

## The Symmetry of Interatomic Lattice Potentials in General Crystal Structures. 2. The Cases of F.C.C., B.C.C. and H.C.P. Disordered Structures

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### Abstract

On the basis of the approach developed in the previous paper [Bugaev & Chepul'skii (1995). *Acta Cryst.*, **A51**, 456–462] within the framework of the multicomponent lattice gas model, the symmetry properties of the unary and binary mixing potentials and of the Fourier transforms of the binary potential for disordered interstitial-substitutional solid solutions with f.c.c., b.c.c. and h.c.p. crystal lattices are analyzed.

### 1. Introduction

In the previous study (Bugaev & Chepul'skii, 1995) (hereafter denoted paper 1), within the framework of the multicomponent lattice gas model, the symmetry properties of many-particle mixing potentials for a solid solution with a given arbitrary crystal structure were considered. The relationships between the matrix elements of mixing potentials and of their Fourier transforms caused by the space symmetry of the crystal structure were obtained. The aim of this paper is to make specific the above-mentioned relationships for the f.c.c., b.c.c. and h.c.p. disordered crystal structures, taking into account the possible distribution of the atom components (substitutional and interstitial) among the sites and octahedral and tetrahedral interstices of the crystal lattice. Consideration of all these types of position within the framework of the unified scheme is dictated by an aspiration to make the results of this work applicable to traditional substitutional or interstitial alloys and also to the alloys in which the atoms of one or other component can change their coordination under the variations of external thermodynamic parameters. Examples are some metal–hydrogen alloys in which the H atoms can occupy both octahedral and tetrahedral interstices of the crystal lattice of one metal (*e.g.* Fromm & Gebhardt, 1976). As another example, one can consider so-called hybrid substitutional-interstitial solid solutions in which the atoms of one component can occupy both the sites and the interstices (McLellan, 1989). We restrict the consideration to the cases of binary and unary mixing potentials since they hold a central position in the advanced theories of solid solutions.

In §2, the results obtained in paper 1 concerning the symmetry properties of the injection and binary mixing

potentials and the transformation rules for the Fourier components of the latter are summarized.

In §3, the lattice gas model is implemented for the distribution of atoms of corresponding components at sites and at interstices (for both octahedral and tetrahedral coordinations of interstitial atoms) in f.c.c., b.c.c. and h.c.p. crystal lattices. This consideration involves the cases of substitutional, interstitial and composite interstitial-substitutional solid solutions simultaneously. Interchange rules between positions of different types due to the symmetry operations are obtained.

In §4, it is shown that, at each considered f.c.c., b.c.c. and h.c.p. disordered structure, the injection energies for positions belonging to the same type of position (site, octahedral or tetrahedral interstices) are equal. The symmetry analysis also allows us to list the coordination shells where noncentrality (anisotropy) is possible for interatomic interactions of the components (both interstitial and substitutional) in the above-mentioned crystal structures.

In §5, the selection of the independent matrix elements of the Fourier transforms of the binary mixing energies for the f.c.c., b.c.c. and h.c.p. disordered structures is performed (on the basis of the symmetry requirements imposed on these matrix elements) and the explicit analytical interrelations between the dependent and independent elements are obtained. The results can be used to control the symmetry adequacy of interatomic potentials obtained both on the basis of the semi-phenomenological consideration and within the first-principle theories of the solid solutions with corresponding crystal structures.

In §6, the matrices of the Fourier transforms of binary mixing energies for the case of the high-symmetry points of the reciprocal lattice of disordered f.c.c., b.c.c. and h.c.p. structures are constructed, taking into account the symmetry relationships between corresponding matrix elements. The importance of the similar separate analysis of this particular case is determined by the fact that the corresponding independent matrix elements are the basic parameters of the advanced theories of solid solutions (*e.g.* de Fontaine, 1979; Khachatryan, 1978, 1983; Yukhnovskii & Gurskii, 1991). In these theories, the symmetry information on a structure of the Fourier transforms of the binary mixing potentials is sufficient

for the choice of the convenient sets of basis functions for expansions into series within the concentration-waves method when analyzing the possible channels of structural instabilities in solid solutions.

## 2. Symmetry of unary and binary mixing potentials

The potential  $E$  of the multicomponent solid solution within the generalized model of a lattice gas, taking into account the one- and two-particle interactions, can be obtained from formulae (1.9), (1.34) and (1.36):\*

$$E = V_0 + \sum_p \sum_{\alpha=\alpha_1}^{Z_p} \Phi_p^\alpha N_p^\alpha + \frac{1}{2} \sum_{\mathbf{R}_1, \mathbf{R}_2} \sum_{p_1, p_2} \sum_{\alpha_1=\alpha_1^{p_1}}^{Z_{p_1}} \sum_{\alpha_2=\alpha_2^{p_2}}^{Z_{p_2}} w_{p_1 p_2}^{\alpha_1 \alpha_2}(\mathbf{R}_1 - \mathbf{R}_2) \times C_{\alpha_1}(p_1, \mathbf{R}_1) C_{\alpha_2}(p_2, \mathbf{R}_2). \quad (1)$$

Here,  $V_0$  is the potential of the solid solution in which any sublattice  $p$  is completed by the particles of type  $\alpha_0^p$ ,  $N_p^\alpha$  is the total number of  $\alpha$  particles in the  $p$  sublattice,  $\Phi_p^\alpha$  is the potential of injection of the  $\alpha$  particle into the  $p$  position (the unary mixing potential),  $w_{p_1 p_2}^{\alpha_1 \alpha_2}(\mathbf{R}_1 - \mathbf{R}_2)$  is the binary mixing potential, which we shall call in this work the mixing potential of the solution. The quantities  $C_\alpha(p, \mathbf{R})$  are defined by (1.3):

$$C_\alpha(p, \mathbf{R}) \equiv \begin{cases} 1 & \text{if the position } (p, \mathbf{R}) \text{ is occupied by} \\ & \text{an } \alpha\text{-type atom} \\ 0 & \text{in the opposite case;} \end{cases} \quad (2)$$

the summations over  $\mathbf{R}$  and  $p$  are taken over  $N$  primitive unit cells and  $\nu$  sublattices, respectively, and the summation over  $\alpha$  is taken over  $\alpha_1^p, \alpha_2^p, \dots, \alpha_{Z_p}^p$  types of atoms allowed for in the occupation within the sublattices  $p$ , excluding the type  $\alpha_0^p$ .

In accordance with paper 1, the choice of the primitive unit cell (determined by the set of radius vectors  $\mathbf{R}$ ) in the multicomponent solid solution (MSS) in the given structural state should be performed in such a way that the set  $\{\mathbf{R}\}$  coincides with the set of translation periods of the space symmetry group  $G$ . Thus, in the disordered state, the MSS space symmetry coincides with the space symmetry of the MSS crystal lattice and we can use the primitive unit cell of this lattice without any changes. In this case, unlike the case of the ordered state, the sublattices  $p$  are distinguished by the crystallographic factor only.

The symmetry relationships for the components of the injection and mixing potentials in accordance with

(1.35), (1.37) and (1.38) have the following form:

$$\Phi_{p'}^\alpha = \Phi_p^\alpha, \quad (3)$$

$$w_{p'q}^{\alpha\beta}(\mathbf{R}) = w_{qp}^{\beta\alpha}(-\mathbf{R}), \quad (4)$$

$$w_{p'q'}^{\alpha\beta}(\mathbf{R}') = w_{pq}^{\alpha\beta}(\mathbf{R}), \quad (5)$$

where the primed quantities can be obtained from non-primed ones as a result of the symmetry transformation  $g = \{S|\tau(S) + \mathbf{R}_m\}$  (see paper 1, §3) belonging to the symmetry group  $G$ :

$$\mathbf{X}(p', \mathbf{R}') \equiv g\mathbf{X}(p, \mathbf{R}) \quad (6)$$

$[\mathbf{X}(p, \mathbf{R}) = \mathbf{R} + \mathbf{h}_p$  are the radius vectors of the positions  $(p, \mathbf{R})$ ,  $\mathbf{h}_p$  are the vectors of the primitive unit-cell basis].

The matrix  $\|\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k})\|$  of the mixing-potential Fourier transforms is defined by (1.39) as

$$\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k}) = \sum_{\mathbf{R}} w_{pq}^{\alpha\beta}(\mathbf{R}) \exp[-i(\mathbf{k}, \mathbf{R})]. \quad (7)$$

The relationships between the elements of this matrix according to (1.40)–(1.43) can be represented as

$$\tilde{w}_{p'q'}^{\alpha\beta}(S\mathbf{k}) = \tilde{w}_{pq}^{\alpha\beta}(\mathbf{k}) \exp[i(S\mathbf{k}, \mathbf{h}_{p'} - \mathbf{h}_{q'}) - i(\mathbf{k}, \mathbf{h}_p - \mathbf{h}_q)], \quad (8)$$

$$\tilde{w}_{pq}^{\alpha\beta}(-\mathbf{k}) = \tilde{w}_{pq}^{\alpha\beta*}(\mathbf{k}), \quad (9)$$

$$\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k}) = \tilde{w}_{qp}^{\beta\alpha}(-\mathbf{k}), \quad (10)$$

$$\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k} + \mathbf{b}) = \tilde{w}_{pq}^{\alpha\beta}(\mathbf{k}), \quad (11)$$

where  $\mathbf{b}$  is an arbitrary vector of the reciprocal lattice.

## 3. The rules of position types interchange under the symmetry transformations in f.c.c., b.c.c. and h.c.p. disordered structures

Under sufficiently high temperatures (but lower than the melting temperature), solid solutions are, as a rule, in the disordered state.\* If the temperature is lowered, the series of step-by-step phase transformations of the ordering type take place. Thus, the disordered state is an initial state for all following ordered states of solution. Therefore, it would be reasonable to consider disordered solid solutions first.

Let us consider the disordered interstitial-substitutional solid solution based on f.c.c., b.c.c. or h.c.p. lattices. Suppose corresponding atoms (interstitial and substitutional) are distributed among the sites  $m$ , octahedral  $o$  and tetrahedral  $t$  interstices of these lattices. In Figs.

\*The references for the formulae from paper 1 are presented in the form (1.XX). The number after the point is the equation number in paper 1.

\*The exclusions are some intermetallic and ceramic chemical compounds, in which the disordered state cannot occur.

1(a)–(c), the relative arrangement of the sites and interstices within the primitive unit cell formed by the elementary translation vectors  $\mathbf{a}_i$  ( $i = 1, 2, 3$ ) of f.c.c., b.c.c. and h.c.p. lattices, respectively, is shown.\* The coordinates of the vectors that specify the positions of sites and interstices within the primitive unit cell are:†

f.c.c.

$$\mathbf{h}_m = (0, 0, 0); \quad \mathbf{h}_o = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right);$$

$$\mathbf{h}_{t_1} = \left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right); \quad \mathbf{h}_{t_2} = \left(\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right);$$

b.c.c.

$$\mathbf{h}_m = (0, 0, 0);$$

$$\mathbf{h}_{o_1} = \left(0, \frac{1}{2}, \frac{1}{2}\right); \quad \mathbf{h}_{o_2} = \left(\frac{1}{2}, 0, \frac{1}{2}\right); \quad \mathbf{h}_{o_3} = \left(\frac{1}{2}, \frac{1}{2}, 0\right);$$

$$\mathbf{h}_{t_1} = \left(\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right); \quad \mathbf{h}_{t_2} = \left(\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right); \quad \mathbf{h}_{t_3} = \left(\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right);$$

$$\mathbf{h}_{t_4} = \left(\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right); \quad \mathbf{h}_{t_5} = \left(\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right); \quad \mathbf{h}_{t_6} = \left(\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right);$$

h.c.p.

$$\mathbf{h}_{m_1} = \left(\frac{2}{3}, \frac{1}{3}, \frac{3}{4}\right)_H; \quad \mathbf{h}_{m_2} = \left(\frac{1}{3}, \frac{2}{3}, \frac{1}{4}\right)_H;$$

$$\mathbf{h}_{o_1} = (0, 0, 0)_H; \quad \mathbf{h}_{o_2} = \left(0, 0, \frac{1}{2}\right)_H;$$

$$\mathbf{h}_{t_1} = \left(\frac{1}{3}, \frac{2}{3}, \frac{1}{2} + \Delta\right)_H; \quad \mathbf{h}_{t_2} = \left(\frac{2}{3}, \frac{1}{3}, \Delta\right)_H;$$

$$\mathbf{h}_{t_3} = \left(\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - \Delta\right)_H; \quad \mathbf{h}_{t_4} = \left(\frac{1}{3}, \frac{2}{3}, 1 - \Delta\right)_H,$$

\* In the h.c.p. lattice, the vector  $\mathbf{a}_3$  is directed alongside the sixfold axis ( $c$  axis),  $\mathbf{a}_1$  and  $\mathbf{a}_2$  are normal to  $\mathbf{a}_3$  and form an angle of  $120^\circ$ , the origin of the primitive unit cell is placed at the center of the inversion of the h.c.p. crystal (at  $o_1$  interstice).

