Characterization of Structure Types by Lattice Complexes with Increased Self-Coordination Numbers

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Most of the 402 characteristic Wyckoff positions were analyzed for the numbers 1, 2, 3, *etc.* of lattice complexes with increased self-coordination numbers T_i of the $i = 1-3$ shells. The Wyckoff letters of standardized inorganic structures with the proper space group number get an additional number 1, 2, 3, *etc.*, if the x, y, z, c/a, $\cos\gamma$, *etc.* parameters are close to the parameters of these lattice complexes. The lattice complexes 1, 2, 3, *etc.* or combinations of several of these complexes are sphere, layer or rod packings. The plate- or needle-like habit of single crystals can frequently be correlated with layered or rod-like packings. Combinations of lattice complexes can be analyzed for attractive or repulsive interactions by structure maps.

Key words: Wyckoff Sequence, Characteristic Lattice Complexes, Crystal Habit, Sphere Packings, Structure Map

Introduction

Compilations of standardized inorganic structures like TYPIX [1], SICS [2] or the Landolt-Börnstein compilation of structure types [3] have become available in recent years, to compare new structures with the large number of known structures. The standardization of the structures is essential for the selection of the structure type. Standardized isopointal structures with the same sequence of Wyckoff letters can contribute to a known structure type, if the ratios of lattice parameters and the positional parameters are similar [1 – 3]. The deviation of the parameters of a structure type, however, is not well defined.

The metals Mg and Zn of Wyckoff position 194-*c* (short symbol for position (2*c*) of space group number 194 of $P6_3/mmc$) for example with the ratios of lattice constants $c/a = 1.6241$ and 1.8563 are listed as different entries (TYPIX) or as a single entry of most other compilations and textbooks. The same applies for the 194-*c* position of isopointal structures with the Wyckoff sequences 194-*ca* like NiAs ($c/a = 1.393$) or FeS ($c/a = 1.688$) and 194-*dc* of BN ($c/a = 2.660$). The structure types of the present investigation will be defined by structures which are close to theoretical structures with maximum self-coordination numbers. The metal atoms of an ideal hexagonal close packing (hcp) with $c/a = \sqrt{8/3} \approx 1.6330$ for example have 12 nearest neighbors (six in the same layer and six in neighboring layers), 6 next-nearest neighbors (in the same layer) and 2 third neighbors (in the two next-nearest layers). This sphere packing is characterized by the three self-coordination numbers (T_1 T_2 T_3) (12 6 2) in the present investigation. The (T_1 T_2 T_3) values are decreased to (6 6 6) at the different c/a values of Mg or Zn. The $T_1 = 12$ neighbors at axial ratio $c/a = \sqrt{8/3}$ decrease to $T_1 = T_2 = 6$ neighbors at slightly different ratios. Increased T_3 values (6 6 8) or (6 6 12) are obtained again at $c/a = 4/3$ or $c/a = \sqrt{20/3}$. The $c/a = 1.6241$, 1.8563 and 1.688 values of Mg, Zn and FeS are close to $c/a \approx 1.6330$ of the hcp packing, while the c/a values of NiAs (1.393) and BN (2.660) are close to the (6 6 8) ($c/a = 4/3$) or (6 6 12) ($c/a \approx 2.580$) packings with increased T_i values. Certain c/a values frequently occur [4, 5]. A similar relation for x y z values can be suggested by comparison of cubic structure types [3]. Two lattice complexes with increased self-coordination numbers #1$\widehat{=}$ (4 6 3) and #2$\widehat{=}$ (12 6 24), for example, were determined for the characteristic Wyckoff position (32*e*) x x x of space group number 227($Fd\overline{3}m$) at $x = (\sqrt{6}-2)/8$ and $x = 1/4$. The Wyckoff letter *e* of standardized inorganic structures like H_2O (227-*e*1*a*), Ti_2C (227-*e*2*c*) or $MgAl_2O_4$ (227-*e*2*cb*) get the numbers 1 or 2, if the x value is close to that of the (4 6 3) or (12 6 24) sphere packings. The determination of (T_1 T_2

T_3) lattice complexes with increased T_i values will be explained in some detail and applied for the analysis of cubic structure types of the Landolt-Börnstein compilation [3]. The non-invariant Wyckoff positions get the numbers 1, 2, *etc.* like 227-*e*2*cb* of the 227-*e* position of oxygen atoms in $MgAl_2O_4$, if the $x\ y\ z$ values are close to the lattice complexes with increased ($T_1\ T_2\ T_3$) values.

