	*C*	*D*	*E*	*D*	*E*/2	0	*I*	*J*	*K*	*L*	2*I*	11*	*K*	*L*/2	0	*S*	*T*	*U*	*V*
*E*87	12	*A*	0	*C*	*D*	*E*	*F*	*G*	*H*	4*	*J*	*K*	*L*	4*	10*	*K*	*N*	*M*	15*	0	2*N*	0
*E*88	12	*A*	*B*	*C*	*A*/2	*E*	*F*	*E*/2	*H*	5*	*J*	*H*/2	*L*	8*	11*	*P*	*L*/2	*R*	*S*	16*	*U*	*U*/2
*E*89	21	*A*	*B*	*C*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	*L*	*M*	*N*	*P*	*Q*	*R*	*S*	*T*	*U*	*V*

* *Notes.* 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 $-4H+6K$.

Table 2*B*. *Symmetry restrictions on coefficients in sixth-rank symmetric polar tensors*

		A	*B*	*C*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	*L*	*M*	*N*	*P*	*Q*	*R*	*S*	*T*	*U*	*V*	*W*	*X*	*Y*	*Z*	*a*	*b*	*c*
		1	2	3	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	2	2	2	2	2
	Number	1	2	3	1	1	1	1	1	1	1	1	1	1	1	1	1	1	2	2	2	2	3	2	2	2	2	2	3
	of	1	2	3	1	1	1	1	1	1	1	1	1	2	2	2	2	3	2	2	2	2	3	3	2	2	2	3	3
	independent	1	2	3	1	1	1	1	1	2	2	2	3	2	2	2	3	3	2	2	2	3	3	3	2	2	3	3	3
Cross	para-	1	2	3	1	1	2	2	3	2	2	3	3	2	2	3	3	3	2	2	3	3	3	3	2	2	3	3	3
reference	meters	1	2	3	2	3	2	3	3	2	3	3	3	2	3	3	3	3	2	3	3	3	3	3	3	3	3	3	3
*F*1	3	*A*	*A*	*A*	0	0	*F*	0	*F*	0	0	0	0	*F*	0	*P*	0	*F*	0	0	0	0	0	0	0	*F*	0	*F*	0
*F*2	4	*A*	*A*	*A*	0	0	*F*	0	*H*	0	0	0	0	*H*	0	*P*	0	*F*	0	0	0	0	0	0	0	*F*	0	*H*	0
*F*3	5	*A*	*A*	*C*	*A*/2	0	*F*	0	*H*	1*	0	*H*/2	0	*F*	0	*H*/2	0	*R*	*A*/2	0	*H*/2	0	*R*/2	0	0	*H*	0	*R*	0
*F*4	6	*A*	*A*	*C*	*D*	0	*F*	0	*H*	2*	0	*H*/2	0	5*	0	*H*/2	0	*R*	11*	0	*H*/2	0	*R*/2	0	0	*H*	0	*R*	0
*F*5	6	*A*	*A*	*C*	0	0	*F*	0	*H*	0	0	0	0	*F*	0	*P*	0	*R*	0	0	0	0	0	0	0	*H*	0	*R*	0
*F*6	6	*A*	*B*	*A*	0	0	*F*	0	*H*	0	0	0	0	*M*	0	*P*	0	*H*	0	0	0	0	0	0	0	*M*	0	*F*	0
*F*7	6	*A*	*B*	*B*	0	0	*F*	0	*F*	0	0	0	0	*M*	0	*P*	0	*M*	0	0	0	0	0	0	0	*Z*	0	*Z*	0
*F*8	7	*A*	*A*	*A*	*D*	*D*	*F*	*G*	*F*	*I*	*J*	*I*	*F*	*J*	*P*	*J*	*F*	*D*	*G*	*J*	*J*	*G*	*D*	*D*	*F*	*I*	*F*	*D*	
*F*9	7	*A*	*A*	*A*	*D*	$-D$	*F*	*G*	*F*	*I*	*J*	$-J$	$-I$	*F*	*J*	*P*	*J*	*F*	*D*	*G*	$-J$	*J*	$-G$	$-D$	$-D$	*F*	$-I$	*F*	$-D$
*F*10	7	*A*	*A*	*A*	*D*	$-D$	*F*	*G*	*F*	*I*	*J*	$-J$	$-I$	*F*	$-J$	*P*	$-J$	*F*	*D*	$-G$	$-J$	$-J$	*G*	$-D$	*D*	*F*	*I*	*F*	*D*
*F*11	7	*A*	*A*	*A*	*D*	*D*	*F*	*G*	*F*	*I*	*J*	*J*	*I*	*F*	$-J$	*P*	$-J$	*F*	*D*	$-G$	*J*	$-J$	$-G$	*D*	$-D$	*F*	$-I$	*F*	$-D$
*F*12	7	*A*	*A*	*C*	*A*/2	*E*	*F*	*E*/2	*H*	1*	*E*/10	*H*/2	*I*	*F*	$-E/10$	*H*/2	*I*/2	*R*	*A*/2	$-E/2$	*H*/2	$-I/2$	*R*/2	0	$-E$	*H*	$-I$	*R*	0
*F*13	7	*A*	*A*	*C*	*A*/2	0	*F*	*G*	*H*	1*	*G*	*H*/2	0	*F*	*G*	*H*/2	*Q*	*R*	*A*/2	*G*	*H*/2	*Q*	*R*/2	0	0	*H*	0	*R*	0
*F*14	8	*A*	*A*	*C*	*D*	0	*F*	0	*H*	0	0	*K*	0	*F*	0	*P*	0	*R*	$-D$	0	$-K$	0	0	0	0	*H*	0	*R*	0
*F*15	8	*A*	*B*	*A*	0	*E*	*F*	0	*H*	0	*J*	0	0	*M*	0	*P*	0	*H*	0	0	0	$-J$	0	$-E$	0	*M*	0	*F*	0
*F*16	8	*A*	*B*	*B*	0	0	*F*	0	*H*	0	0	0	0	*M*	*N*	*P*	$-N$	*M*	0	0	0	0	0	0	*Y*	*Z*	0	*Z*	$-Y$
*F*17	10	*A*	*A*	*A*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	*I*	*H*	*K*	*P*	*J*	*F*	*E*	*G*	*J*	*K*	*G*	*D*	*D*	*F*	*I*	*H*	*E*