† The coordinates are given on a crystallographic basis  $\{\mathbf{a}_i\}$ , i.e.  $\mathbf{h}_x = (X_1, X_2, X_3) \equiv X_1\mathbf{a}_1 + X_2\mathbf{a}_2 + X_3\mathbf{a}_3$  (where  $X$  is any of the positions in question).

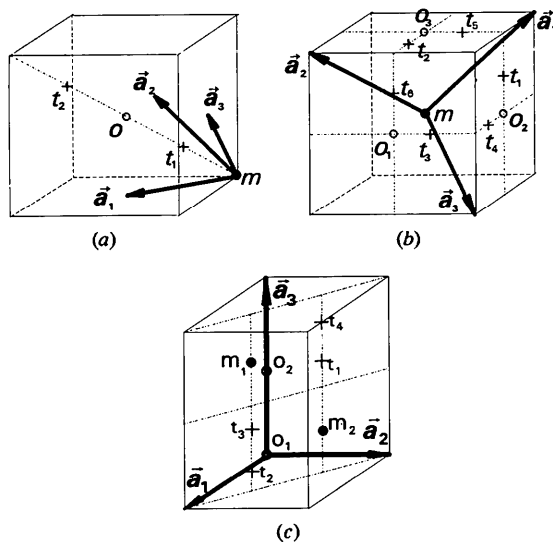


Fig. 1. Relative arrangement of the sites and interstices within the primitive unit cell [formed by the vectors  $\mathbf{a}_i$  ( $i = 1, 2, 3$ ) of elementary translations] of (a) f.c.c., (b) b.c.c. and (c) h.c.p. crystal lattices.

where  $\Delta \equiv (1/3)(a/c)^2$  and  $a$  and  $c$  are the translation periods of the h.c.p. lattice in the basis plane and in the normal direction to it, respectively.

The space symmetry groups of f.c.c., b.c.c. and h.c.p. lattices (and, therefore, of corresponding disordered solutions based on them) are  $O_h^5 = Fm\bar{3}m$ ,  $O_h^9 = Im\bar{3}m$  and  $D_{6h}^4 = P6_3/mmc$ , respectively (*International Tables for X-ray Crystallography*, 1952). In Tables 1–3, the interchange rules for the sites and interstices of the different types are shown for the cases of f.c.c., b.c.c. and h.c.p. lattices, respectively, under the lattice symmetry transformations. In these tables, in every row corresponding to the symmetry transformations  $\{S|\tau(S)\}^*$  (from the space group of the lattice under consideration), one finds the vector  $\mathbf{k}' \equiv S\mathbf{k}$  in the third column and in the following columns the types of site and interstice that correspond to the new [obtained as a result of the symmetry transformations  $\{S|\tau(S)\}$ ] positions of all types of site and interstice. For example, under the symmetry operation  $i(\bar{x}, \bar{y}, \bar{z})$  for the h.c.p. lattice,

$$(k_1, k_2, k_3) \rightarrow (-k_1, -k_2, k_3); \quad m_1 \rightarrow m'_1 = m_2;$$

$$o_1 \rightarrow o'_1 = o_1 \dots$$

Note that the interchange rules for the positions in f.c.c. and h.c.p. lattices are the same for those elements  $\{S|\tau(S)\}$  of the corresponding space groups that have the point-group transformations  $S$  belonging to the same class (indicated by the horizontal heavy lines in Tables 1–3).

#### 4. Symmetry of injection and mixing potentials

From Tables 1–3 and the general symmetry rules (3) for injection potentials, we obtain

f.c.c.

$$\Phi_{t_1}^\alpha = \Phi_{t_2}^\alpha,$$

b.c.c.

$$\Phi_{o_1}^\alpha = \Phi_{o_2}^\alpha = \Phi_{o_3}^\alpha, \quad \Phi_{t_1}^\alpha = \Phi_{t_2}^\alpha = \Phi_{t_3}^\alpha = \Phi_{t_4}^\alpha = \Phi_{t_5}^\alpha = \Phi_{t_6}^\alpha,$$

h.c.p.

$$\Phi_{m_1}^\alpha = \Phi_{m_2}^\alpha, \quad \Phi_{o_1}^\alpha = \Phi_{o_2}^\alpha, \quad \Phi_{t_1}^\alpha = \Phi_{t_2}^\alpha = \Phi_{t_3}^\alpha = \Phi_{t_4}^\alpha.$$

Thus, in every case of disordered solid solution under consideration, the injection potentials for the positions of the same type (one of  $m$ ,  $o$  or  $t$ ) are equal.

It follows from the symmetry properties (5) that the mixing potential of any two types of particle that are situated at two positions in the crystal lattice must be equal to the mixing potential of the same particles situated at two other positions if even one symmetry transformation, which sends one of these two pairs of

\* The designations of the elements of the point groups  $O_h(m\bar{3}m)$  and  $D_{6h}(6/mmm)$  are the same as ones adopted by McWeeny (1963).

Table 1. The rules of position interchange under the symmetry transformations of the disordered f.c.c. crystal structure

$O_2^*$	$O_2^\dagger$	$k_1, k_2, k_3 \ddagger$	$m'$	$o'$	$t_1 \S$	$t_2$
$\{U 0\}$	$xyz$	$k_1, k_2, k_3$	$m$	$o$	$t_1$	$t_2$
$\{C_3^{xy} 0\}$	$zxy$	$k_3, k_1, k_2$	$m$	$o$	$t_1$	$t_2$
$\{\bar{C}_3^{xy} 0\}$	$yzx$	$k_2, k_3, k_1$	$m$	$o$	$t_1$	$t_2$
$\{C_3^{yz} 0\}$	$\bar{zxy}$	$k_1 - k_2, k_3 - k_2, -k_2$	$m$	$o$	$t_1$	$t_2$
$\{\bar{C}_3^{yz} 0\}$	$\bar{yzx}$	$k_1 - k_3, -k_3, k_2 - k_3$	$m$	$o$	$t_1$	$t_2$
$\{C_3^{zx} 0\}$	$\bar{zxy}$	$-k_3, k_2 - k_3, k_1 - k_3$	$m$	$o$	$t_1$	$t_2$
$\{\bar{C}_3^{zx} 0\}$	$\bar{yzx}$	$k_3 - k_1, k_2 - k_1, -k_1$	$m$	$o$	$t_1$	$t_2$
$\{C_3^{xy} 0\}$	$\bar{zxy}$	$k_2 - k_1, -k_1, k_3 - k_1$	$m$	$o$	$t_1$	$t_2$
$\{\bar{C}_3^{xy} 0\}$	$\bar{yzx}$	$-k_2, k_1 - k_2, k_3 - k_2$	$m$	$o$	$t_1$	$t_2$
$\{C_4^z 0\}$	$xzy$	$k_3 - k_2, k_3, k_3 - k_1$	$m$	$o$	$t_2$	$t_1$
$\{\bar{C}_4^z 0\}$	$xzy$	$k_2 - k_3, k_2 - k_1, k_2$	$m$	$o$	$t_2$	$t_1$
$\{C_4^x 0\}$	$zyx$	$k_1 - k_2, k_1 - k_3, k_1$	$m$	$o$	$t_2$	$t_1$
$\{\bar{C}_4^x 0\}$	$\bar{zyx}$	$k_3, k_3 - k_1, k_3 - k_2$	$m$	$o$	$t_2$	$t_1$
$\{C_4^y 0\}$	$\bar{yxz}$	$k_2, k_2 - k_3, k_2 - k_1$	$m$	$o$	$t_2$	$t_1$
$\{\bar{C}_4^y 0\}$	$\bar{yxz}$	$k_1 - k_3, k_1, k_1 - k_2$	$m$	$o$	$t_2$	$t_1$
$\{C_2^z 0\}$	$x\bar{y}\bar{z}$	$-k_1, k_3 - k_1, k_2 - k_1$	$m$	$o$	$t_1$	$t_2$
$\{C_2^y 0\}$	$\bar{x}\bar{y}\bar{z}$	$k_3 - k_2, -k_2, k_1 - k_2$	$m$	$o$	$t_1$	$t_2$
$\{C_2^x 0\}$	$\bar{x}\bar{y}\bar{z}$	$k_2 - k_3, k_1 - k_3, -k_3$	$m$	$o$	$t_1$	$t_2$
$\{C_2^{xy} 0\}$	$yx\bar{z}$	$k_3 - k_1, k_3 - k_2, k_3$	$m$	$o$	$t_2$	$t_1$
$\{C_2^{yz} 0\}$	$\bar{y}\bar{x}\bar{z}$	$-k_2, -k_1, -k_3$	$m$	$o$	$t_2$	$t_1$
$\{C_2^{zx} 0\}$	$\bar{z}\bar{y}\bar{x}$	$k_2 - k_1, k_2, k_2 - k_3$	$m$	$o$	$t_2$	$t_1$
$\{C_2^{xy} 0\}$	$\bar{z}\bar{y}\bar{x}$	$-k_3, -k_2, -k_1$	$m$	$o$	$t_2$	$t_1$
$\{C_2^{yz} 0\}$	$\bar{x}\bar{z}\bar{y}$	$k_1, k_1 - k_2, k_1 - k_3$	$m$	$o$	$t_2$	$t_1$
$\{C_2^{zx} 0\}$	$\bar{x}\bar{z}\bar{y}$	$-k_1, -k_3, -k_2$	$m$	$o$	$t_2$	$t_1$

$O_2^*$	$O_2^\dagger$	$k_1, k_2, k_3 \ddagger$	$m'$	$o'$	$t_1 \S$	$t_2$
$\{I 0\}$	$\bar{x}\bar{y}\bar{z}$	$-k_1, -k_2, -k_3$	$m$	$o$	$t_2$	$t_1$
$\{S_6^{xy} 0\}$	$\bar{y}\bar{z}\bar{x}$	$k_2, k_3, k_1$	$m$	$o$	$t_2$	$t_1$
$\{\bar{S}_6^{xy} 0\}$	$\bar{z}\bar{x}\bar{y}$	$k_3, k_1, k_2$	$m$	$o$	$t_2$	$t_1$
$\{S_6^{yz} 0\}$	$\bar{y}\bar{z}\bar{x}$	$k_3 - k_1, k_3, k_3 - k_2$	$m$	$o$	$t_2$	$t_1$
$\{\bar{S}_6^{yz} 0\}$	$\bar{z}\bar{x}\bar{y}$	$k_2 - k_1, k_2 - k_3, k_2$	$m$	$o$	$t_2$	$t_1$
$\{S_6^{zx} 0\}$	$\bar{y}\bar{z}\bar{x}$	$k_1 - k_3, k_1 - k_2, k_1$	$m$	$o$	$t_2$	$t_1$
$\{\bar{S}_6^{zx} 0\}$	$\bar{z}\bar{x}\bar{y}$	$k_3, k_3 - k_2, k_3 - k_1$	$m$	$o$	$t_2$	$t_1$
$\{S_6^{xy} 0\}$	$\bar{y}\bar{z}\bar{x}$	$k_2, k_2 - k_1, k_2 - k_3$	$m$	$o$	$t_2$	$t_1$
$\{\bar{S}_6^{xy} 0\}$	$\bar{z}\bar{x}\bar{y}$	$k_1 - k_2, k_1, k_1 - k_3$	$m$	$o$	$t_2$	$t_1$
$\{S_4^z 0\}$	$\bar{x}\bar{z}\bar{y}$	$k_3 - k_2, k_1 - k_2, -k_2$	$m$	$o$	$t_1$	$t_2$
$\{\bar{S}_4^z 0\}$	$\bar{x}\bar{z}\bar{y}$	$k_2 - k_3, -k_3, k_1 - k_3$	$m$	$o$	$t_1$	$t_2$
$\{S_4^x 0\}$	$\bar{z}\bar{y}\bar{x}$	$-k_3, k_1 - k_3, k_2 - k_3$	$m$	$o$	$t_1$	$t_2$
$\{\bar{S}_4^x 0\}$	$\bar{z}\bar{y}\bar{x}$	$k_2 - k_1, k_3 - k_1, -k_1$	$m$	$o$	$t_1$	$t_2$
$\{S_4^y 0\}$	$\bar{y}\bar{x}\bar{z}$	$k_3 - k_1, -k_1, k_2 - k_1$	$m$	$o$	$t_1$	$t_2$
$\{\bar{S}_4^y 0\}$	$\bar{y}\bar{x}\bar{z}$	$-k_2, k_3 - k_2, k_1 - k_2$	$m$	$o$	$t_1$	$t_2$
$\{C_2^x 0\}$	$\bar{x}\bar{y}\bar{z}$	$k_1, k_1 - k_2, k_1 - k_2$	$m$	$o$	$t_2$	$t_1$
$\{C_2^y 0\}$	$\bar{x}\bar{y}\bar{z}$	$k_2 - k_3, k_2, k_2 - k_1$	$m$	$o$	$t_2$	$t_1$
$\{C_2^z 0\}$	$\bar{x}\bar{y}\bar{z}$	$k_3 - k_2, k_3 - k_1, k_3$	$m$	$o$	$t_2$	$t_1$
$\{C_2^{xy} 0\}$	$yx\bar{z}$	$k_2, k_1, k_3$	$m$	$o$	$t_1$	$t_2$
$\{C_2^{yz} 0\}$	$\bar{y}\bar{x}\bar{z}$	$k_1 - k_3, k_2 - k_3, -k_3$	$m$	$o$	$t_1$	$t_2$
$\{C_2^{zx} 0\}$	$\bar{z}\bar{y}\bar{x}$	$k_3, k_2, k_1$	$m$	$o$	$t_1$	$t_2$
$\{C_2^{xy} 0\}$	$\bar{z}\bar{y}\bar{x}$	$k_1 - k_2, -k_2, k_3 - k_2$	$m$	$o$	$t_1$	$t_2$
$\{C_2^{yz} 0\}$	$\bar{x}\bar{z}\bar{y}$	$k_1, k_3, k_2$	$m$	$o$	$t_1$	$t_2$
$\{C_2^{zx} 0\}$	$\bar{x}\bar{z}\bar{y}$	$-k_1, k_2 - k_1, k_3 - k_1$	$m$	$o$	$t_1$	$t_2$

