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Direct Methods: the Identification of Space-Group-Specific Inconsistent Three-Phase Structure Invariants

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Abstract

Certain space groups often permit the generation of pairs of triple relationships involving the same three parent reflections in different symmetry forms, giving rise to two equally probable invariant estimates which, because of the space-group symmetry, must disagree by an *a priori* known phase shift. The 230 space groups have been examined to identify those which permit inconsistent triples, and the complete list which describes the forms of the pair of triples and their phase inconsistency is given.

Introduction

Direct-methods procedures in crystallography are usually dependent on the ability to identify and utilize a body of linear phase-invariant relationships which have a variable but high expected probability of being correct. The triple phase invariants

$$\Phi_{\mathbf{h},\mathbf{k}} = \varphi_{\mathbf{h}} - \varphi_{\mathbf{k}} + \varphi_{\mathbf{k}-\mathbf{h}} \quad (1)$$

form the most important class of phase-determining relationships, and usually provide a sufficiently large excess of invariants, $\Phi_{\mathbf{h},\mathbf{k}} \simeq 0$ (modulo 2π), to enable the individual φ's to be determined. The average or expected value associated with a triple invariant is linked to the product of the $|E|$ magnitudes of the three main terms

$$A_{\mathbf{h},\mathbf{k}} = 2\sigma_3/\sigma_2^{3/2}|E_{\mathbf{h}}E_{\mathbf{k}}E_{\mathbf{l}}| \quad (2)$$

with

$$\sigma_n = \sum_j^N Z_j^n,$$

Z_j being the atomic number of the jth atom of the structure having N atoms in the primitive unit cell. The distribution of $\Phi_{\mathbf{h},\mathbf{k}}$ values for a non-centrosymmetric structure (Cochran, 1955) is given as

$$P(\Phi_{\mathbf{h},\mathbf{k}}) = \exp\,(A_{\mathbf{h},\mathbf{k}} \cos \Phi)/[2\pi I_0(A_{\mathbf{h},\mathbf{k}})], \quad (3)$$

leading to an *a priori* cosine estimate (Hauptman, 1966) of

$$\varepsilon[\cos\,(\Phi_{\mathbf{h},\mathbf{k}})] = I_1(A_{\mathbf{h},\mathbf{k}})/I_0(A_{\mathbf{h},\mathbf{k}}). \quad (4)$$

Aberrant phase invariants are those for which $\Phi_{\mathbf{h},\mathbf{k}}$ is sufficiently far from 0 (modulo 2π) to cause tangent-formula phase-refinement methods to diverge from a solution given a basis set of essentially correct starting phases. Empirical estimates of these cosine invariants (Karle & Hauptman, 1957; Vaughan, 1958; Hauptman, 1964, 1972) may be obtained from an algebraic average over the normal quadrupole relationships

$$\Phi_{\mathbf{h},\mathbf{k}} + \Phi_{\mathbf{k},\mathbf{l}} + \Phi_{\mathbf{l},\mathbf{h}} + \Phi_{\mathbf{h}-\mathbf{k},\mathbf{l}-\mathbf{k}} = 0 \quad (5)$$

using sets of six $|E|$ magnitudes taken from fourth-order Karle–Hauptman determinants possessing the invariant $\Phi_{\mathbf{h},\mathbf{k}}$ to be determined.

Inconsistent phase relationships are less precisely identified with a particular phase invariant, and are a consequence of space-group translational symmetry through which a known phase shift must be absorbed in a phasing loop involving a number of phase invariants. The simplest example of an inconsistent phase relationship is two $\sum_1$ invariants which indicate contradictory signs. A more familiar example is given by inconsistent quadrupoles (Viterbo & Woolfson, 1973)

$$\Phi_{\mathbf{h},\mathbf{k}} + \Phi_{\mathbf{k},\mathbf{l}} + \Phi_{\mathbf{l},\mathbf{h}'} + \Phi_{\mathbf{h}-\mathbf{k},(\mathbf{l}-\mathbf{k})'} = n\pi/24 \quad (6)$$

where $\mathbf{h}'$ is a non-Friedel symmetry-related form of the vector $\mathbf{h}$. An illustration in the space group $P2_12_12_1$ is