Characteristic Lattice Complexes with Increased Self-Coordination Numbers

The characteristic lattice complexes with increased T_i values like the 3D (12 6 2) packing of the Mg structure type will be outlined by some examples in 1D or 2D. Atoms in a one-dimensional row (1D) with lattice constant $a = 1$ and inversion centers at $x = 0$ and $x = 1/2$ can occupy the Wyckoff positions (1*a*) $x = 0$, (1*b*) $x = 1/2$ or (2*c*) with the coordinates x and $\overline{x}$ of the two positions. The A and B atoms of an AB compound like a theoretical 1D NaCl can occupy the (1*a*) and (1*b*) positions. Each A atom has the self-coordination numbers ($T_1\ T_2\ T_3$) (2 2 2) of nearest, second and third A–A neighbors at distances $d_i = 1$, 2 and 3. The same applies for the B–B neighbors of (1*b*) position. The row of alternating A and B positions with maximum Madelung factor MF = $2\ln 2$ in 1D can also be considered as a lattice complex (2 2 2) for a combination of A and B atoms (A = B) and distances $d_i = 0.5$, 1 and 1.5 of first, second and third neighbors. The (2 2 2) combination of A and B positions of an AB_2 compound with A and B atoms in Wyckoff positions (1*a*) $x = 0$ and (2*c*) x and $\overline{x}$ is only possible for $x = 1/3$. Decreased T_i values (1 1 2) are obtained for the B atoms with distances $d_i = 2x$, $1 - 2x$ and 1 between nearest, second and third B–B neighbors for x values within the range $0 < x < 0.25$ and $d_i = 1 - 2x$, $2x$ and 1 for increased x values $0.25 < x < 0.5$. Theoretical 1D AB_2 structures CdO_2, FeS_2, PdF_2, SiO_2 or CO_2 with A atoms in (1*a*) $x = 0$ and B atoms in (2*c*) x, $\overline{x}$ positions with $x = 0.6$ (CdO_2), 0.35 (FeS_2), 0.28 (PdF_2), 0.26 (SiO_2) and 0.1 (CO_2) can contribute to three structure types. The x value of CdO_2 is varied to $\overline{x} = 0.4$ (standardized) for the comparison of the O–O and S–S dumb-bells of CdO_2 and FeS_2 with the center of the dumb-bells in (1*b*) $x = 0.5$ position. The CO_2 structure can be characterized by a linear O=C=O molecule with the center of the molecule A, the C atom, in (1*a*) $x = 0$ position. This structure with A = CO_2 can be compared with A = N_2 or D_2 dumb-bells or organic structures with the center of the molecules in the same position. The T_i values of the N_2, D_2, O_2 or S_2 dumb-bells are (1 1 2). Increased T_i values (2 2 2) are obtained for the (2*c*) position at $x = 0.25$. The PdF_2 and SiO_2 structures with x values close to the ideal $x = 0.25$ value contribute to the idealized AB_2 structure type with Wyckoff positions (1*a*) $x = 0$ and (2*c*) $x = 0.25$. The three structure types of the CdO_2, SiO_2 and CO_2 structures in 3D with Wyckoff positions 205-*a* and 205-*c* have a face-centered cubic (fcc) sphere packing of A atoms with ($T_1\ T_2\ T_3$) values (12 6 24) and a sphere packing of 205-*c* $x\ x\ x$ position with ($T_1\ T_2\ T_3$) values (7 6 3) at $x = (\sqrt{5} - 1)/8$ [6]. The well-known FeS_2 (pyrite) with S_2 dumb-bells instead of SiO_2 or PdF_2 is listed as structure type in most compilations. A large variety of compounds with different x values are given in the SICS compilation [2]. The (1 1 2) values of the 1D dumb-bells of N_2 or D_2 can be compared with the (1 6 6) values of the 3D N_2 or D_2 structure (205-*c*).