\* The elements of the corresponding symmetry group represented in the Seitz (1936) notation.

† The elements of the corresponding symmetry group represented in the *International Tables for X-ray Crystallography* (1952) notation.

‡ Transformations of the coordinates of vectors with respect to the basis of the reciprocal lattice under corresponding symmetry transformations.

§ Type of position in which the position of  $t_1$  type transforms under corresponding symmetry transformations.

positions to another, exists. Therefore, if we fix the position of any one particle and draw imaginary coordination shells around it, in the general case not all positions in each chosen coordination shell can coincide owing to the application of all symmetry transformations of the solid solution, which retain the position of the origin of the shells to be fixed. Thus, the important outcome of the crystal symmetry is the property of noncentrality (anisotropy) of the interparticle interactions in the lattice gas, which exhibits a dependence of the pairwise mixing potential on the orientation (with respect to the crystal lattice) of the vector that connects the positions of particles in a pair.

Using (5), we can obtain the coordination shells where the noncentrality of the interatomic interactions can take place. Hereafter, the necessary condition of noncentrality is the case when the set of positions within the corresponding coordination shell may be divided into groups of positions that cannot be made to coincide with

each other by any symmetry transformation (with the origin of the shell stationary) of the solid solution. In Tables 4(a)–(c), the results of a similar consideration for the disordered solid solution are shown. Each row of these tables is characterized by the type of position chosen as the origin of the coordination shell ( $m$ ,  $o$  or  $t$  is given at the beginning of the row). Each column is characterized by the position type forming the coordination shell ( $m$ ,  $o$  or  $t$  is given at the top of the column). At the intersection of every row with columns  $n_1$ ,  $n_2$ ,  $n_3$  and columns  $r_1$ ,  $r_2$ ,  $r_3$ , the numbers and the radii, respectively, of the first three coordination shells (composed of the positions of those types that characterize the column and formed around the positions of those types that characterize the row), the possible noncentrality of interatomic interaction is specified.

Thus, for example, in the case of the h.c.p. lattice, choosing position  $t$  as the origin (any  $t$  position:  $t_1$ ,  $t_2$ ,  $t_3$ ,  $t_4$ ) and considering the coordination shells formed by the

Table 2. As Table 1 but for the b.c.c. structure

$O_2^*$	$O_2^\dagger$	$k_1', k_2', k_3'$	$m'$	$\alpha_1'$	$\alpha_2'$	$\alpha_3'$	$t_1'$	$t_2'$	$t_3'$	$t_4'$	$t_5'$	$t_6'$	$t_7'$	$t_8'$
$\{U 0\}$	$xyz$	$k_1, k_2, k_3$	$m$	$\alpha_1$	$\alpha_2$	$\alpha_3$	$t_1$	$t_2$	$t_3$	$t_4$	$t_5$	$t_6$	$t_7$	$t_8$
$\{C_3^m 0\}$	$zxy$	$k_3, k_1, k_2$	$m$	$\alpha_2$	$\alpha_3$	$\alpha_1$	$t_2$	$t_3$	$t_1$	$t_6$	$t_5$	$t_4$	$t_8$	$t_7$
$\{\bar{C}_3^m 0\}$	$yzx$	$k_2, k_3, k_1$	$m$	$\alpha_3$	$\alpha_1$	$\alpha_2$	$t_3$	$t_1$	$t_2$	$t_4$	$t_6$	$t_5$	$t_7$	$t_8$
$\{C_3^m 0\}$	$\bar{z}\bar{y}\bar{x}$	$k_1, k_3, -k_1 - k_2 - k_3$	$m$	$\alpha_2$	$\alpha_3$	$\alpha_1$	$t_6$	$t_5$	$t_1$	$t_2$	$t_3$	$t_4$	$t_8$	$t_7$
$\{\bar{C}_3^m 0\}$	$\bar{y}\bar{z}\bar{x}$	$k_1, -k_1 - k_2 - k_3, k_2$	$m$	$\alpha_3$	$\alpha_1$	$\alpha_2$	$t_5$	$t_4$	$t_6$	$t_3$	$t_1$	$t_2$	$t_8$	$t_7$
$\{C_3^m 0\}$	$\bar{z}\bar{x}\bar{y}$	$-k_1 - k_2 - k_3, k_2, k_1$	$m$	$\alpha_2$	$\alpha_3$	$\alpha_1$	$t_2$	$t_6$	$t_4$	$t_5$	$t_3$	$t_1$	$t_8$	$t_7$
$\{\bar{C}_3^m 0\}$	$\bar{y}\bar{z}\bar{y}$	$k_3, k_2, -k_1 - k_2 - k_3$	$m$	$\alpha_3$	$\alpha_1$	$\alpha_2$	$t_6$	$t_1$	$t_5$	$t_3$	$t_4$	$t_2$	$t_8$	$t_7$
$\{C_3^m 0\}$	$\bar{z}\bar{x}\bar{y}$	$k_2, -k_1 - k_2 - k_3, k_3$	$m$	$\alpha_2$	$\alpha_3$	$\alpha_1$	$t_6$	$t_5$	$t_4$	$t_2$	$t_6$	$t_1$	$t_8$	$t_7$
$\{\bar{C}_3^m 0\}$	$\bar{y}\bar{z}\bar{x}$	$-k_1 - k_2 - k_3, k_1, k_3$	$m$	$\alpha_3$	$\alpha_1$	$\alpha_2$	$t_6$	$t_4$	$t_2$	$t_3$	$t_1$	$t_5$	$t_8$	$t_7$
$\{C_2^m 0\}$	$x\bar{z}\bar{y}$	$-k_2, k_1 + k_2 + k_3, -k_1$	$m$	$\alpha_1$	$\alpha_3$	$\alpha_2$	$t_3$	$t_6$	$t_4$	$t_5$	$t_2$	$t_1$	$t_8$	$t_7$
$\{\bar{C}_2^m 0\}$	$xz\bar{y}$	$-k_3, -k_1, k_1 + k_2 + k_3$	$m$	$\alpha_1$	$\alpha_3$	$\alpha_2$	$t_6$	$t_5$	$t_1$	$t_3$	$t_2$	$t_4$	$t_8$	$t_7$
$\{C_2^m 0\}$	$z\bar{y}\bar{x}$	$-k_2, -k_3, k_1 + k_2 + k_3$	$m$	$\alpha_3$	$\alpha_2$	$\alpha_1$	$t_6$	$t_1$	$t_5$	$t_2$	$t_4$	$t_3$	$t_8$	$t_7$
$\{\bar{C}_2^m 0\}$	$\bar{y}\bar{z}\bar{x}$	$k_1 + k_2 + k_3, -k_1, -k_2$	$m$	$\alpha_3$	$\alpha_2$	$\alpha_1$	$t_2$	$t_4$	$t_6$	$t_5$	$t_1$	$t_3$	$t_8$	$t_7$
$\{C_2^m 0\}$	$\bar{y}\bar{z}\bar{x}$	$k_1 + k_2 + k_3, -k_3, -k_1$	$m$	$\alpha_2$	$\alpha_1$	$\alpha_3$	$t_4$	$t_6$	$t_2$	$t_1$	$t_3$	$t_5$	$t_8$	$t_7$
$\{\bar{C}_2^m 0\}$	$\bar{y}\bar{z}\bar{z}$	$-k_3, k_1 + k_2 + k_3, -k_2$	$m$	$\alpha_2$	$\alpha_1$	$\alpha_3$	$t_4$	$t_5$	$t_6$	$t_1$	$t_8$	$t_2$	$t_3$	$t_7$
$\{C_2^m 0\}$	$x\bar{y}\bar{z}$	$-k_1 - k_2 - k_3, k_3, k_2$	$m$	$\alpha_1$	$\alpha_2$	$\alpha_3$	$t_4$	$t_2$	$t_6$	$t_1$	$t_5$	$t_3$	$t_8$	$t_7$
$\{C_2^m 0\}$	$\bar{x}\bar{y}\bar{z}$	$k_3, -k_1 - k_2 - k_3, k_1$	$m$	$\alpha_1$	$\alpha_2$	$\alpha_3$	$t_4$	$t_6$	$t_5$	$t_1$	$t_2$	$t_3$	$t_8$	$t_7$
$\{C_2^m 0\}$	$\bar{x}\bar{y}\bar{z}$	$k_2, k_1, -k_1 - k_2 - k_3$	$m$	$\alpha_1$	$\alpha_2$	$\alpha_3$	$t_1$	$t_6$	$t_5$	$t_4$	$t_2$	$t_3$	$t_8$	$t_7$
$\{C_2^m 0\}$	$y\bar{x}\bar{z}$	$-k_1, -k_2, k_1 + k_2 + k_3$	$m$	$\alpha_2$	$\alpha_1$	$\alpha_3$	$t_1$	$t_6$	$t_5$	$t_4$	$t_3$	$t_2$	$t_8$	$t_7$
$\{C_2^m 0\}$	$\bar{y}\bar{x}\bar{z}$	$-k_2, -k_1, -k_3$	$m$	$\alpha_2$	$\alpha_1$	$\alpha_3$	$t_1$	$t_3$	$t_2$	$t_4$	$t_6$	$t_5$	$t_8$	$t_7$
$\{C_2^m 0\}$	$\bar{z}\bar{y}\bar{x}$	$-k_1, k_1 + k_2 + k_3, -k_3$	$m$	$\alpha_3$	$\alpha_2$	$\alpha_1$	$t_5$	$t_4$	$t_3$	$t_2$	$t_1$	$t_6$	$t_8$	$t_7$
$\{C_2^m 0\}$	$\bar{z}\bar{y}\bar{x}$	$-k_3, -k_2, -k_1$	$m$	$\alpha_3$	$\alpha_2$	$\alpha_1$	$t_2$	$t_1$	$t_3$	$t_5$	$t_4$	$t_6$	$t_8$	$t_7$
$\{C_2^m 0\}$	$\bar{x}\bar{z}\bar{y}$	$k_1 + k_2 + k_3, -k_2, -k_3$	$m$	$\alpha_1$	$\alpha_3$	$\alpha_2$	$t_6$	$t_2$	$t_4$	$t_5$	$t_3$	$t_1$	$t_8$	$t_7$
$\{C_2^m 0\}$	$\bar{x}\bar{z}\bar{y}$	$-k_1, -k_3, -k_2$	$m$	$\alpha_1$	$\alpha_3$	$\alpha_2$	$t_5$	$t_2$	$t_1$	$t_6$	$t_3$	$t_4$	$t_8$	$t_7$