$$\begin{aligned}\Phi_1 &= \varphi_{2,1,1} + \varphi_{\bar{6},1,\bar{8}} + \varphi_{4,\bar{2},7}\\ \Phi_2 &= \varphi_{6,\bar{1},8} + \varphi_{\bar{4},\bar{5},\bar{7}} + \varphi_{\bar{2},6,\bar{1}}\\ \Phi_3 &= \varphi_{4,5,7} + \varphi_{2,\bar{1},1} + \varphi_{\bar{6},\bar{4},\bar{8}}\\ \Phi_4 &= \varphi_{\bar{4},2,\bar{7}} + \varphi_{\bar{2},\bar{6},\bar{1}} + \varphi_{6,4,8}\end{aligned} \quad (7)$$

where

$$\Phi_1 + \Phi_2 + \Phi_3 + \Phi_4 = \pi \text{ (modulo } 2\pi). \quad (8)$$

Quartet invariants which are related to these inconsistent quadruples may also be seen to be inconsistent:

$$\begin{aligned}\Phi_1 &= \varphi_{2,1,1} + \varphi_{4,\bar{2},7} + \varphi_{\bar{4},\bar{5},\bar{7}} + \varphi_{\bar{2},6,\bar{1}}\\ \Phi_2 &= \varphi_{2,1,1} + \varphi_{\bar{4},\bar{2},\bar{7}} + \varphi_{4,\bar{5},7} + \varphi_{\bar{2},6,\bar{1}}\end{aligned} \quad (9)$$

$$\Phi_1 = \Phi_2 + \pi \text{ (modulo } 2\pi), \quad (10)$$

and characteristically involve a cross term, *e.g.* $E_{0,7,0}$,

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which is a space-group extinction. It is less well known that certain three-phase relationships in chiral space groups have been shown to produce unique phase-invariant probability estimates off the real plane (Pontenagel & Krabbendam, 1983). For example, in the space group $P4_1$ it was shown that the most probable phase of the triple product $E_{2,2,1}E_{\bar{4},0,1,}E_{2,\bar{2},\bar{2}}$ was $-45°$ as a consequence of an inconsistent phase shift relating two distinct symmetry-permitted forms of the same three reciprocal-lattice vectors. Hitherto, single three-phase invariants, apart from pairs of contradictory $\sum_1$ relationships, had not been shown to be inconsistent within phasing loops smaller than a quadruple. We here report the reciprocal-lattice conditions for generating and computing the phase-shift inconsistency for all such possible triples in the 230 space groups. These special relationships are also shown to occur in non-chiral and centrosymmetric space groups.

Inconsistent three-phase invariants

Symmetry-equivalent transformations in reciprocal space are often separated into parent- and daughter-form operations. A parent transformation affects only the signs of the h, k and l components of a lattice vector, and not the magnitudes; a daughter operation transforms a vector as a mixed function of the h, k and l components. Examples of the latter are the trigonal transformation h, k, l to $k, -h-k, l$ or the tetragonal transformation h, k, l to k, h, l in which the h and k indices are interchanged. The question may be raised whether, given the triple invariant $\mathbf{h}+\mathbf{k}+\mathbf{l}=0$, the same three vectors may be combined in a non-identical manner, $\mathbf{h}+\mathbf{k}.\mathbf{R}_j+\mathbf{l}.\mathbf{R}_k=0$, where $\mathbf{R}_i$ is the inverse of the rotational matrix of the ith equivalent position of the space group or its Friedel equivalent. Clearly no *independent* solutions

$$\mathbf{k}.(\mathbf{R}_j-\mathbf{I})+\mathbf{l}.(\mathbf{R}_k-\mathbf{I})=0 \tag{11}$$

exist if $\mathbf{R}_j$ and $\mathbf{R}_k$ both represent parent transformations, as $\mathbf{k}$ would be forced to be a symmetry transformation of $\mathbf{l}$ and define a $\sum_1$ invariant. The situation is different if either $\mathbf{R}_j$ or $\mathbf{R}_k$ or both represent daughter transformations, for example in space group $P4_12_12$:

$$\begin{aligned}\Phi_1&=\varphi_{2,1,1}+\varphi_{\bar{1},2,3}+\varphi_{\bar{1},\bar{3},\bar{4}}\\ \Phi_2&=\varphi_{2,1,1}+\varphi_{1,\bar{2},3}+\varphi_{\bar{3},1,\bar{4}}\end{aligned} \tag{12}$$