Usually the compound, which was investigated first, is chosen as structure type in the present investigation. Most structures like CO_2, N_2 or O_2 with the center of the molecule or cluster at the carbon position of CO_2 are not included in the present investigation because of the deviation of the x value from $x = 0.25$ of the ideal structure in 1D. These structures can be characterized like the structure of an element A in the varied Wyckoff positions (1*a*) $x = 0$ in 1D or 205-*a* instead of 205-*c* (N_2 or D_2) or 205-*ca* (CO_2) in 3D. The same applies for Fe(S_2) with the center of the S_2 dumb-bell in 205-*b* position, which is identical to the NaCl structure (225-*ba*). Other structures like NH_4I or $NaClO_4$ containing NH_4 or ClO_4 groups with rotational disorder or split sites can be compared with a 1D structure with N or Cl positions in (1*a*) $x = 0$ and H or O atoms in (2*c*) $x = 0.1$ with an occupancy of 0.5. Non-standardized structures like 1D SiO_2 with the different Wyckoff positions (1*b*) $x = 0.5$ and (2*c*) $x = 0.24$ or with all atoms in (1*a*) x position of a space group without inversion center at $x = 0.26$ (Si), $x = 0$ and $x = 0.52$ (O atoms) cannot be compared with the standardized structures. All atoms of the (1*a*) x position of the 1D space group without inversion center have the ($T_1\ T_2\ T_3$) (2 2 2) self-coordination values. The missing symmetry (inversion center) would be detected for the approximation of the $x = 0.52$ value to $x = 0.5$ and the (2 2 2) values for both oxygen positions. The discussion of the different structures in 1D shows that all kinds of A–A or B–B packings can be analyzed by consideration of (1*a*) $x = 0$ and (2*c*) x, $\overline{x}$ positions with T_i values (2 2 2) or

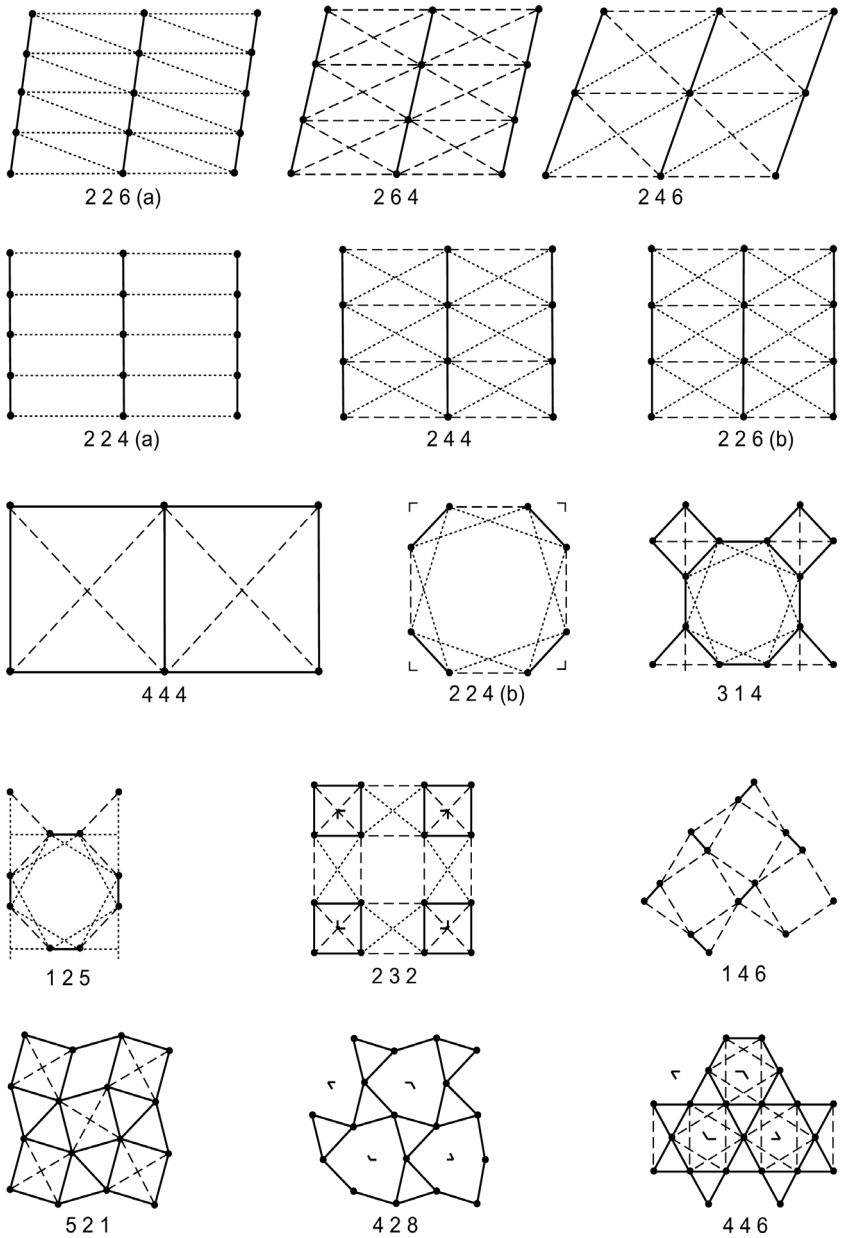

Fig. 1. 2D packings of A atoms with increased (T_1 T_2 T_3) values of Wyckoff positions 2-*a* (2 2 6 (a), 2 6 4, 2 4 6), 6-*a* (2 2 4 (a), 2 4 4, 2 2 6 (b), 4 4 4), 11-*d* (2 2 4 (b), 3 1 4, 1 2 5), 11-*f* (2 3 2, 4 4 4), 12-*c* (1 4 6, 5 2 1, 4 4 4), 15-*c* (4 2 8, 4 4 6). The T_1 nearest, T_2 next-nearest and T_3 third A–A neighbors are connected by solid, dashed and dotted lines, respectively.