$O_2^*$	$O_2^\dagger$	$k_1', k_2', k_3'$	$m'$	$\alpha_1'$	$\alpha_2'$	$\alpha_3'$	$t_1'$	$t_2'$	$t_3'$	$t_4'$	$t_5'$	$t_6'$	$t_7'$	$t_8'$
$\{I 0\}$	$\bar{x}\bar{y}\bar{z}$	$-k_1, -k_2, -k_3$	$m$	$\alpha_1$	$\alpha_2$	$\alpha_3$	$t_4$	$t_6$	$t_8$	$t_1$	$t_2$	$t_3$	$t_5$	$t_7$
$\{S_6^m 0\}$	$\bar{y}\bar{z}\bar{x}$	$-k_2, -k_3, -k_1$	$m$	$\alpha_3$	$\alpha_1$	$\alpha_2$	$t_6$	$t_4$	$t_5$	$t_3$	$t_1$	$t_2$	$t_8$	$t_7$
$\{\bar{S}_6^m 0\}$	$\bar{z}\bar{x}\bar{y}$	$-k_3, -k_1, -k_2$	$m$	$\alpha_2$	$\alpha_3$	$\alpha_1$	$t_6$	$t_5$	$t_1$	$t_2$	$t_3$	$t_4$	$t_8$	$t_7$
$\{S_6^m 0\}$	$\bar{y}\bar{z}\bar{x}$	$-k_1, k_1 + k_2 + k_3, -k_2$	$m$	$\alpha_3$	$\alpha_1$	$\alpha_2$	$t_6$	$t_1$	$t_2$	$t_3$	$t_4$	$t_5$	$t_8$	$t_7$
$\{\bar{S}_6^m 0\}$	$\bar{z}\bar{x}\bar{y}$	$-k_1, -k_3, k_1 + k_2 + k_3$	$m$	$\alpha_2$	$\alpha_3$	$\alpha_1$	$t_2$	$t_3$	$t_4$	$t_5$	$t_6$	$t_1$	$t_8$	$t_7$
$\{S_6^m 0\}$	$\bar{y}\bar{z}\bar{x}$	$-k_3, -k_2, k_1 + k_2 + k_3$	$m$	$\alpha_3$	$\alpha_1$	$\alpha_2$	$t_3$	$t_4$	$t_2$	$t_6$	$t_1$	$t_5$	$t_8$	$t_7$
$\{\bar{S}_6^m 0\}$	$\bar{z}\bar{x}\bar{y}$	$k_1 + k_2 + k_3, -k_2, -k_1$	$m$	$\alpha_2$	$\alpha_3$	$\alpha_1$	$t_6$	$t_5$	$t_1$	$t_2$	$t_3$	$t_4$	$t_8$	$t_7$
$\{S_6^m 0\}$	$\bar{y}\bar{z}\bar{x}$	$k_1 + k_2 + k_3, -k_1, -k_3$	$m$	$\alpha_3$	$\alpha_1$	$\alpha_2$	$t_3$	$t_1$	$t_6$	$t_4$	$t_5$	$t_2$	$t_8$	$t_7$
$\{\bar{S}_6^m 0\}$	$\bar{z}\bar{x}\bar{y}$	$-k_2, k_1 + k_2 + k_3, -k_3$	$m$	$\alpha_2$	$\alpha_3$	$\alpha_1$	$t_2$	$t_6$	$t_1$	$t_3$	$t_4$	$t_5$	$t_8$	$t_7$
$\{S_2^m 0\}$	$\bar{x}\bar{z}\bar{y}$	$k_3, k_1, -k_1 - k_2 - k_3$	$m$	$\alpha_1$	$\alpha_3$	$\alpha_2$	$t_3$	$t_2$	$t_4$	$t_6$	$t_5$	$t_1$	$t_8$	$t_7$
$\{\bar{S}_2^m 0\}$	$\bar{x}\bar{z}\bar{y}$	$k_2, -k_1 - k_2 - k_3, k_1$	$m$	$\alpha_1$	$\alpha_3$	$\alpha_2$	$t_6$	$t_2$	$t_1$	$t_3$	$t_5$	$t_4$	$t_8$	$t_7$
$\{S_2^m 0\}$	$\bar{z}\bar{y}\bar{x}$	$-k_1 - k_2 - k_3, k_1, k_2$	$m$	$\alpha_3$	$\alpha_2$	$\alpha_1$	$t_6$	$t_1$	$t_3$	$t_2$	$t_4$	$t_5$	$t_8$	$t_7$
$\{\bar{S}_2^m 0\}$	$\bar{z}\bar{y}\bar{x}$	$k_2, k_3, -k_1 - k_2 - k_3$	$m$	$\alpha_3$	$\alpha_2$	$\alpha_1$	$t_2$	$t_4$	$t_5$	$t_3$	$t_1$	$t_6$	$t_8$	$t_7$
$\{S_2^m 0\}$	$\bar{y}\bar{z}\bar{x}$	$k_3, -k_1 - k_2 - k_3, k_2$	$m$	$\alpha_2$	$\alpha_1$	$\alpha_3$	$t_1$	$t_6$	$t_2$	$t_4$	$t_5$	$t_3$	$t_8$	$t_7$
$\{\bar{S}_2^m 0\}$	$\bar{y}\bar{z}\bar{x}$	$-k_1 - k_2 - k_3, k_3, k_1$	$m$	$\alpha_2$	$\alpha_1$	$\alpha_3$	$t_1$	$t_5$	$t_6$	$t_4$	$t_3$	$t_2$	$t_8$	$t_7$
$\{\sigma^m 0\}$	$\bar{x}\bar{y}\bar{z}$	$k_1 + k_2 + k_3, -k_3, -k_2$	$m$	$\alpha_1$	$\alpha_2$	$\alpha_3$	$t_1$	$t_5$	$t_3$	$t_4$	$t_2$	$t_6$	$t_8$	$t_7$
$\{\sigma^m 0\}$	$\bar{x}\bar{y}\bar{z}$	$-k_3, k_1 + k_2 + k_3, -k_1$	$m$	$\alpha_1$	$\alpha_2$	$\alpha_3$	$t_1$	$t_2$	$t_6$	$t_4$	$t_5$	$t_3$	$t_8$	$t_7$
$\{\sigma^m 0\}$	$\bar{x}\bar{y}\bar{z}$	$-k_2, -k_1, k_1 + k_2 + k_3$	$m$	$\alpha_1$	$\alpha_2$	$\alpha_3$	$t_4$	$t_2$	$t_5$	$t_1$	$t_6$	$t_3$	$t_8$	$t_7$
$\{\sigma^m 0\}$	$y\bar{x}\bar{z}$	$k_2, k_1, k_3$	$m$	$\alpha_2$	$\alpha_1$	$\alpha_3$	$t_4$	$t_6$	$t_5$	$t_1$	$t_3$	$t_2$	$t_8$	$t_7$
$\{\sigma^m 0\}$	$\bar{y}\bar{x}\bar{z}$	$k_1, k_2, -k_1 - k_2 - k_3$	$m$	$\alpha_2$	$\alpha_1$	$\alpha_3$	$t_4$	$t_5$	$t_2$	$t_1$	$t_6$	$t_3$	$t_8$	$t_7$
$\{\sigma^m 0\}$	$z\bar{y}\bar{x}$	$k_3, k_2, k_1$	$m$	$\alpha_3$	$\alpha_2$	$\alpha_1$	$t_6$	$t_4$	$t_5$	$t_2$	$t_1$	$t_3$	$t_8$	$t_7$
$\{\sigma^m 0\}$	$\bar{z}\bar{y}\bar{x}$	$k_1, -k_1 - k_2 - k_3, k_3$	$m$	$\alpha_3$	$\alpha_2$	$\alpha_1$	$t_2$	$t_1$	$t_6$	$t_5$	$t_4$	$t_3$	$t_8$	$t_7$
$\{\sigma^m 0\}$	$\bar{x}\bar{z}\bar{y}$	$k_1, k_3, k_2$	$m$	$\alpha_1$	$\alpha_3$	$\alpha_2$	$t_6$	$t_5$	$t_4$	$t_3$	$t_2$	$t_1$	$t_8$	$t_7$
$\{\sigma^m 0\}$	$\bar{x}\bar{z}\bar{y}$	$-k_1, -k_2 - k_3, k_2, k_3$	$m$	$\alpha_1$	$\alpha_3$	$\alpha_2$	$t_3$	$t_6$	$t_1$	$t_5$	$t_4$	$t_2$	$t_8$	$t_7$

\* The elements of the corresponding symmetry group represented in the Seitz (1936) notation.  
 † The elements of the corresponding symmetry group represented in the *International Tables for X-ray Crystallography* (1952) notation.  
 ‡ Transformations of the coordinates of vectors with respect to the basis of the reciprocal lattice under corresponding symmetry transformations.  
 § Type of position in which the position of  $t_1$  type transforms under corresponding symmetry transformations.

$o$  positions (all types of octahedral interstices, *i.e.* both  $o_1$  and  $o_2$ ) around the origin, we obtain the possible noncentrality of interactions at the third, fifth and seventh coordination shells with the radii  $(a/2)(11/2)^{1/2}$ ,  $(a/2)(57/6)^{1/2}$  and  $(a/2)(27/2)^{1/2}$ , respectively.\*

From Table 4(a), one can find, for example, that, in the case of the f.c.c. lattice, the noncentrality in interatomic interaction (under the increase of the radii of corresponding shells) for tetrahedral coordination can appear at the third coordination shell first. For the cases when the atoms occupy the positions of the same class ( $m$ ,  $o$  or  $t$ ), the noncentrality can appear first at the ninth shell and, for the positions of different types, at the fourth shell.

\* It is important to note that in the case of the h.c.p. lattice the corresponding results depend on the ratio of  $c$  to  $a$ . The noncentrality shells presented in Table 4(c) correspond to the case of the ideal ratio  $c/a = (8/3)^{1/2} \approx 1.63$ .

It follows from the consideration summarized in Tables 4(a)–(c) that the noncentrality of interatomic interaction can take place even at sufficiently closely spaced interatomic distances and, thus, must be taken into account under the consistent statistical-thermodynamic analysis of the solid solution. For example, in the case of the h.c.p. lattice [Table 4(c)], noncentrality is possible at the first shell for the cases of atomic coordinations of the types site–site and site–tetrahedral interstice.

Note that only necessary conditions of the existence of noncentrality have been used here. Therefore, under the microscopic calculations of interatomic interaction energies, it may be that at some predicted coordination shells [see Tables 4(a)–(c)] the noncentrality is lacking.\*

\* The inverse situation cannot occur: other shells of the noncentrality (within the given radius) that are different from those obtained cannot exist.