$$\Phi_1=\Phi_2+\pi \text{ (modulo } 2\pi). \tag{13}$$

Given that examples of inconsistent triples could exist, (11) was exhaustively applied to all 230 space groups using Burzlaff & Hountas's (1982) equivalent-position generation routine to determine if solutions existed and whether a non-zero phase shift, $\mathbf{k}.\mathbf{t}_j+\mathbf{l}.\mathbf{t}_k$, was resultant, where the $\mathbf{t}_i$ are the associated translation components. The results for all space groups satisfying (11) are given in Table 1, together with information in Tables 2 and 3 which defines the form of the pairs of inconsistent triples and the value of the phase-invariant discrepancy based on the particular reflections involved. In the previous example, the first two parent reflections are 211 and 213. The necessary conditions relating these first two parent reflections can be found in Table 1(b) under the first entry for space group $P4_12_12$ (HK-A-B-4). The HK entry indicates that $h_1=h_2$, $k_1=k_2$; the A condition in Table 2 gives the form of the second reflection in the first triple as $\bar{1}23$ $(-k_2, h_2, l_2)$, and the B condition gives its form as $1\bar{2}3$ $(k_2, -h_2, l_2)$ in the second triple. The number 4 indicates that the phase shift is equal to $2\pi(\frac{3}{4}l_1+\frac{1}{4}l_2)$ (modulo 2π), or 180°.

Discussion

Inconsistent phase relationships provide a valuable framework for identifying, if not correcting, potential phasing traps in direct-methods analyses. Given that the number of inconsistent relationships generated from a basis of triple invariants usually represents a small percentage of the normal consistent ones (Viterbo & Woolfson, 1973), it is often feasible simply to remove all those triples which enter into inconsistent relationships from the phasing process without adversely introducing a large number of holes into subsequent phase extension maps. Should it be a problem that a structure in a particular space group does generate a large percentage of inconsistent relationships, cosine-invariant estimation methods may be used to help identify the most aberrant triple invariant in the relation so that the more reliable ones can be retained.

An inherent weakness of cosine-invariant estimation techniques, both algebraic methods and those derived from probability distributions, is that they generally assume only $P1$ or $P\bar{1}$ symmetry. Algebraic triples formulae, for example, will produce the same three-phase cosine estimates from a monoclinic data set, regardless of the space group assumed within the lattice type for the structure. That is because the formulae use only the $|E|$ magnitudes of the vectors defining normal quadrupoles, and the quadrupoles generated for any space group within a Laue group will be the same; space-group-specific information such as phase relationships among the symmetry-related reflections and phase restrictions are not utilized. In spite of this weakness, these formulae can, however, make a clear distinction between the estimates of a pair of inconsistent triples, simply because the $|E|$ values selected by their second neighborhoods are different.

Recent methods which propose to utilize the maximum space-group symmetry in deriving the joint probability distributions of structure factors may offer an advantage over the $P1$ and $P\bar{1}$ approximations

Table 1. *Conditions, styles and phase shifts for all space groups which can form daughter triple pairs*

HK, *HL* denote conditions of $h_1 = h_2$ and $k_1 = k_2$, $h_1 = h_2$ and $l_1 = l_2$ respectively. Single letters *A* to *P* are triple styles and numerals 0 to 19 are used for phase shifts. All symbols, except *HK* and *HL*, refer to Tables 2 and 3.