(1 1 2), the characteristic lattice complexes [7] in 1D. The T_i values (2 2 2) of (1*a*) $x = 0$ are also obtained for (1*b*) $x = 0.5$ or (1*a*) x positions (in a 1D space group without inversion center). The investigation of the x values of (2*c*) x, $\bar{x}$ positions within the asymmetric range $0 < x \leq 0.25$ is sufficient because of identical B–B structures for increased x values. The asymmetric ranges are different for different characteristic lattice complexes [8].

2D structures are characterized by the lattice parameters a, b with the angle γ between a and b and the x, y parameters of different Wyckoff positions. Some packings of A atoms with increased self-coordination numbers T_1 T_2 T_3 of first, second and third A–A neighbors are shown in Fig. 1. The four positions of A atoms in Wyckoff position 11-*d* (space group *p*4*mm*) with the xy coordinates $x0$; $\bar{x}0$; $0x$; $0\bar{x}$ in 2 2 4 (b), 3 1 4 and 1 2 5 packings can be compared with the two posi-

tions x and $\overline{x}$ of 2-c position in 1D. Clusters of four or two atoms are obtained for x values close to $x = 0$ or $x = 0.5$, respectively. The T_2 or T_3 numbers are increased at $x = 1/4$ (2 2 4) or $(-1+\sqrt{3})/2$ (1 2 5). A 2D circle packing [16] with T_i values (3 1 4) is formed at $x = (2-\sqrt{2})/2$. The intermediate (T_1 T_2 T_3) values (2 1 1) and (1 2 1) are decreased. Similar results with circle packings of A atoms at intermediate x values are obtained for Wyckoff positions 11-f (4 4 4), 12-c (5 2 1 and 4 4 4), 15-c (4 2 8 and 4 4 6). The T_1 nearest neighbors are connected in two dimensions. The other packings with $T_1 < 3$ are rod packings with $T_1 = 2$ neighbors (first and second row of Fig. 1) or isolated A_2 or A_4 clusters with $T_1 = 1$ or 2 A neighbors within the clusters. The rod packings (2 2 4, 2 4 4 and 2 2 6) and the circle packing (4 4 4) are obtained for A atoms in the Wyckoff position $x = y = 0$ of 6-a of a rectangular lattice (*pmm*) with ratios of lattice constants $b/a = 1/3$, $1/2$, $1/\sqrt{3}$ or 1. The intermediate T_i values (2 2 2, 2 2 2, 2 2 4) are decreased. For $a = 1$, $b = 1/2$ as an example the A atom at $x = y = 0$ has $T_1 = 2$ nearest neighbors at the b axis with $y = \pm 1$, $T_2 = 2$ neighbors at $y = \pm 2$ plus $T_2 = 2$ neighbors at the a axis with $x = \pm 1$ and $T_3 = 4$ neighbors at diagonal positions with distances $\sqrt{1+0.5^2}$. The square-net circle packing with T_i values (4 4 4) at distances 1, $\sqrt{2}$ and 2 is obtained at $b/a = 1$.