*F*18	10	*A*	*A*	*A*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	$-I$	*H*	$-K$	*P*	*J*	*F*	$-E$	*G*	$-J$	$-K$	$-G$	$-D$	$-D$	*F*	$-I$	*H*	*E*
*F*19	10	*A*	*A*	*A*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	$-I$	*H*	*K*	*P*	$-J$	*F*	$-E$	$-G$	$-J$	$-K$	*G*	$-D$	*D*	*F*	*I*	*H*	$-E$
*F*20	10	*A*	*A*	*A*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	*I*	*H*	$-K$	*P*	$-J$	*F*	*E*	$-G$	*J*	*K*	$-G$	*D*	$-D$	*F*	$-I$	*H*	$-E$
*F*21	10	*A*	*A*	*C*	*D*	*E*	*F*	*G*	*H*	2*	4*	*H*/2	*L*	5*	7*	*H*/2	*Q*	*R*	11*	13*	*H*/2	18*	*R*/2	0	$-E$	*H*	$-L$	*R*	0
*F*22	10	*A*	*B*	*C*	0	0	*F*	0	*H*	0	0	0	0	*M*	0	*P*	0	*R*	0	0	0	0	0	0	0	*Z*	0	*b*	0
*F*23	10	*A*	*A*	*C*	*D*	0	*F*	0	*H*	*I*	0	*K*	0	*F*	0	*P*	0	*R*	*D*	0	*K*	0	*W*	0	0	*H*	0	*R*	0
*F*24	10	*A*	*B*	*A*	0	*E*	*F*	0	*H*	0	*J*	0	*L*	*M*	0	*P*	0	*H*	0	*T*	0	*J*	0	*E*	0	*M*	0	*F*	0
*F*25	10	*A*	*B*	*B*	0	0	*F*	*G*	*F*	0	0	0	0	*M*	*N*	*P*	*N*	*M*	0	0	0	0	0	0	*Y*	*Z*	*a*	*Z*	*Y*
*F*26	10	*A*	*B*	*C*	*D*	0	*F*	0	*H*	3*	0	*K*	0	6*	0	*P*	0	*R*	*B*/2	0	16*	0	*W*	0	0	22*	0	2*W*	0
*F*27	10	*A*	*B*	*C*	*A*/2	0	*F*	0	*H*	1*	0	*H*/2	0	*M*	0	*P*	0	*R*	12*	0	17*	0	*R*/2	0	0	*Z*	0	*b*	0
*F*28	16	*A*	*B*	*C*	*D*	0	*F*	0	*H*	*I*	0	*K*	0	*M*	0	*P*	0	*R*	*S*	0	*U*	0	*W*	0	0	*Z*	0	*b*	0
*F*29	16	*A*	*B*	*C*	0	*E*	*F*	0	*H*	0	*J*	0	*L*	*M*	0	*P*	0	*R*	0	*T*	0	*V*	0	*X*	0	*Z*	0	*b*	0
*F*30	16	*A*	*B*	*C*	0	0	*F*	*G*	*H*	0	0	0	0	*M*	*N*	*P*	*Q*	*R*	0	0	0	0	0	0	*Y*	*Z*	*a*	*b*	*c*
*F*31	16	*A*	*A*	*C*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	*L*	*F*	$-J$	*P*	*Q*	*R*	*D*	$-G$	*K*	$-Q$	*W*	*X*	$-E$	*H*	$-L$	*R*	$-X$
*F*32	16	*A*	*A*	*C*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	*L*	*F*	*J*	*P*	*Q*	*R*	*D*	*G*	*K*	*Q*	*W*	*X*	*E*	*H*	*L*	*R*	*X*
*F*33	16	*A*	*B*	*A*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	*L*	*M*	*N*	*P*	$-K$	*H*	*S*	*T*	$-N$	*J*	$-G$	*E*	$-S$	*M*	$-I$	*F*	$-D$
*F*34	16	*A*	*B*	*A*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	*L*	*M*	*N*	*P*	*K*	*H*	*S*	*T*	*N*	*J*	*G*	*E*	*S*	*M*	*I*	*F*	*D*
*F*35	16	*A*	*B*	*B*	*D*	$-D$	*F*	*G*	*F*	*I*	*J*	$-J$	$-I$	*M*	*N*	*P*	*N*	*M*	*S*	*T*	*U*	$-U$	$-T$	$-S$	*Y*	*Z*	*a*	*Z*	*Y*
*F*36	16	*A*	*B*	*B*	*D*	*D*	*F*	*G*	*F*	*I*	*J*	*J*	*I*	*M*	*N*	*P*	*N*	*M*	*S*	*T*	*U*	*U*	*T*	*S*	*Y*	*Z*	*a*	*Z*	*Y*
*F*37	16	*A*	*B*	*C*	*D*	*E*	*F*	*G*	*H*	3*	*J*	*K*	*L*	6*	8*	*P*	*Q*	*R*	*B*/2	14*	16*	19*	*W*	*X*	20*	22*	23*	2*W*	2*X*
*F*38	16	*A*	*B*	*C*	*A*/2	0	*F*	*G*	*H*	1*	*G*	*H*/2	0	*M*	*N*	*P*	*Q*	*R*	12*	15*	17*	*Q*	*R*/2	0	*Y*	*Z*	*a*	*b*	*c*
*F*39	16	*A*	*B*	*C*	*D*	*E*	*F*	*G*	*H*	3*	*J*	*K*	*L*	6*	9*	*P*	*Q*	*R*	*B*/2	9*	16*	*Q*	*W*	*X*	0	22*	0	2*W*	0
*F*40	16	*A*	*B*	*C*	*A*/2	*E*	*F*	*E*/2	*H*	1*	*J*	*H*/2	*L*	*M*	10*	*P*	*L*/2	*R*	12*	*T*	17*	*V*	*R*/2	*X*	21*	*Z*	24*	*b*	*X*/2
*F*41	28	*A*	*B*	*C*	*D*	*E*	*F*	*G*	*H*	*I*	*J*	*K*	*L*	*M*	*N*	*P*	*Q*	*R*	*S*	*T*	*U*	*V*	*W*	*X*	*Y*	*Z*	*a*	*b*	*c*