(*a*) Centrosymmetric space groups

Space group	Triple pair Number 1	Number 2	Number 3	Number 4
$P4/m$	HK-A-B-0	HK-C-D-0		
$P4_2/m$	HK-A-B-1	HK-C-D-1		
$P4/n$	HK-A-B-0	HK-C-D-0		
$P4_2/n$	HK-A-B-1	HK-C-D-1		
$I4/m$	HK-A-B-0	HK-C-D-0		
$I4_1/a$	HK-A-B-2	HK-C-D-3		
$P4/mmm$	HK-A-B-0	HK-C-D-0		
$P4/mcc$	HK-A-B-0	HK-C-D-0		
$P4/nbm$	HK-A-B-0	HK-C-D-0		
$P4/nnc$	HK-A-B-0	HK-C-D-0		
$P4/mbm$	HK-A-B-0	HK-C-D-0		
$P4/mnc$	HK-A-B-0	HK-C-D-0		
$P4/nmm$	HK-A-B-0	HK-C-D-0		
$P4/ncc$	HK-A-B-0	HK-C-D-0		
$P4_2/mmc$	HK-A-B-1	HK-C-D-1		
$P4_2/mcm$	HK-A-B-1	HK-C-D-1		
$P4_2/nbc$	HK-A-B-1	HK-C-D-1		
$P4_2/nnm$	HK-A-B-1	HK-C-D-1		
$P4_2/mbc$	HK-A-B-1	HK-C-D-1		
$P4_2/mnm$	HK-A-B-1	HK-C-D-1		
$P4_2/nmc$	HK-A-B-1	HK-C-D-1		
$P4_2/ncm$	HK-A-B-1	HK-C-D-1		
$I4/mmm$	HK-A-B-0	HK-C-D-0		
$I4/mcm$	HK-A-B-0	HK-C-D-0		
$I4_1/amd$	HK-A-B-2	HK-C-D-3		
$I4_1/acd$	HK-A-B-4	HK-C-D-5		
$P\bar{3}$	HK-E-F-0			
$R\bar{3}$	HK-E-F-0			
$P\bar{3}1m$	HK-E-F-0			
$P\bar{3}1c$	HK-E-F-0			
$P\bar{3}m1$	HK-E-F-0			
$P\bar{3}c1$	HK-E-F-0			
$R\bar{3}m$	HK-E-F-0			
$R\bar{3}c$	HK-E-F-0			
$P6/m$	HK-G-H-0	HK-E-F-0	HK-I-J-0	HK-K-L-0
$P6_3/m$	HK-G-H-1	HK-E-F-0	HK-I-J-1	HK-K-L-0
$P6/mmm$	HK-G-H-0	HK-I-J-0	HK-E-F-0	HK-K-L-0
$P6/mcc$	HK-G-H-0	HK-I-J-0	HK-E-F-0	HK-K-L-0
$P6_3/mcm$	HK-G-H-1	HK-I-J-1	HK-E-F-0	HK-K-L-0
$P6_3/mmc$	HK-G-H-1	HK-I-J-1	HK-E-F-0	HK-K-L-0
$Pm3m$	HL-M-N-0	HK-A-B-0	HL-O-P-0	HK-C-D-0
$Pn3n$	HL-M-N-0	HK-A-B-0	HL-O-P-0	HK-C-D-0
$Pm3n$	HL-M-N-6	HK-A-B-1	HL-O-P-6	HK-C-D-1
$Pn3m$	HL-M-N-6	HK-A-B-1	HL-O-P-6	HK-C-D-1
$Fm3m$	HL-M-N-0	HK-A-B-0	HL-O-P-0	HK-C-D-0
$Fm3c$	HL-M-N-0	HK-A-B-1	HL-O-P-7	HK-C-D-8
$Fd3m$	HL-M-N-9	HK-A-B-3	HL-O-P-10	HK-C-D-11
$Fd3c$	HL-M-N-9	HK-A-B-5	HL-O-P-10	HK-C-D-12
$Im3m$	HL-M-N-0	HK-A-B-0	HL-O-P-0	HK-C-D-0
$Ia3d$	HL-M-N-9	HK-A-B-2	HL-O-P-13	HK-C-D-3