The next example in 2D for the characteristic Wyckoff position (1a) of $p2$ with space group number 2 (= 2-a) was investigated for the special case $a = b = 1$ lattice constants and varied angles γ [9]. The square net with T_i values (4 4 4) and distances $d_i = 1$, $\sqrt{2}$ and 2 of the nearest, second and third A–A neighbors are obtained at $\gamma = 90°$. The T_i values are decreased to (4 2 2) within the range $60° < \gamma < 90°$ and reach (6 6 6) at $\gamma = 60°$ (hexagonal net with $d_i = 1$, $\sqrt{3}$ and 2). The T_i values vary further to (2 4 4), (*2 4 6*), (2 4 2), (*2 6 4*), (2 2 4), (*2 2 6*) and (2 2 2) (first row of Fig. 1). The $\cos\gamma$ values for increased T_i values (italic) are 3/4, 7/8 and 17/18, respectively. Identical packings are obtained for negative $\cos\gamma$ values in the range $90° < \gamma < 180°$. There is a large gap of $\Delta\gamma = 30°$ between the (4 4 4) and (6 6 6) circle packings. The $\cos\gamma = 0.25$ value ($\gamma \approx 75°$) is the limit between both. The range of γ values between the (2 6 4) and (2 2 6) packings at $\gamma \approx 29°$ and 19.2° is decreased. The (2 2 2) values at low $\gamma < 19.2°$ (or γ close to 180°) correspond to the linear chain. The observation of the same (T_1 T_2 T_3) values for Wyckoff position 9-a at the ratios of lattice constants $b/a = \tan\gamma/2$ show that identical packings can occur in different characteristic Wyckoff positions [9]. The ratio of lattice parameters b/a could be varied for the 2-a position besides the variation of $\cos\gamma$, to search for other characteristic lattice complexes with increased T_i values. The solutions can be obtained in a similar way as the trial-and-error or least-squares refinement of crystal structures. First the distances d_i of $i = 1-4$ shells of A–A neighbors are calculated. The smallest ratio d_{i+1}/d_i is then decreased further by variation of the parameters b/a and $\cos\gamma$ for the final value $d_{i+1}/d_i = 1$ at increased T_i values. A slightly increased ratio has to be taken, if it decreases faster. The b/a and $\cos\gamma$ values of the increased T_i values are the starting points for a second run of a trial-and-error calculation. The boundaries between the different packings meet at certain b/a and $\cos\gamma$ or x and y values in other Wyckoff positions with two parameters [8, 10]. The numbers of runs for the final packing with increased T_i values correspond to the numbers of variables x, y, z, $\cos\alpha$, $\cos\beta$, $\cos\gamma$, b/a, c/b and c/a. All lattice complexes with increased T_i values were determined for less than two parameters in 2D and 3D [9]. The parameters of sphere packings with increased T_i values were determined by Fischer, Koch and Sowa by different methods [8, 10–16]. The increased (T_1 T_2 T_3) values of each characteristic Wyckoff position are listed in Table 1. The structures of the Landolt-Börnstein compilation of structure types with less than two parameters are analyzed for these values in Table 2. In some cases two or more Wyckoff positions can be combined to a sphere packing. The Cs and Cl atoms (221-*ba*) of the CsCl structure for example form the bcc lattice of W (229-*a*), the Cu and Au atoms of Cu_3Au (221-*ca*) the fcc lattice of Cu (225-*a*) (Table 2). Some examples of combinations of two or more Wyckoff positions can be found in Table 3.

The NaCl structure with Wyckoff positions 225-*ba* for Na and Cl atoms can be combined to the primitive cubic packing with T_i values (6 12 8) (A = B atoms) of Wyckoff position 221-*a*. The distances $d_i = 1$, $\sqrt{2}$ and $\sqrt{3}$ correspond to the primitice cubic packing with lattice constant $a = 1$. The packings with increased T_i values (2 2 6), (2 6 8), (2 4 10), (6 12 8), (4 6 8) and (4 4 6) are obtained for the Wyckoff position 123-*a* with a tetragonal distortion of the primitive cubic packing at $c/a = 1/3, 1/2, 1/\sqrt{3}, 1, \sqrt{2}$ or 2 [6]. The (2 2 2) values of the linear chain are obtained at $c/a < 1/3$, the (4 4 4) values of the square net at $c/a > 2$. The first and eighth values (2 2 2) and (4 4 4) of 123-*a* are taken for more than 10% deviation from $c/a = 1/3$ or 2 in

Table 1. Numbers 1, 2, 3, *etc.* of lattice complexes with increased self-coordination numbers (T_1 T_2 T_3) of the first, second and third shell for characteristic Wyckoff positions (WP) of space group (SG) numbers.