Table 3. As Table 1 but for the h.c.p. structure ( $\tau = a_3/2$ )

$D_{6h}^*$	$D_{6h}^\dagger$	$k_1, k_2, k_3$	$m_1'$	$m_2'$	$\alpha_1'$	$\alpha_2'$	$t_1'$	$t_2'$	$t_3'$	$t_4'$
$\{U 0\}$	$x, y, z$	$k_1, k_2, k_3$	$m_2$	$m_2$	$\alpha_1$	$\alpha_2$	$t_1$	$t_2$	$t_3$	$t_4$
$\{C_2 z\}$	$\bar{x}, \bar{y}, 1/2+z$	$-k_1, -k_2, k_3$	$m_2$	$m_2$	$\alpha_1$	$\alpha_2$	$t_2$	$t_1$	$t_4$	$t_3$
$\{C_2 0\}$	$\bar{y}, x-y, z$	$-k_1, -k_2, k_1, k_3$	$m_1$	$m_2$	$\alpha_1$	$\alpha_2$	$t_1$	$t_2$	$t_3$	$t_4$
$\{\bar{C}_2 0\}$	$y-x, \bar{x}, z$	$k_2, -k_1-k_2, k_3$	$m_1$	$m_2$	$\alpha_1$	$\alpha_2$	$t_1$	$t_2$	$t_3$	$t_4$
$\{C_2 z\}$	$x-y, x, 1/2+z$	$-k_2, k_1+k_2, k_3$	$m_2$	$m_2$	$\alpha_2$	$\alpha_1$	$t_2$	$t_1$	$t_4$	$t_3$
$\{\bar{C}_2 z\}$	$y, y-x, 1/2+z$	$k_1+k_2, -k_1, k_3$	$m_2$	$m_2$	$\alpha_2$	$\alpha_1$	$t_2$	$t_1$	$t_4$	$t_3$
$\{C_2^{(y)} 0\}$	$x-y, \bar{y}, \bar{z}$	$k_1, -k_1-k_2, -k_3$	$m_2$	$m_1$	$\alpha_1$	$\alpha_2$	$t_3$	$t_4$	$t_1$	$t_2$
$\{C_2^{(x)} 0\}$	$y, x, \bar{z}$	$k_2, k_1, -k_3$	$m_2$	$m_1$	$\alpha_1$	$\alpha_2$	$t_3$	$t_4$	$t_1$	$t_2$
$\{C_2^{(y)} z\}$	$\bar{x}, y-x, \bar{z}$	$-k_1-k_2, k_2, -k_3$	$m_2$	$m_1$	$\alpha_1$	$\alpha_2$	$t_3$	$t_4$	$t_1$	$t_2$
$\{C_2^{(x)} z\}$	$x, x-y, 1/2-z$	$k_1+k_2, -k_2, -k_3$	$m_1$	$m_2$	$\alpha_2$	$\alpha_1$	$t_4$	$t_3$	$t_2$	$t_1$
$\{C_2^{(y)} z\}$	$y-x, y, 1/2-z$	$-k_1, k_1+k_2, -k_3$	$m_1$	$m_2$	$\alpha_2$	$\alpha_1$	$t_4$	$t_3$	$t_2$	$t_1$
$\{C_2^{(x)} z\}$	$\bar{y}, \bar{x}, 1/2-z$	$-k_2, -k_1, -k_3$	$m_1$	$m_2$	$\alpha_2$	$\alpha_1$	$t_4$	$t_3$	$t_2$	$t_1$
$\{I 0\}$	$\bar{x}, \bar{y}, \bar{z}$	$-k_1, -k_2, -k_3$	$m_2$	$m_1$	$\alpha_1$	$\alpha_2$	$t_3$	$t_4$	$t_1$	$t_2$
$\{C_2 z\}$	$x, y, 1/2-z$	$k_1, k_2, -k_3$	$m_1$	$m_2$	$\alpha_2$	$\alpha_1$	$t_4$	$t_3$	$t_2$	$t_1$
$\{S_6 0\}$	$y, y-x, \bar{z}$	$k_1+k_2, -k_1, -k_3$	$m_2$	$m_1$	$\alpha_1$	$\alpha_2$	$t_3$	$t_4$	$t_1$	$t_2$
$\{\bar{S}_6 0\}$	$x-y, x, \bar{z}$	$-k_2, k_1+k_2, -k_3$	$m_2$	$m_1$	$\alpha_1$	$\alpha_2$	$t_3$	$t_4$	$t_1$	$t_2$
$\{S_6 z\}$	$y-x, \bar{x}, 1/2-z$	$k_2, -k_1-k_2, -k_3$	$m_1$	$m_2$	$\alpha_2$	$\alpha_1$	$t_4$	$t_3$	$t_2$	$t_1$
$\{\bar{S}_6 z\}$	$\bar{y}, x-y, 1/2-z$	$-k_1-k_2, k_1, k_3$	$m_1$	$m_2$	$\alpha_2$	$\alpha_1$	$t_4$	$t_3$	$t_2$	$t_1$
$\{C_2^{(y)} 0\}$	$y-x, y, z$	$-k_1, k_1+k_2, k_3$	$m_1$	$m_2$	$\alpha_1$	$\alpha_2$	$t_1$	$t_2$	$t_3$	$t_4$
$\{C_2^{(x)} 0\}$	$\bar{y}, \bar{x}, z$	$-k_2, -k_1, k_3$	$m_1$	$m_2$	$\alpha_1$	$\alpha_2$	$t_1$	$t_2$	$t_3$	$t_4$
$\{C_2^{(y)} z\}$	$x, x-y, z$	$k_1+k_2, -k_2, k_3$	$m_1$	$m_2$	$\alpha_1$	$\alpha_2$	$t_1$	$t_2$	$t_3$	$t_4$
$\{C_2^{(x)} z\}$	$x-y, \bar{y}, 1/2+z$	$k_1, -k_1-k_2, k_3$	$m_2$	$m_1$	$\alpha_2$	$\alpha_1$	$t_2$	$t_1$	$t_4$	$t_3$
$\{C_2^{(y)} z\}$	$y, x, 1/2+z$	$k_2, k_1, k_3$	$m_2$	$m_1$	$\alpha_2$	$\alpha_1$	$t_2$	$t_1$	$t_4$	$t_3$
$\{C_2^{(x)} z\}$	$\bar{x}, y-x, 1/2+z$	$-k_1-k_2, k_2, k_3$	$m_2$	$m_1$	$\alpha_2$	$\alpha_1$	$t_2$	$t_1$	$t_4$	$t_3$

\* The elements of the corresponding symmetry group represented in the Seitz (1936) notation.

† The elements of the corresponding symmetry group represented in the *International Tables for X-ray Crystallography* (1952) notation.

‡ Transformations of the coordinates of vectors with respect to the basis of the reciprocal lattice under corresponding symmetry transformations.

§ Type of position in which the position of  $t_1$  type transforms under corresponding symmetry transformations.

So, for example, in Blanter (1985), in the case of octahedral coordination of the interstitial atoms in the b.c.c. lattice, the noncentrality of the strain-induced (elastic) interaction takes place at the sixth, seventh *etc.* coordination shells, though, as may be seen from Table 4(b), the fifth shell is also present besides the above-mentioned ones.

### 5. Matrix of mixing-potential Fourier transforms for reciprocal-lattice arbitrary points of disordered f.c.c., b.c.c. and h.c.p. solid solutions

Under the theoretical development of interatomic potentials (or of mixing potentials) in solid solutions, the methods that permit one to find first the Fourier transforms of these potentials are used, as a rule (*e.g.* Khachatryan, 1978, 1983; Krasko & Makhnovetskii,

1974). For the symmetry adequacy of such methods, it is necessary (as shown in paper 1) to take into consideration the conditions imposed by the space symmetry of the solid solution on the potentials of interatomic interactions of its atomic components. For the Fourier transforms of the potentials, these requirements are expressed by (8)–(11). Using these equations and Tables 1–3, one can find the minimal number of independent elements of the matrix  $\|\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k})\|$  for the cases of f.c.c., b.c.c. and h.c.p. disordered solid solutions, and also the analytical relationships between corresponding matrix elements. The results of this procedure are presented in Tables 5, 6 and 7. Each of these tables is the fragment of the matrix  $\|\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k})\|$  under some given  $\alpha, \beta$  and  $\mathbf{k}$ . The indices  $p$  and  $q$  enumerate the rows and columns of the tables and run over the meanings

f.c.c.:

$$\{m, o, t_1, t_2\};$$

b.c.c.:

$$\{m, o_1, o_2, o_3, t_1, t_2, t_3, t_4, t_5, t_6\};$$

h.c.p.:

$$\{m_1, m_2, o_1, o_2, t_1, t_2, t_3, t_4\}.$$

The next elements are chosen as independent\*

f.c.c.:

$$\{\tilde{w}_{mm}, \tilde{w}_{mo}, \tilde{w}_{om}, \tilde{w}_{mt_1}, \tilde{w}_{t_1m}, \tilde{w}_{oo}, \tilde{w}_{ot_1}, \tilde{w}_{t_1o}, \tilde{w}_{t_1t_4}\};$$

b.c.c.:

$$\{\tilde{w}_{mm}, \tilde{w}_{mo_1}, \tilde{w}_{o_1m}, \tilde{w}_{o_1o_1}, \tilde{w}_{o_1o_2}, \tilde{w}_{mt_1}, \tilde{w}_{o_1t_1}, \tilde{w}_{o_1t_2}, \tilde{w}_{t_1m}, \tilde{w}_{t_1o_1}, \tilde{w}_{t_1t_1}, \tilde{w}_{t_1t_2}, \tilde{w}_{t_1t_4}, \tilde{w}_{t_2o_1}\};$$

h.c.p.:

$$\{\tilde{w}_{m_1m_1}, \tilde{w}_{m_1m_2}, \tilde{w}_{m_1o_1}, \tilde{w}_{o_1m_1}, \tilde{w}_{m_1t_1}, \tilde{w}_{m_1t_2}, \tilde{w}_{t_1m_1}, \tilde{w}_{t_2m_1}, \tilde{w}_{o_1t_1}, \tilde{w}_{o_1t_2}, \tilde{w}_{t_1o_1}, \tilde{w}_{t_1o_2}, \tilde{w}_{t_1t_1}, \tilde{w}_{t_1t_2}, \tilde{w}_{t_1t_3}, \tilde{w}_{t_1t_4}\}.$$

All the remaining elements of the matrix  $\|\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k})\|$  are expressed in terms of the independent ones by the use of the relationships presented in Tables 5–7 in corresponding cells. The symbol  $\tilde{w}$  is used for the designation of the complex quantities and the symbol  $\tilde{V}$  for the real ones. As an example, for the case of the h.c.p. lattice we get from Table 7

$$\begin{aligned} \tilde{w}_{o_2t_2}^{\alpha\beta}(k_1, k_2, k_3) &= \tilde{w}_{o_1t_1}^{\alpha\beta}(-k_1, -k_2, k_3) \\ &\times \exp[i2\pi(-k_1 - k_2 + k_3)], \end{aligned}$$

where  $k_1, k_2$  and  $k_3$  are the coordinates of the vector  $\mathbf{k}$  with respect to the basis of the reciprocal lattice.

\* The indices  $\alpha, \beta$  and the variable  $\mathbf{k}$  are omitted for clarity.

Table 4. The numbers and the radii of the first three coordination shells of the possible noncentrality for the pairwise interaction of atoms at sites (*m*) and octahedral (*o*) and tetrahedral (*t*) interstices within disordered f.c.c., b.c.c. and h.c.p. crystal structures

(a) F.c.c. structure

fcc	<i>m</i>						<i>o</i>						<i>t</i>					
	<i>n</i> <sub>1</sub>	<i>r</i> <sub>1</sub>	<i>n</i> <sub>2</sub>	<i>r</i> <sub>2</sub>	<i>n</i> <sub>3</sub>	<i>r</i> <sub>3</sub>	<i>n</i> <sub>1</sub>	<i>r</i> <sub>1</sub>	<i>n</i> <sub>2</sub>	<i>r</i> <sub>2</sub>	<i>n</i> <sub>3</sub>	<i>r</i> <sub>3</sub>	<i>n</i> <sub>1</sub>	<i>r</i> <sub>1</sub>	<i>n</i> <sub>2</sub>	<i>r</i> <sub>2</sub>	<i>n</i> <sub>3</sub>	<i>r</i> <sub>3</sub>
<i>m</i>	9	$\frac{3a}{\sqrt{2}}$	13	$\frac{a}{2}\sqrt{26}$	16	$\frac{a}{2}\sqrt{34}$	4	$\frac{3a}{2}$	7	$\frac{a}{2}\sqrt{17}$	10	$\frac{5a}{2}$	4	$\frac{3a}{4}\sqrt{3}$	7	$\frac{a}{4}\sqrt{51}$	8	$\frac{a}{4}\sqrt{59}$
<i>o</i>	4	$\frac{3a}{2}$	7	$\frac{a}{2}\sqrt{17}$	10	$\frac{5a}{2}$	9	$\frac{3a}{\sqrt{2}}$	13	$\frac{a}{2}\sqrt{26}$	16	$\frac{a}{2}\sqrt{34}$	4	$\frac{3a}{4}\sqrt{3}$	7	$\frac{a}{4}\sqrt{51}$	8	$\frac{a}{4}\sqrt{59}$
<i>t</i>	4	$\frac{3a}{4}\sqrt{3}$	7	$\frac{a}{4}\sqrt{51}$	8	$\frac{a}{4}\sqrt{59}$	4	$\frac{3a}{4}\sqrt{3}$	7	$\frac{a}{4}\sqrt{51}$	8	$\frac{a}{4}\sqrt{59}$	3	$\frac{a}{2}\sqrt{3}$	6	$\frac{a}{2}\sqrt{6}$	8	$\frac{3a}{2}$