(*b*) Non-centrosymmetric space groups

Space group	Triple pair Number 1	Number 2	Number 3	Number 4
$P4$	HK-A-B-0	HK-C-D-0		
$P4_1$	HK-A-B-4	HK-C-D-2		
$P4_2$	HK-A-B-1	HK-C-D-1		
$P4_3$	HK-A-B-2	HK-C-D-4		
$I4$	HK-A-B-0	HK-C-D-0		
$I4_1$	HK-A-B-4	HK-C-D-2		
$P\bar{4}$	HK-A-B-0	HK-C-D-0		
$I\bar{4}$	HK-A-B-0	HK-C-D-0		
$P422$	HK-A-B-0	HK-C-D-0		
$P42_12$	HK-A-B-0	HK-C-D-0		
$P4_122$	HK-A-B-4	HK-C-D-2		
$P4_12_12$	HK-A-B-4	HK-C-D-2		
$P4_222$	HK-A-B-1	HK-C-D-1		
$P4_22_12$	HK-A-B-1	HK-C-D-1		
$P4_322$	HK-A-B-2	HK-C-D-4		
$P4_32_12$	HK-A-B-2	HK-C-D-4		
$I422$	HK-A-B-0	HK-C-D-0		
$I4_122$	HK-A-B-4	HK-C-D-2		
$P4mm$	HK-A-B-0	HK-C-D-0		
$P4bm$	HK-A-B-0	HK-C-D-0		
$P4_2cm$	HK-A-B-1	HK-C-D-1		
$P4_2nm$	HK-A-B-1	HK-C-D-1		
$P4cc$	HK-A-B-0	HK-C-D-0		
$P4nc$	HK-A-B-0	HK-C-D-0		
$P4_2mc$	HK-A-B-1	HK-C-D-1		
$P4_2bc$	HK-A-B-1	HK-C-D-1		
$I4mm$	HK-A-B-0	HK-C-D-0		
$I4cm$	HK-A-B-0	HK-C-D-0		
$I4_1md$	HK-A-B-2	HK-C-D-2		
$I4_1cd$	HK-A-B-2	HK-C-D-5		
$P\bar{4}2m$	HK-A-B-0	HK-C-D-0		
$P\bar{4}2c$	HK-A-B-0	HK-C-D-0		
$P\bar{4}2_1m$	HK-A-B-0	HK-C-D-0		
$P\bar{4}2_1c$	HK-A-B-0	HK-C-D-0		
$P\bar{4}m2$	HK-A-B-0	HK-C-D-0		
$P\bar{4}c2$	HK-A-B-0	HK-C-D-0		
$P\bar{4}b2$	HK-A-B-0	HK-C-D-0		
$P\bar{4}n2$	HK-A-B-0	HK-C-D-0		
$I\bar{4}m2$	HK-A-B-0	HK-C-D-0		
$I\bar{4}c2$	HK-A-B-0	HK-C-D-0		
$I\bar{4}2m$	HK-A-B-0	HK-C-D-0		
$I\bar{4}2d$	HK-A-B-0	HK-C-D-0		
$P3$	HK-E-F-0			
$P3_1$	HK-E-F-14			
$P3_2$	HK-E-F-15			
$R3$	HK-E-F-0			
$P312$	HK-E-F-0			
$P321$	HK-E-F-0			
$P3_112$	HK-E-F-14			
$P3_121$	HK-E-F-14			
$P3_212$	HK-E-F-15			
$P3_221$	HK-E-F-15			
$R32$	HK-E-F-0			
$P3m1$	HK-E-F-0			
$P31m$	HK-E-F-0			
$P3c1$	HK-E-F-0			
$P31c$	HK-E-F-0			
$R3m$	HK-E-F-0			
$R3c$	HK-E-F-0			
$P6$	HK-G-H-0	HK-E-F-0	HK-K-L-0	HK-I-J-0
$P6_1$	HK-G-H-16	HK-E-F-14	HK-K-L-15	HK-I-J-17
$P6_5$	HK-G-H-17	HK-E-F-15	HK-K-L-14	HK-I-J-16
$P6_2$	HK-G-H-14	HK-E-F-15	HK-K-L-14	HK-I-J-15
$P6_4$	HK-G-H-15	HK-E-F-14	HK-K-L-15	HK-I-J-14
$P6_3$	HK-G-H-1	HK-E-F-0	HK-K-L-0	HK-I-J-1
$P\bar{6}$	HK-K-L-0	HK-E-F-0	HK-G-H-0	HK-I-J-0
$P622$	HK-G-H-0	HK-E-F-0	HK-K-L-0	HK-I-J-0
$P6_122$	HK-G-H-16	HK-E-F-14	HK-K-L-15	HK-I-J-17
$P6_522$	HK-G-H-17	HK-E-F-15	HK-K-L-14	HK-I-J-16
$P6_222$	HK-G-H-14	HK-E-F-15	HK-K-L-14	HK-I-J-15
$P6_422$	HK-G-H-15	HK-E-F-14	HK-K-L-15	HK-I-J-14
$P6_322$	HK-G-H-1	HK-E-F-0	HK-K-L-0	HK-I-J-1
$P6mm$	HK-G-H-0	HK-E-F-0	HK-K-L-0	HK-I-J-0
$P6cc$	HK-G-H-0	HK-E-F-0	HK-K-L-0	HK-I-J-0
$P6_3cm$	HK-G-H-1	HK-E-F-0	HK-K-L-0	HK-I-J-1
$P6_3mc$	HK-G-H-1	HK-E-F-0	HK-K-L-0	HK-I-J-1
$P\bar{6}m2$	HK-K-L-0	HK-E-F-0	HK-G-H-0	HK-I-J-0
$P\bar{6}c2$	HK-K-L-0	HK-E-F-0	HK-G-H-1	HK-I-J-1
$P\bar{6}2m$	HK-K-L-0	HK-E-F-0	HK-G-H-0	HK-I-J-0
$P\bar{6}2c$	HK-K-L-0	HK-E-F-0	HK-G-H-1	HK-I-J-1
$P432$	HL-M-N-0	HK-A-B-0	HL-O-P-0	HK-C-D-0
$P4_232$	HL-M-N-6	HK-A-B-1	HL-O-P-6	HK-C-D-1
$F432$	HL-M-N-0	HK-A-B-0	HL-O-P-0	HK-C-D-0
$F4_132$	HL-M-N-13	HK-A-B-3	HL-O-P-13	HK-C-D-3
$I432$	HL-M-N-0	HK-A-B-0	HL-O-P-0	HK-C-D-0
$P4_332$	HL-M-N-18	HK-A-B-4	HL-O-P-13	HK-C-D-3