SG-WP	1, 4	2, 5	3, 6
1-a	(12 6 24)	(10 4 8)	(8 12 6)
	(8 6 12)	(6 12 8)	
2-i	(12 6 24)	(12 6 2)	(11 2 3)
	(10 9 12)	(10 4 8)	(9 8 12)
	(8 12 6)	(8 12 4)	(8 6 12)
	(8 6 6)	(6 12 8)	(6 4 8)
	(6 2 6)	(5 6 6)	(4 12 12)
12-i	(11 2 3)		
43-b	(11 2 3)		
62-c	(10 4 2)		
63-c	(10 8 4)	(10 4 2)	
64-f	(11 2 3)		
70-a	(10 4 8)		
70-g	(10 4 8)		
78-a	(12 6 24)	(10 4 8)	(8 4 4)
80-b	(7 4 2)	(6 12 12)	(6 12 8)
81-h	(12 6 24)	(11 2 3)	
82-g	(12 6 24)	(10 4 8)	(10 1 5)
	(9 6 8)	(9 5 20)	
83-j	(7 12 5)		
83-l	(7 12 5)		
84-j	(12 6 24)	(11 2 3)	
84-k	(9 8 12)	(7 12 5)	
85-g	(10 1 5)	(9 5 20)	(7 4 2)
86-g	(12 6 24)	(11 2 3)	(10 1 5)
	(9 8 12)	(9 5 20)	(7 4 2)
87-h	(10 1 5)	(9 5 20)	(7 4 2)
87-i	(7 12 5)	(7 6 10)	(7 2 7)
88-f	(12 6 24)	(10 4 8)	(9 4 2)
	(8 6 2)	(8 4 1)	(8 2 3)
	(8 2 2)		
89-p	(8 1 2)	(7 4 2)	(7 2 2)
90-g	(8 1 9)	(7 12 5)	(7 7 6)
93-p	(9 8 12)	(7 1 2)	(6 12 8)
	(6 5 4)	(6 2 12)	(5 7 2)
94-g	(12 6 24)	(10 4 8)	(9 8 12)
	(7 12 5)	(7 4 2)	
95-a	(12 6 24)	(10 4 8)	(6 2 2)
95-c	(8 12 4)	(6 4 8)	
95-d	(12 6 24)	(10 8 4)	(10 4 8)
	(7 1 2)	(6 2 12)	(6 2 2)
	(6 1 4)		
96-a	(12 6 24)	(10 4 8)	(8 4 4)
96-b	(12 6 24)	(11 2 3)	(10 4 8)
	(8 12 4)	(7 2 2)	
97-k	(7 4 2)	(7 3 4)	(7 2 7)
	(6 12 8)	(6 6 2)	(6 6 1)
	(6 1 2)	(5 7 2)	(5 4 1)
98-d	(6 12 8)	(5 2 2)	
98-f	(6 12 12)	(6 12 8)	(6 4 2)
98-g	(12 6 24)	(10 4 8)	(8 2 2)
	(7 2 3)	(7 1 2)	(6 12 8)
	(6 3 4)	(6 2 12)	(6 2 1)
	(5 2 4)		
109-b	(7 4 2)	(6 12 12)	
109-c	(6 12 8)	(6 2 7)	
110-b	(12 6 24)	(11 2 3)	(8 3 2)
	(7 2 4)		
111-n	(12 6 24)	(10 4 8)	
111-o	(7 1 2)	(6 2 12)	(5 7 2)
112-n	(12 6 24)	(10 4 8)	(9 6 8)
	(8 1 2)	(7 4 2)	(7 2 2)
113-e	(12 6 24)	(11 2 3)	
113-f	(8 1 9)	(7 7 6)	
114-e	(12 6 24)	(11 2 3)	(10 4 8)
	(9 6 8)		
115-j	(7 1 2)	(6 2 12)	
115-l	(6 12 8)	(6 5 4)	
116-j	(9 8 12)	(8 1 2)	(7 4 2)
	(7 2 2)	(7 1 2)	(6 2 12)
117-i	(12 6 24)	(10 4 8)	(7 12 5)
	(7 4 2)		
118-i	(9 8 12)	(8 1 9)	(7 12 5)
	(7 7 6)	(6 12 12)	
119-i	(8 1 9)	(7 7 6)	(6 12 12)
119-j	(6 12 8)	(6 6 2)	(5 7 4)
120-i	(12 6 24)	(10 4 8)	(7 4 2)
	(7 3 4)	(7 2 7)	
121-i	(12 6 24)	(10 4 8)	(9 6 8)
	(8 1 2)	(7 4 2)	
121-j	(7 4 2)	(7 3 4)	(7 1 2)
	(6 12 8)	(6 6 1)	(6 2 12)
122-d	(12 6 24)	(10 4 8)	(8 4 2)
122-e	(12 6 24)	(11 2 3)	(9 8 12)
	(8 3 2)	(8 2 2)	(7 2 4)
	(7 2 3)	(7 2 2)	
123-a	(2 2 2)	(2 2 6)	(2 6 8)
	(2 4 10)	(6 12 8)	(4 6 8)
	(4 4 6)	(4 4 4)	
123-g	(6 12 8)		
123-j	(6 12 8)		
123-l	(5 7 2)		
123-p	(5 7 2)		
123-r	(6 12 8)		
123-s	(5 7 2)		
123-u	(7 2 7)	(5 7 2)	(5 4 1)
124-m	(8 1 2)	(7 4 2)	(7 2 2)
125-m	(8 1 2)	(7 4 2)	
125-n	(7 4 2)	(7 3 4)	
126-k	(8 1 2)	(7 4 2)	(7 2 2)
	(7 1 1)	(6 2 1)	
127-g	(7 12 5)		
127-i	(6 12 8)		
127-k	(7 12 5)		
127-l	(6 12 8)		
128-k	(8 1 9)	(7 12 5)	(7 7 6)
128-i	(7 12 5)	(6 12 8)	(6 6 1)
129-c	(12 6 24)	(10 4 8)	
129-i	(8 1 9)	(7 7 6)	
129-j	(6 12 8)	(6 5 4)	
129-k	(6 6 2)	(5 7 2)	
130-g	(8 2 1)	(8 1 9)	(8 1 2)
	(7 7 6)	(7 4 2)	(7 2 7)
	(7 2 2)	(7 1 3)	
131-j	(7 1 2)	(6 2 12)	
131-o	(5 7 2)		
131-q	(6 12 8)	(6 5 4)	
131-r	(6 12 8)	(5 7 2)	