(b) B.c.c. structure

bcc	<i>m</i>						<i>o</i>						<i>t</i>					
	<i>n</i> <sub>1</sub>	<i>r</i> <sub>1</sub>	<i>n</i> <sub>2</sub>	<i>r</i> <sub>2</sub>	<i>n</i> <sub>3</sub>	<i>r</i> <sub>3</sub>	<i>n</i> <sub>1</sub>	<i>r</i> <sub>1</sub>	<i>n</i> <sub>2</sub>	<i>r</i> <sub>2</sub>	<i>n</i> <sub>3</sub>	<i>r</i> <sub>3</sub>	<i>n</i> <sub>1</sub>	<i>r</i> <sub>1</sub>	<i>n</i> <sub>2</sub>	<i>r</i> <sub>2</sub>	<i>n</i> <sub>3</sub>	<i>r</i> <sub>3</sub>
<i>m</i>	10	$\frac{3a}{2}\sqrt{3}$	13	$3a$	18	$\frac{a}{2}\sqrt{51}$	5	$\frac{3a}{2}$	9	$\frac{a}{2}\sqrt{17}$	10	$\frac{3a}{\sqrt{2}}$	4	$\frac{a}{4}\sqrt{29}$	6	$\frac{3a}{4}\sqrt{5}$	7	$\frac{a}{4}\sqrt{53}$
<i>o</i>	5	$\frac{3a}{2}$	9	$\frac{a}{2}\sqrt{17}$	10	$\frac{3a}{\sqrt{2}}$	4	$a$	5	$\frac{a}{2}\sqrt{5}$	7	$a\sqrt{2}$	3	$\frac{3a}{4}$	5	$\frac{a}{4}\sqrt{17}$	7	$\frac{5a}{4}$
<i>t</i>	4	$\frac{a}{4}\sqrt{29}$	6	$\frac{3a}{4}\sqrt{5}$	7	$\frac{a}{4}\sqrt{53}$	3	$\frac{3a}{4}$	5	$\frac{a}{4}\sqrt{17}$	7	$\frac{5a}{4}$	5	$\frac{a}{4}\sqrt{10}$	7	$\frac{a}{4}\sqrt{14}$	8	$a$

(c) H.c.p. structure

hcp	<i>m</i>						<i>o</i>						<i>t</i>					
	<i>n</i> <sub>1</sub>	<i>r</i> <sub>1</sub>	<i>n</i> <sub>2</sub>	<i>r</i> <sub>2</sub>	<i>n</i> <sub>3</sub>	<i>r</i> <sub>3</sub>	<i>n</i> <sub>1</sub>	<i>r</i> <sub>1</sub>	<i>n</i> <sub>2</sub>	<i>r</i> <sub>2</sub>	<i>n</i> <sub>3</sub>	<i>r</i> <sub>3</sub>	<i>n</i> <sub>1</sub>	<i>r</i> <sub>1</sub>	<i>n</i> <sub>2</sub>	<i>r</i> <sub>2</sub>	<i>n</i> <sub>3</sub>	<i>r</i> <sub>3</sub>
<i>m</i>	1	$a$	4	$a\sqrt{3}$	8	$a\sqrt{\frac{17}{3}}$	7	$\frac{3a}{\sqrt{2}}$	8	$a\sqrt{\frac{11}{2}}$	10	$a\sqrt{\frac{39}{6}}$	1	$\frac{3a}{2\sqrt{6}}$	3	$\frac{a}{2}\sqrt{\frac{11}{2}}$	5	$\frac{a}{2}\sqrt{\frac{57}{6}}$
<i>o</i>	7	$\frac{3a}{\sqrt{2}}$	8	$a\sqrt{\frac{11}{2}}$	10	$a\sqrt{\frac{39}{6}}$	6	$a\sqrt{\frac{11}{3}}$	9	$a\sqrt{\frac{17}{3}}$	12	$a\sqrt{7}$	3	$\frac{a}{2}\sqrt{\frac{11}{2}}$	5	$\frac{a}{2}\sqrt{\frac{57}{6}}$	7	$\frac{a}{2}\sqrt{\frac{27}{2}}$
<i>t</i>	1	$\frac{3a}{2\sqrt{6}}$	3	$\frac{a}{2}\sqrt{\frac{11}{2}}$	5	$\frac{a}{2}\sqrt{\frac{57}{6}}$	3	$\frac{a}{2}\sqrt{\frac{11}{2}}$	5	$\frac{a}{2}\sqrt{\frac{57}{6}}$	7	$\frac{a}{2}\sqrt{\frac{27}{2}}$	3	$a$	5	$a\sqrt{\frac{3}{2}}$	7	$a\sqrt{2}$

In the particular case of  $\alpha = \beta$ , according to (9) and (10) the additional requirement on the matrix elements  $\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k})$  is

$$\tilde{w}_{pq}^{\alpha\alpha*}(\mathbf{k}) = \tilde{w}_{qp}^{\alpha\alpha}(\mathbf{k}), \quad (12)$$

i.e. the corresponding block of the matrix must be Hermitian.

From (9) and (10), one can also connect the matrix elements  $\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k})$  with the different sets  $\{\alpha\beta\}$  distinguished from each other by exchanging the elements only:

$$\tilde{w}_{pq}^{\beta\alpha}(\mathbf{k}) = \tilde{w}_{pq}^{\alpha\beta*}(\mathbf{k}). \quad (13)$$

Table 5. The matrix of the mixing-potential Fourier transforms  $\|\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k})\|$  for the disordered f.c.c. structure under the fixed  $\alpha, \beta$  and  $\mathbf{k}$ , where  $\mathbf{k}$  is an arbitrary point in the corresponding reciprocal lattice

	<i>m</i>	<i>o</i>	<i>t</i> <sub>1</sub>	<i>t</i> <sub>2</sub>
<i>m</i>	$\tilde{V}_{mm}(k_1, k_2, k_3)$	$\tilde{V}_{mo}(k_1, k_2, k_3) \cdot e^{-i2\pi(k_1+k_2+k_3)}$	$\tilde{w}_{m1}(k_1, k_2, k_3)$	$\tilde{w}_{m2}^*(k_1, k_2, k_3) \cdot e^{-i2\pi(k_1+k_2+k_3)}$
<i>o</i>	$\tilde{V}_{om}(k_1, k_2, k_3) \cdot e^{i2\pi(k_1+k_2+k_3)}$	$\tilde{V}_{oo}(k_1, k_2, k_3)$	$\tilde{w}_{o1}(k_1, k_2, k_3)$	$\tilde{w}_{o2}^*(k_1, k_2, k_3)$
<i>t</i> <sub>1</sub>	$\tilde{w}_{1m}(k_1, k_2, k_3)$	$\tilde{w}_{1o}(k_1, k_2, k_3)$	$\tilde{w}_{11}(k_1, k_2, k_3)$	$\tilde{w}_{12}(k_1, k_2, k_3)$
<i>t</i> <sub>2</sub>	$\tilde{w}_{2m}^*(k_1, k_2, k_3) \cdot e^{i2\pi(k_1+k_2+k_3)}$	$\tilde{w}_{2o}^*(k_1, k_2, k_3)$	$\tilde{w}_{21}^*(k_1, k_2, k_3)$	$\tilde{w}_{22}^*(k_1, k_2, k_3)$



Table 8. Matrices of the mixing-potential Fourier transforms  $\|\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k})\|$  for the disordered f.c.c. crystal structure with fixed  $\alpha, \beta$

(a)  $\mathbf{k} = (0, 0, 0)$  ( $\Gamma$ )

$\Gamma$	$m$	$o$	$t_1$	$t_2$
$m$	$V_{mm}$	$V_{mo}$	$V_{m1}$	$V_{m2}$
$o$	$V_{om}$	$V_{oo}$	$V_{o1}$	$V_{o2}$
$t_1$	$V_{1m}$	$V_{1o}$	$V_{11}$	$V_{12}$
$t_2$	$V_{2m}$	$V_{2o}$	$V_{21}$	$V_{22}$

(b)  $\mathbf{k} = (1/2, 1/2, 1/2)$  ( $L$ )

$L$	$m$	$o$	$t_1$	$t_2$
$m$	$V_{mm}$	0	$V_{m1}$	$-V_{m2}$
$o$	0	$V_{oo}$	$V_{o1}$	$V_{o2}$
$t_1$	$V_{1m}$	$V_{1o}$	$V_{11}$	$V_{12}$
$t_2$	$-V_{1m}$	$V_{1o}$	$V_{11}$	$V_{12}$

(c)  $\mathbf{k} = (1/2, 1/2, 0)$  ( $X$ )

$X$	$m$	$o$	$t_1$	$t_2$
$m$	$V_{mm}$	$V_{mo}$	0	0
$o$	$V_{om}$	$V_{oo}$	0	0
$t_1$	0	0	$V_{11}$	$V_{12}$
$t_2$	0	0	$V_{11}$	$V_{11}$

(d)  $\mathbf{k} = (1/4, 3/4, 1/2)$  ( $W$ )

$W$	$m$	$o$	$t_1$	$t_2$
$m$	$V_{mm}$	0	0	0
$o$	0	$V_{oo}$	0	0
$t_1$	0	0	$V_{11}$	0
$t_2$	0	0	0	$V_{11}$

The rules of transformation for the independent matrix components  $\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k})$  due to the application of the elements of the corresponding symmetry group can be obtained from Tables 1-3 using (8).

Note that, as may be seen from Tables 5 and 7, the block  $\|\tilde{w}_{t_i t_j}^{\alpha\beta}(\mathbf{k})\|$ , which corresponds to the octahedral interstices for the cases of f.c.c. and h.c.p. lattices, has the form

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix},$$

where  $A$  and  $B$  are the matrices of  $2 \times 2$  dimensions.

From Tables 5-7, one can also obtain the following analytical relationships

f.c.c.:

$$\text{Re } \tilde{w}_{mo}^{\alpha\beta}(\mathbf{k}) / \text{Im } \tilde{w}_{mo}^{\alpha\beta}(\mathbf{k}) = -\cotan \pi(k_1 + k_2 + k_3); \tag{14}$$

b.c.c.:

$$\begin{aligned} \text{Re } \tilde{w}_{o1o2}^{\alpha\beta}(\mathbf{k}) / \text{Im } \tilde{w}_{o1o2}^{\alpha\beta}(\mathbf{k}) &= \cotan \pi(k_2 - k_1), \\ \text{Re } \tilde{w}_{mo1}^{\alpha\beta}(\mathbf{k}) / \text{Im } \tilde{w}_{mo1}^{\alpha\beta}(\mathbf{k}) &= -\cotan \pi(k_2 + k_3); \end{aligned} \tag{15}$$

Table 9. Matrices of the mixing-potential Fourier transforms  $\|\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k})\|$  for disordered b.c.c. crystal structure with fixed  $\alpha, \beta$

(a)  $\mathbf{k} = (0, 0, 0)$  ( $\Gamma$ )

$\Gamma$	$m$	$a_1$	$a_2$	$a_3$	$t_1$	$t_2$	$t_3$	$t_4$	$t_5$	$t_6$
$m$	$V_{mm}$	$V_{m1}$	$V_{m2}$	$V_{m3}$	$V_{m4}$	$V_{m5}$	$V_{m6}$	$V_{m1}$	$V_{m2}$	$V_{m3}$
$a_1$	$V_{a1m}$	$V_{a11}$	$V_{a12}$	$V_{a13}$	$V_{a14}$	$V_{a15}$	$V_{a16}$	$V_{a11}$	$V_{a12}$	$V_{a13}$
$a_2$	$V_{a2m}$	$V_{a21}$	$V_{a22}$	$V_{a23}$	$V_{a24}$	$V_{a25}$	$V_{a26}$	$V_{a21}$	$V_{a22}$	$V_{a23}$
$a_3$	$V_{a3m}$	$V_{a31}$	$V_{a32}$	$V_{a33}$	$V_{a34}$	$V_{a35}$	$V_{a36}$	$V_{a31}$	$V_{a32}$	$V_{a33}$
$t_1$	$V_{t1m}$	$V_{t11}$	$V_{t12}$	$V_{t13}$	$V_{t14}$	$V_{t15}$	$V_{t16}$	$V_{t14}$	$V_{t15}$	$V_{t16}$
$t_2$	$V_{t2m}$	$V_{t21}$	$V_{t22}$	$V_{t23}$	$V_{t24}$	$V_{t25}$	$V_{t26}$	$V_{t24}$	$V_{t25}$	$V_{t26}$
$t_3$	$V_{t3m}$	$V_{t31}$	$V_{t32}$	$V_{t33}$	$V_{t34}$	$V_{t35}$	$V_{t36}$	$V_{t34}$	$V_{t35}$	$V_{t36}$
$t_4$	$V_{t4m}$	$V_{t41}$	$V_{t42}$	$V_{t43}$	$V_{t44}$	$V_{t45}$	$V_{t46}$	$V_{t44}$	$V_{t45}$	$V_{t46}$
$t_5$	$V_{t5m}$	$V_{t51}$	$V_{t52}$	$V_{t53}$	$V_{t54}$	$V_{t55}$	$V_{t56}$	$V_{t54}$	$V_{t55}$	$V_{t56}$
$t_6$	$V_{t6m}$	$V_{t61}$	$V_{t62}$	$V_{t63}$	$V_{t64}$	$V_{t65}$	$V_{t66}$	$V_{t64}$	$V_{t65}$	$V_{t66}$