Table 1 (*cont.*)

Space group	Triple pair			
(*b*) Non-centrosymmetric space groups				
	Number 1	Number 2	Number 3	Number 4
$P4_132$	*HL-M-N*-9	*HK-A-B*-2	*HL-O-P*-19	*HK-C-D*-5
$I4_132$	*HL-M-N*-9	*HK-A-B*-2	*HL-O-P*-19	*HK-C-D*-5
$P\bar{4}3m$	*HL*-0-*P*-0	*HK-C-D*-0	*HL-M-N*-0	*HK-A-B*-0
$F\bar{4}3m$	*HL*-0-*P*-0	*HK-C-D*-0	*HL-M-N*-0	*HK-A-B*-0
$I\bar{4}3m$	*HL*-0-*P*-0	*HK-C-D*-0	*HL-M-N*-0	*HK-A-B*-0
$P\bar{4}3n$	*HL*-0-*P*-6	*HK-C-D*-1	*HL-M-N*-6	*HK-A-B*-1
$F\bar{4}3c$	*HL*-0-*P*-0	*HK-C-D*-0	*HL-M-N*-0	*HK-A-B*-0
$I\bar{4}3d$	*HL*-0-*P*-19	*HK-C-D*-5	*HL-M-N*-9	*HK-A-B*-2

Table 2. *Styles of triples in Table* 1

The first reflection is always h_1, k_1, l_1.