Table 1 (continued).

SG-WP	1, 4	2, 5	3, 6
132-i	(12 6 24)	(10 4 8)	
132-n	(7 1 2)	(6 2 12)	(5 7 2)
132-o	(9 8 12)	(6 12 8)	
132-p	(5 7 2)		
133-k	(9 8 12)	(8 1 2)	(7 4 2)
	(7 3 4)	(7 2 7)	(7 1 2)
	(6 12 8)	(6 2 12)	(6 2 2)
	(6 2 1)	(5 7 2)	(5 4 1)
134-m	(9 8 12)	(7 1 2)	(6 12 8)
	(6 5 4)	(6 2 12)	
134-n	(6 12 8)	(6 6 2)	(6 6 1)
	(6 5 4)	(5 7 2)	
135-h	(12 6 24)	(10 4 8)	(7 12 5)
	(7 4 2)		
135-i	(9 8 12)	(7 12 5)	(7 2 7)
	(6 12 8)		
136-f	(12 6 24)	(11 2 3)	
136-i	(8 1 9)	(7 7 6)	
136-j	(9 8 12)	(7 12 5)	
136-k	(6 12 8)	(6 6 1)	
137-g	(12 6 24)	(10 4 8)	
137-h	(7 1 2)	(6 12 8)	(6 5 4)
	(6 2 12)	(5 7 2)	
138-i	(9 8 12)	(8 1 2)	(7 4 2)
138-j	(8 1 9)	(7 7 6)	(7 4 2)
	(7 3 4)		
139-a	(2 2 2)	(2 2 10)	(2 10 8)
	(2 8 6)	(10 4 8)	(8 6 12)
	(12 6 24)	(4 12 20)	(4 4 12)
	(4 4 4)		
139-e	(9 8 12)	(6 12 8)	
139-h	(6 12 8)	(6 5 4)	
139-i	(8 1 9)	(7 7 6)	
139-l	(6 6 2)	(5 7 2)	
139-m	(6 12 8)	(5 7 2)	
139-n	(6 12 8)	(6 6 1)	
139-o	(5 7 2)		
140-h	(8 1 2)	(7 4 2)	
140-k	(7 4 2)	(7 3 4)	(6 12 8)
140-l	(7 2 7)	(5 7 2)	(5 4 1)
140-m	(6 12 8)	(6 5 2)	(5 7 2)
141-a	(2 2 2)	(2 2 6)	(2 6 4)
	(2 4 6)	(6 4 8)	(4 6 8)
	(4 4 10)	(4 12 2)	(4 12 12)
	(4 4 16)	(8 12 4)	(4 4 4)
141-c	(2 2 2)	(2 2 6)	(2 6 4)
	(2 4 6)	(6 4 2)	(4 2 6)
	(4 4 4)	(4 2 6)	(6 12 12)
	(2 4 12)	(2 4 4)	
141-e	(12 6 24)	(10 8 4)	(10 4 8)
	(7 12 6)		
141-f	(6 12 8)	(5 2 2)	
141-g	(6 12 8)	(6 2 7)	
141-h	(12 6 24)	(10 4 8)	(8 2 2)
	(7 2 3)	(6 3 4)	(6 2 1)
141-i	(8 1 9)	(7 7 6)	(7 1 2)
	(6 12 8)	(6 2 12)	(6 1 4)
	(6 1 3)		
142-e	(12 6 24)	(10 4 8)	(6 12 8)
	(6 2 2)		
142-f	(8 3 2)	(7 2 4)	