* *Notes.* 1 $-A/4+3F/2$; 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 $-L/4+3V/2$.

Results

Calculations were carried out only for contravariant coefficients; only these enter into the standard crystallographic least-squares procedure. The present tabulation covers all crystallographic settings of special positions for tensors up to rank 6 and all cubic, hexagonal, tetragonal and trigonal settings for tensors up to rank 8. The orientation of the symmetry elements in the lattice must be identified (*e.g.* by inspection of *International Tables for X-ray Crystallography*, 1952) before the tables can be used.

There is a key attributed to each site symmetry given in Table 1. The symmetry relations of this site

may be looked up under the corresponding entry in Table 2.* The order of the coefficients corresponds exactly to the order of assignment of independency, *i.e.* in the case of linear relationships the independent parameters always enter on the left-hand side of the dependent ones. It is worth noting that three of the non-centrosymmetric groups have null third-rank tensors but one free coefficient as some higher level (rank 5 for 422, rank 7 for 622, rank 9 for 432).

It should also be remembered that, in a least-squares refinement of a non-centrosymmetric structure, one parameter corresponding to a non-zero entry for the point group has to be kept fixed (Hazell & Willis, 1978).

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* The tables containing the symmetry restrictions of the seventh- and eighth-rank tensors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38913 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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The Solution of the One-Dimensional Sign Problem for Fourier Transforms

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Abstract

An iterative procedure for the determination of the signs of scattering amplitudes is considered. It is assumed that the scattering density is a one-dimensional antisymmetric function with a limited range of definition. The convergence of the method to a rigorous solution is proved. The stability of the procedure with respect to various experimental errors is shown in model examples. The proof can be generalized for a one-dimensional phase determination of a continuous intensity distribution.

Introduction

When non-crystalline objects are investigated by diffraction methods, the intensity of coherent scattering $I(\mathbf{s})$ can often be measured as a continuous function of scattering vector $\mathbf{s}$ (for instance, intensity distribution along layer lines for one-dimensionally periodic structures, intensity of small-angle scattering). The restoration of the scattering density distribution frequently requires the solution of the phase problem. The latter is analogous to the phase problem in crystal-structure analysis and lies in finding the phases of scattering amplitudes $A(\mathbf{s})$ when their moduli are known from the experimental intensities. In the present paper the case will be considered when the scattering density is a one-dimensional antisymmetric function, so that its connection with the scattering amplitude is given by the sine–Fourier transform

$$A(s) = \mathcal{F}_s[\rho(r)] = \int_0^\infty \rho(r) \sin sr \, dr \qquad (1)$$

and $A(s)$ is a real function.

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