	Second reflection			Third reflection		
A	$-k_2$,	h_2,	l_2;	$-h_1+k_2$,	$-k_1-h_2$,	$-l_1-l_2$;
B	k_2,	$-h_2$,	l_2;	$-h_1-k_2$,	$-k_1+h_2$,	$-l_1-l_2$;
C	$-k_2$,	h_2,	$-l_2$;	$-h_1+k_2$,	$-k_1-h_2$,	$-l_1+l_2$;
D	k_2,	$-h_2$,	$-l_2$;	$-h_1-k_2$,	$-k_1+h_2$,	$-l_1+l_2$;
E	k_2,	$-h_2-k_2$,	l_2;	$-h_1-k_2$,	$-k_1+h_2+k_2$,	$-l_1-l_2$;
F	$-h_2-k_2$,	h_2,	l_2;	$-h_1+h_2+k_2$,	$-k_1-h_2$,	$-l_1-l_2$;
G	$-k_2$,	h_2+k_2,	l_2;	$-h_1+k_2$,	$-k_1-h_2-k_2$,	$-l_1-l_2$;
H	h_2+k_2,	$-h_2$,	l_2;	$-h_1-h_2-k_2$	$-k_1+h_2$,	$-l_1-l_2$;
I	$-k_2$,	h_2+k_2,	$-l_2$;	$-h_1+k_2$,	$-k_1-h_2-k_2$,	$-l_1+l_2$;
J	h_2+k_2,	$-h_2$,	$-l_2$;	$-h_1-h_2-k_2$,	$-k_1+h_2$,	$-l_1+l_2$;
K	$-h_2-k_2$,	h_2,	$-l_2$;	$-h_1+h_2+k_2$,	$-k_1-h_2$,	$-l_1+l_2$;
L	k_2,	$-h_2-k_2$,	$-l_2$;	$-h_1-k_2$,	$-k_1+h_2+k_2$,	$-l_1+l_2$;
M	l_2,	k_2,	$-h_2$;	$-h_1-l_2$,	$-k_1-k_2$,	$-l_1+h_2$;
N	$-l_2$,	k_2,	h_2;	$-h_1+l_2$,	$-k_1-k_2$,	$-l_1-h_2$;
O	l_2,	$-k_2$,	$-h_2$;	$-h_1-l_2$,	$-k_1+k_2$,	$-l_1+h_2$;
P	$-l_2$,	$-k_2$,	h_2;	$-h_1+l_2$,	$-k_1+k_2$,	$-l_1-h_2$;

Table 3. *Phase shift between the triple pairs in Table* 1

	Phase shift
0	0
1	$\frac{1}{2}l_1+\frac{1}{2}l_2$
2	$\frac{1}{4}l_1+\frac{3}{4}l_2$
3	$\frac{1}{4}l_1+\frac{1}{2}h_2+\frac{1}{2}k_2+\frac{3}{4}l_2$
4	$\frac{3}{4}l_1+\frac{1}{4}l_2$
5	$\frac{3}{4}l_1+\frac{1}{2}h_2+\frac{1}{2}k_2+\frac{1}{4}l_2$
6	$\frac{1}{2}k_1+\frac{1}{2}k_2$
7	$\frac{1}{2}h_2+\frac{1}{2}l_2$
8	$\frac{1}{2}l_1+\frac{1}{2}h_2+\frac{1}{2}k_2+\frac{1}{2}l_2$
9	$\frac{1}{4}k_1+\frac{3}{4}k_2$
10	$\frac{1}{4}k_1+\frac{1}{2}h_2+\frac{3}{4}k_2$
11	$\frac{1}{4}l_1+\frac{1}{2}k_2+\frac{3}{4}l_2$
12	$\frac{3}{4}l_1+\frac{1}{2}h_2+\frac{1}{4}l_2$
13	$\frac{1}{4}k_1+\frac{1}{2}h_2+\frac{3}{4}k_2+\frac{1}{2}l_2$
14	$\frac{2}{3}l_1+\frac{1}{3}l_2$
15	$\frac{1}{3}l_1+\frac{2}{3}l_2$
16	$\frac{5}{6}l_1+\frac{1}{6}l_2$
17	$\frac{1}{6}l_1+\frac{5}{6}l_2$
18	$\frac{3}{4}k_1+\frac{1}{4}k_2$
19	$\frac{3}{4}k_1+\frac{1}{2}h_2+\frac{1}{4}k_2+\frac{1}{2}l_2$

(Castleden, 1987; Peschar & Schenk, 1987). The first neighborhood estimate, *i.e.* the joint probability distribution provided by the three *E* values of a pair of inconsistent triples, should provide a lower estimate than the $P1$ or $P\bar{1}$ formula for the cosine invariant. This lowered estimate would be consistent with the phase inconsistency but would not distinguish which of the two triples is more reliable, as both estimates must be equal. One will of necessity have to derive a second neighborhood distribution to obtain this differentiation. These same conditions may also be seen to apply to $P1$ triples formula distributions based on one-wavelength anomalous-dispersion data (Hauptman, 1982), where suitable conditioning of the distribution will be required if one wishes to utilize the inconsistent triples information. The simplest remedy, however, as stated above, may be to ignore these inconsistent relations when applying these formulae. In this regard the data given in the tables will enable one to identify the inconsistent triples for all 230 space groups.

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