(b)  $\mathbf{k} = (0, 0, \frac{1}{2})$  ( $N$ )

$N$	$m$	$a_1$	$a_2$	$a_3$	$t_1$	$t_2$	$t_3$	$t_4$	$t_5$	$t_6$
$m$	$V_{mm}$	0	0	$V_{m3}$	0	$V_{m2}$	$-V_{m2}$	0	$-V_{m1}$	$V_{m1}$
$a_1$	0	$V_{a1m}$	$V_{a12}$	0	$V_{a11}$	$V_{a12}$	$V_{a13}$	$V_{a14}$	$V_{a15}$	$V_{a16}$
$a_2$	0	$V_{a2m}$	$V_{a21}$	0	$V_{a21}$	$V_{a22}$	$V_{a23}$	$V_{a24}$	$V_{a25}$	$V_{a26}$
$a_3$	$V_{a3m}$	0	0	$V_{a33}$	0	$-V_{a32}$	$V_{a31}$	0	$V_{a33}$	$-V_{a33}$
$t_1$	0	$V_{t1m}$	$V_{t12}$	0	$V_{t11}$	$V_{t12}$	$V_{t13}$	$V_{t14}$	$V_{t15}$	$V_{t16}$
$t_2$	$V_{t2m}$	$V_{t21}$	$V_{t22}$	$-V_{t23}$	$V_{t21}$	$V_{t22}$	$V_{t23}$	$V_{t24}$	$V_{t25}$	$V_{t26}$
$t_3$	$-V_{t3m}$	$V_{t31}$	$V_{t32}$	$V_{t33}$	$V_{t31}$	$V_{t32}$	$V_{t33}$	$V_{t34}$	$V_{t35}$	$V_{t36}$
$t_4$	0	$V_{t4m}$	$V_{t42}$	0	$V_{t41}$	$V_{t42}$	$V_{t43}$	$V_{t44}$	$V_{t45}$	$-iV_{t46}$
$t_5$	$-V_{t5m}$	$V_{t51}$	$V_{t52}$	$V_{t53}$	$V_{t51}$	$V_{t52}$	$V_{t53}$	$V_{t54}$	$V_{t55}$	$V_{t56}$
$t_6$	$V_{t6m}$	$V_{t61}$	$V_{t62}$	$-V_{t63}$	$V_{t61}$	$V_{t62}$	$V_{t63}$	$iV_{t64}$	$V_{t65}$	$V_{t66}$

(c)  $\mathbf{k} = (1/2, 1/2, -1/2)$  ( $H$ )

$H$	$m$	$a_1$	$a_2$	$a_3$	$t_1$	$t_2$	$t_3$	$t_4$	$t_5$	$t_6$
$m$	$V_{mm}$	$V_{m1}$	$V_{m2}$	$V_{m3}$	0	0	0	0	0	0
$a_1$	$V_{a1m}$	$V_{a11}$	$V_{a12}$	$V_{a13}$	$V_{a14}$	0	$-V_{a12}$	$-V_{a11}$	0	$V_{a11}$
$a_2$	$V_{a2m}$	$V_{a21}$	$V_{a22}$	$V_{a23}$	$-V_{a21}$	$V_{a21}$	0	$V_{a21}$	$-V_{a21}$	0
$a_3$	$V_{a3m}$	$V_{a31}$	$V_{a32}$	$V_{a33}$	0	$-V_{a31}$	$V_{a31}$	0	$V_{a31}$	$-V_{a31}$
$t_1$	0	$V_{t1m}$	$-V_{t12}$	0	$V_{t11}$	0	0	$V_{t14}$	0	0
$t_2$	0	0	$V_{t21}$	$-V_{t23}$	0	$V_{t21}$	0	0	$V_{t24}$	0
$t_3$	0	$-V_{t3m}$	0	$V_{t33}$	0	0	$V_{t31}$	0	0	$V_{t34}$
$t_4$	0	$-V_{t4m}$	$V_{t42}$	0	$V_{t44}$	0	0	$V_{t44}$	0	0
$t_5$	0	0	$-V_{t51}$	$V_{t53}$	0	$V_{t54}$	0	0	$V_{t54}$	0
$t_6$	0	$V_{t6m}$	0	$-V_{t63}$	0	0	$V_{t64}$	0	0	$V_{t64}$

(d)  $\mathbf{k} = (1/4, 1/4, 1/4)$  ( $P$ )

$P$	$m$	$a_1$	$a_2$	$a_3$	$t_1$	$t_2$	$t_3$	$t_4$	$t_5$	$t_6$
$m$	$V_{mm}$	0	0	0	0	0	0	0	0	0
$a_1$	0	$V_{a1m}$	$V_{a12}$	$V_{a13}$	$iV_{a14}$	0	$-V_{a12}$	$-V_{a11}$	0	$iV_{a14}$
$a_2$	0	$V_{a2m}$	$V_{a21}$	$V_{a23}$	$-V_{a21}$	$iV_{a24}$	0	$iV_{a21}$	$-V_{a21}$	0
$a_3$	0	$V_{a3m}$	$V_{a31}$	$V_{a33}$	0	$-V_{a31}$	$iV_{a34}$	0	$iV_{a31}$	$-V_{a31}$
$t_1$	0	$-iV_{t1m}$	$-V_{t12}$	0	$V_{t11}$	0	0	0	0	0
$t_2$	0	0	$-iV_{t21}$	$-V_{t23}$	0	$V_{t21}$	0	0	0	0
$t_3$	0	$-V_{t3m}$	0	$-iV_{t33}$	0	0	$V_{t31}$	0	0	0
$t_4$	0	$-V_{t4m}$	$-iV_{t42}$	0	0	0	0	$V_{t44}$	0	0
$t_5$	0	0	$-V_{t51}$	$-iV_{t53}$	0	0	0	0	$V_{t51}$	0
$t_6$	0	$-iV_{t6m}$	0	$-V_{t63}$	0	0	0	0	0	$V_{t64}$

Table 10. Matrices of the mixing-potential Fourier transforms  $\|\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k})\|$  for the disordered h.c.p. structure with fixed  $\alpha, \beta$ (a)  $\mathbf{k} = (0, 0, 0)$  ( $\Gamma$ )

$\Gamma$	$m_1$	$m_2$	$\alpha_1$	$\alpha_2$	$t_1$	$t_2$	$t_3$	$t_4$
$m_1$	$V_{m_1 m_1}$	$V_{m_1 m_2}$	$V_{m_1 \alpha_1}$	$V_{m_1 \alpha_2}$	$V_{m_1 t_1}$	$V_{m_1 t_2}$	$V_{m_1 t_3}$	$V_{m_1 t_4}$
$m_2$	$V_{m_2 m_1}$	$V_{m_2 m_2}$	$V_{m_2 \alpha_1}$	$V_{m_2 \alpha_2}$	$V_{m_2 t_1}$	$V_{m_2 t_2}$	$V_{m_2 t_3}$	$V_{m_2 t_4}$
$\alpha_1$	$V_{\alpha_1 m_1}$	$V_{\alpha_1 m_2}$	$V_{\alpha_1 \alpha_1}$	$V_{\alpha_1 \alpha_2}$	$V_{\alpha_1 t_1}$	$V_{\alpha_1 t_2}$	$V_{\alpha_1 t_3}$	$V_{\alpha_1 t_4}$
$\alpha_2$	$V_{\alpha_2 m_1}$	$V_{\alpha_2 m_2}$	$V_{\alpha_2 \alpha_1}$	$V_{\alpha_2 \alpha_2}$	$V_{\alpha_2 t_1}$	$V_{\alpha_2 t_2}$	$V_{\alpha_2 t_3}$	$V_{\alpha_2 t_4}$
$t_1$	$V_{t_1 m_1}$	$V_{t_1 m_2}$	$V_{t_1 \alpha_1}$	$V_{t_1 \alpha_2}$	$V_{t_1 t_1}$	$V_{t_1 t_2}$	$V_{t_1 t_3}$	$V_{t_1 t_4}$
$t_2$	$V_{t_2 m_1}$	$V_{t_2 m_2}$	$V_{t_2 \alpha_1}$	$V_{t_2 \alpha_2}$	$V_{t_2 t_1}$	$V_{t_2 t_2}$	$V_{t_2 t_3}$	$V_{t_2 t_4}$
$t_3$	$V_{t_3 m_1}$	$V_{t_3 m_2}$	$V_{t_3 \alpha_1}$	$V_{t_3 \alpha_2}$	$V_{t_3 t_1}$	$V_{t_3 t_2}$	$V_{t_3 t_3}$	$V_{t_3 t_4}$
$t_4$	$V_{t_4 m_1}$	$V_{t_4 m_2}$	$V_{t_4 \alpha_1}$	$V_{t_4 \alpha_2}$	$V_{t_4 t_1}$	$V_{t_4 t_2}$	$V_{t_4 t_3}$	$V_{t_4 t_4}$

(d)  $\mathbf{k} = (1/3, 1/3, 1/2)$  ( $H$ )

$H$	$m_1$	$m_2$	$\alpha_1$	$\alpha_2$	$t_1$	$t_2$	$t_3$	$t_4$
$m_1$	$V_{m_1 m_1}$	0	0	0	0	$V_{m_1 t_2}$	$-V_{m_1 t_3}$	0
$m_2$	0	$V_{m_2 m_2}$	0	0	$-V_{m_2 t_1}$	0	0	$V_{m_2 t_4}$
$\alpha_1$	0	0	$V_{\alpha_1 \alpha_1}$	0	0	0	0	0
$\alpha_2$	0	0	0	$V_{\alpha_2 \alpha_2}$	0	0	0	0
$t_1$	0	$-V_{t_1 m_1}$	0	0	$V_{t_1 t_1}$	0	0	$V_{t_1 t_4}$
$t_2$	$V_{t_2 m_1}$	0	0	0	0	$V_{t_2 t_1}$	$V_{t_2 t_4}$	0
$t_3$	$-V_{t_3 m_1}$	0	0	0	0	$V_{t_3 t_4}$	$V_{t_3 t_1}$	0
$t_4$	0	$V_{t_4 m_1}$	0	0	$V_{t_4 t_4}$	0	0	$V_{t_4 t_1}$

(b)  $\mathbf{k} = (0, 1/2, 0)$  ( $M$ )

$M$	$m_1$	$m_2$	$\alpha_1$	$\alpha_2$	$t_1$	$t_2$	$t_3$	$t_4$
$m_1$	$V_{m_1 m_1}$	$V_{m_1 m_2}$	$V_{m_1 \alpha_1}$	$V_{m_1 \alpha_2}$	$V_{m_1 t_1}$	$V_{m_1 t_2}$	$V_{m_1 t_3}$	$V_{m_1 t_4}$
$m_2$	$V_{m_2 m_1}$	$V_{m_2 m_2}$	$-V_{m_2 \alpha_1}$	$-V_{m_2 \alpha_2}$	$V_{m_2 t_1}$	$V_{m_2 t_2}$	$V_{m_2 t_3}$	$V_{m_2 t_4}$
$\alpha_1$	$V_{\alpha_1 m_1}$	$-V_{\alpha_1 m_2}$	$V_{\alpha_1 \alpha_1}$	$V_{\alpha_1 \alpha_2}$	$V_{\alpha_1 t_1}$	$V_{\alpha_1 t_2}$	$-V_{\alpha_1 t_3}$	$-V_{\alpha_1 t_4}$
$\alpha_2$	$V_{\alpha_2 m_1}$	$-V_{\alpha_2 m_2}$	$V_{\alpha_2 \alpha_1}$	$V_{\alpha_2 \alpha_2}$	$-V_{\alpha_2 t_1}$	$-V_{\alpha_2 t_2}$	$V_{\alpha_2 t_3}$	$V_{\alpha_2 t_4}$
$t_1$	$V_{t_1 m_1}$	$V_{t_1 m_2}$	$V_{t_1 \alpha_1}$	$-V_{t_1 \alpha_2}$	$V_{t_1 t_1}$	$V_{t_1 t_2}$	$V_{t_1 t_3}$	$V_{t_1 t_4}$
$t_2$	$V_{t_2 m_1}$	$V_{t_2 m_2}$	$V_{t_2 \alpha_1}$	$-V_{t_2 \alpha_2}$	$V_{t_2 t_1}$	$V_{t_2 t_2}$	$V_{t_2 t_3}$	$V_{t_2 t_4}$
$t_3$	$V_{t_3 m_1}$	$V_{t_3 m_2}$	$-V_{t_3 \alpha_1}$	$V_{t_3 \alpha_2}$	$V_{t_3 t_1}$	$V_{t_3 t_2}$	$V_{t_3 t_3}$	$V_{t_3 t_4}$
$t_4$	$V_{t_4 m_1}$	$V_{t_4 m_2}$	$-V_{t_4 \alpha_1}$	$V_{t_4 \alpha_2}$	$V_{t_4 t_1}$	$V_{t_4 t_2}$	$V_{t_4 t_3}$	$V_{t_4 t_4}$

(e)  $\mathbf{k} = (0, 1/2, 1/2)$  ( $L$ )

$L$	$m_1$	$m_2$	$\alpha_1$	$\alpha_2$	$t_1$	$t_2$	$t_3$	$t_4$
$m_1$	$V_{m_1 m_1}$	0	$V_{m_1 \alpha_1}$	$-V_{m_1 \alpha_2}$	$V_{m_1 t_1}$	$V_{m_1 t_2}$	$-V_{m_1 t_3}$	$V_{m_1 t_4}$
$m_2$	0	$V_{m_2 m_2}$	$V_{m_2 \alpha_1}$	$V_{m_2 \alpha_2}$	$-V_{m_2 t_1}$	$V_{m_2 t_2}$	$V_{m_2 t_3}$	$V_{m_2 t_4}$
$\alpha_1$	$V_{\alpha_1 m_1}$	$V_{\alpha_1 m_2}$	$V_{\alpha_1 \alpha_1}$	0	$V_{\alpha_1 t_1}$	$V_{\alpha_1 t_2}$	$V_{\alpha_1 t_3}$	$V_{\alpha_1 t_4}$
$\alpha_2$	$-V_{\alpha_2 m_1}$	$V_{\alpha_2 m_2}$	0	$V_{\alpha_2 \alpha_2}$	$-V_{\alpha_2 t_1}$	$V_{\alpha_2 t_2}$	$V_{\alpha_2 t_3}$	$-V_{\alpha_2 t_4}$
$t_1$	$V_{t_1 m_1}$	$-V_{t_1 m_2}$	$V_{t_1 \alpha_1}$	$V_{t_1 \alpha_2}$	$V_{t_1 t_1}$	$V_{t_1 t_2}$	$V_{t_1 t_3}$	$V_{t_1 t_4}$
$t_2$	$V_{t_2 m_1}$	$V_{t_2 m_2}$	$V_{t_2 \alpha_1}$	$V_{t_2 \alpha_2}$	$-V_{t_2 t_1}$	$V_{t_2 t_2}$	$V_{t_2 t_3}$	$-V_{t_2 t_4}$
$t_3$	$-V_{t_3 m_1}$	$V_{t_3 m_2}$	$V_{t_3 \alpha_1}$	$V_{t_3 \alpha_2}$	$V_{t_3 t_1}$	$V_{t_3 t_2}$	$V_{t_3 t_3}$	$V_{t_3 t_4}$
$t_4$	$V_{t_4 m_1}$	$V_{t_4 m_2}$	$V_{t_4 \alpha_1}$	$V_{t_4 \alpha_2}$	$V_{t_4 t_4}$	$-V_{t_4 t_3}$	$-V_{t_4 t_2}$	$V_{t_4 t_1}$

(c)  $\mathbf{k} = (1/3, 1/3, 0)$  ( $K$ )

$K$	$m_1$	$m_2$	$\alpha_1$	$\alpha_2$	$t_1$	$t_2$	$t_3$	$t_4$
$m_1$	$V_{m_1 m_1}$	0	0	0	0	$V_{m_1 t_2}$	$V_{m_1 t_3}$	0
$m_2$	0	$V_{m_2 m_2}$	0	0	$V_{m_2 t_1}$	0	0	$V_{m_2 t_4}$
$\alpha_1$	0	0	$V_{\alpha_1 \alpha_1}$	$V_{\alpha_1 \alpha_2}$	0	0	0	0
$\alpha_2$	0	0	$V_{\alpha_2 \alpha_1}$	$V_{\alpha_2 \alpha_2}$	0	0	0	0
$t_1$	0	$V_{t_1 m_2}$	0	0	$V_{t_1 t_1}$	0	0	$V_{t_1 t_4}$
$t_2$	$V_{t_2 m_1}$	0	0	0	0	$V_{t_2 t_1}$	$V_{t_2 t_4}$	0
$t_3$	$V_{t_3 m_1}$	0	0	0	0	$V_{t_3 t_4}$	$V_{t_3 t_1}$	0
$t_4$	0	$V_{t_4 m_2}$	0	0	$V_{t_4 t_4}$	0	0	$V_{t_4 t_1}$

(f)  $\mathbf{k} = (0, 0, 1/2)$  ( $A$ )

$A$	$m_1$	$m_2$	$\alpha_1$	$\alpha_2$	$t_1$	$t_2$	$t_3$	$t_4$
$m_1$	$V_{m_1 m_1}$	0	$V_{m_1 \alpha_1}$	$-V_{m_1 \alpha_2}$	$V_{m_1 t_1}$	$V_{m_1 t_2}$	$-V_{m_1 t_3}$	$V_{m_1 t_4}$
$m_2$	0	$V_{m_2 m_2}$	$-V_{m_2 \alpha_1}$	$-V_{m_2 \alpha_2}$	$-V_{m_2 t_1}$	$V_{m_2 t_2}$	$V_{m_2 t_3}$	$V_{m_2 t_4}$
$\alpha_1$	$V_{\alpha_1 m_1}$	$-V_{\alpha_1 m_2}$	$V_{\alpha_1 \alpha_1}$	0	$V_{\alpha_1 t_1}$	$V_{\alpha_1 t_2}$	$-V_{\alpha_1 t_3}$	$-V_{\alpha_1 t_4}$
$\alpha_2$	$-V_{\alpha_2 m_1}$	$-V_{\alpha_2 m_2}$	0	$V_{\alpha_2 \alpha_2}$	$V_{\alpha_2 t_1}$	$-V_{\alpha_2 t_2}$	$V_{\alpha_2 t_3}$	$-V_{\alpha_2 t_4}$
$t_1$	$V_{t_1 m_1}$	$-V_{t_1 m_2}$	$V_{t_1 \alpha_1}$	$V_{t_1 \alpha_2}$	$V_{t_1 t_1}$	$V_{t_1 t_2}$	$V_{t_1 t_3}$	$V_{t_1 t_4}$
$t_2$	$V_{t_2 m_1}$	$V_{t_2 m_2}$	$V_{t_2 \alpha_1}$	$-V_{t_2 \alpha_2}$	$-V_{t_2 t_1}$	$V_{t_2 t_2}$	$V_{t_2 t_3}$	$-V_{t_2 t_4}$
$t_3$	$-V_{t_3 m_1}$	$V_{t_3 m_2}$	$-V_{t_3 \alpha_1}$	$V_{t_3 \alpha_2}$	$V_{t_3 t_1}$	$V_{t_3 t_2}$	$V_{t_3 t_3}$	$V_{t_3 t_4}$
$t_4$	$V_{t_4 m_1}$	$V_{t_4 m_2}$	$-V_{t_4 \alpha_1}$	$-V_{t_4 \alpha_2}$	$V_{t_4 t_4}$	$-V_{t_4 t_3}$	$-V_{t_4 t_2}$	$V_{t_4 t_1}$

h.c.p.:

$$\text{Re } \tilde{w}_{\alpha_1 \alpha_2}^{\alpha\beta}(\mathbf{k}) / \text{Im } \tilde{w}_{\alpha_1 \alpha_2}^{\alpha\beta}(\mathbf{k}) = -\cotan \pi k_3; \quad (16)$$

where Re and Im mean the real and imaginary parts of the complex quantity, respectively.

## 6. Matrices of the mixing-potential Fourier transforms for the high-symmetry points of a reciprocal lattice

Under the statistical-thermodynamic analysis of the stability of ordered structures within the method of concentration waves, it is necessary to know the normal concentration modes of the structural instabilities that are specified by the eigenvectors of matrices of the Fourier

transforms  $\|\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k})\|$ . As shown by Sanchez, Gratias & de Fontaine (1982), Khachatryan (1978, 1983), Solov'eva & Shtern (1990) and Zhorovkov (1993), the concentration modes can be found using the information on independent elements of this matrix.

The specific place in such an analysis belongs to the Lifshitz points\* of the reciprocal lattice since these points correspond to the stable ordered structures, which have a wide range of existence in the phase diagrams of solid solutions and are most often observed in experiment (Sanchez, Gratias & de Fontaine, 1982; Khachatryan, 1978, 1983). Therefore, it seems to be useful to construct

\* By definition, the wave-vector group of the Lifshitz point contains the symmetry elements intersecting at one point (Landau & Lifshitz, 1980; Khachatryan, 1978, 1983).

the matrices of the Fourier transforms of mixing energies also for the Lifshitz points. The results of such a consideration are shown in Tables 8(a)–(c), 9(a)–(c) and 10(a)–(f) for the disordered solid solutions with f.c.c., b.c.c. and h.c.p. lattices.

Each of these tables presents the fragment of the matrix  $\|\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k})\|$  at some given  $\alpha$ ,  $\beta$  and given vector  $\mathbf{k}$ , which corresponds to one of the Lifshitz points of the structure under consideration. The convenient designations introduced by Bouckaert, Smoluchowski & Wigner (1936) for the high-symmetry points of reciprocal lattices are used. The symbol  $V$  is used for the designation of the real quantities. The additional requirements on matrix elements  $\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k})$ , as in the case of the non-Lifshitz points, are (12) and (13). Note that for the Lifshitz points all matrix components  $\tilde{w}_{pq}^{\alpha\beta}(\mathbf{k})$  necessary are real or imaginary. Moreover, the elements belonging to the same types of position (one of  $m$ ,  $o$  and  $t$ ) must be real.\*

The analysis carried out in this work concerns the symmetry properties of the mixing potentials of the lowest orders (unary and binary) in disordered structures. Similarly (on the basis of the approach proposed in paper 1), the study of mixing potentials of higher orders and/or for ordered structures can be performed.

\*The block  $\|\tilde{w}_{m,m}(\mathbf{k})\|$  of the Fourier transforms of the mixing potential corresponding to the sites of a disordered h.c.p. binary solution was obtained by Sanchez, Gratias & de Fontaine (1982) and Zhorovkov (1993) both for arbitrary and for the high-symmetry points of reciprocal space. The same results for the block  $\|\tilde{w}_{o,o}(\mathbf{k})\|$  corresponding to the octahedral interstices of disordered b.c.c. binary solution were given by Khachatryan (1978, 1983) for the cases of some high-symmetry points.

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## Structural Classes and Space Groups of Organic Homomolecular Crystals: New Statistical Data

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### Abstract

Structural classes (SC) are very useful for the description and consideration of molecular arrangements in crystals. The distribution of 19 642 organic homomolecular crystals among SC has been investigated. 305 SC having very unequal frequencies were discovered. A full list is given.

### Introduction

The concept of structural class (SC), proposed by Zorky, Belsky, Lazareva & Porai-Koshits (1967), has proved to be very convenient for describing the general features of molecular arrangements connected with space symmetry. We sometimes say that the SC reflects 'the topology' of a molecular crystal (Zorky 1991). The meaning of this

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