SG-WP	1, 4	2, 5	3, 6
142-g	(9 8 12)	(8 1 9)	(7 7 6)
	(7 2 3)	(7 2 1)	(7 1 3)
	(7 1 2)	(7 1 1)	(6 12 8)
	(6 5 4)	(6 3 4)	(6 2 12)
	(6 2 2)	(6 2 1)	
145-a	(12 6 24)	(8 6 12)	
146-b	(8 12 6)	(8 6 16)	(8 4 4)
148-f	(10 5 21)		
152-c	(11 2 3)		
153-a	(10 4 8)	(6 4 4)	
154-a	(12 6 24)	(8 6 12)	
155-d	(8 12 6)	(8 6 16)	(6 4 8)
	(6 2 4)		
160-b	(8 6 16)	(8 4 4)	
160-c	(6 2 6)	(5 6 6)	
161-b	(12 6 2)	(8 6 6)	(8 4 8)
	(8 4 4)	(8 2 2)	
162-k	(12 6 2)	(8 6 6)	
164-d	(12 6 2)	(8 6 6)	
164-i	(8 8 2)	(8 6 2)	(6 8 4)
	(6 4 2)		
166-a	(2 2 2)	(2 2 8)	(2 8 6)
	(2 6 8)	(8 6 12)	(6 8 6)
	(6 6 8)	(6 12 8)	(6 6 12)
	(12 6 24)	(6 6 12)	(6 12 12)
	(6 6 6)		
166-c	(12 6 24)	(10 9 12)	(8 6 12)
166-d	(2 2 2)	(2 2 6)	(2 6 4)
	(2 4 6)	(6 4 8)	(4 6 4)
	(4 4 6)	(4 8 8)	(4 4 10)
	(8 6 16)	(4 4 10)	(4 4 10)
	(4 4 6)		
166-f	(6 2 6)	(5 6 6)	(5 2 2)
166-h	(8 6 16)	(7 7 8)	(7 4 3)
	(7 2 4)	(7 1 2)	(6 4 8)
	(6 2 2)		
167-e	(12 6 2)	(8 6 6)	(8 2 2)
	(6 4 4)	(6 2 2)	
169-a	(12 6 2)	(8 6 6)	(8 2 2)
171-c	(7 4 2)	(6 3 4)	(5 6 6)
	(5 4 4)		
174-j	(8 12 6)		
174-l	(8 12 6)		
175-j	(7 10 5)		
175-l	(7 10 5)		
176-h	(12 6 2)	(10 4 2)	
176-i	(10 9 12)	(7 10 5)	
177-n	(8 1 2)	(7 2 2)	
178-a	(10 4 8)	(6 4 4)	
178-b	(12 6 2)	(8 6 6)	(8 2 2)
	(6 2 2)		
178-c	(11 2 3)	(7 4 1)	(7 2 1)
	(7 1 2)	(6 4 4)	(6 4 2)
	(6 2 2)	(6 1 4)	(6 1 2)
	(6 1 1)	(5 2 2)	
179-c	(11 2 3)		
180-c	(2 2 2)	(2 2 6)	(2 6 4)
	(2 4 6)	(6 4 4)	(4 6 4)
	(4 4 6)	(4 4 4)	(4 4 10)
	(4 10 4)	(10 4 8)	(6 4 10)
	(6 10 4)	(6 6 10)	(6 6 6)

Table 1 (continued).

SG-WP	1, 4	2, 5	3, 6
180-f	(10 4 8)	(9 2 6)	(6 4 4)
180-g	(5 2 2)	(4 2 4)	
180-i	(6 4 2)	(6 3 4)	(5 6 6)
	(5 4 4)	(5 2 2)	
180-k	(7 1 1)	(6 4 2)	(6 3 4)
	(6 2 1)	(5 6 6)	(5 4 4)
	(5 4 2)	(5 2 3)	(5 2 2)
	(5 2 1)	(5 1 2)	
182-i	(10 9 12)	(7 7 8)	(7 4 2)
	(6 10 6)	(6 6 4)	(5 6 6)
187-j	(6 8 4)		
187-l	(5 6 6)		
187-n	(6 8 4)		
187-o	(5 6 6)		
188-c	(10 9 12)	(5 6 6)	
188-k	(12 6 2)	(8 6 6)	
188-l	(10 9 12)	(5 6 6)	
189-f	(8 12 6)		
189-i	(8 12 6)		
189-j	(6 10 6)		
189-l	(6 10 6)		
190-h	(8 12 6)	(8 8 2)	(8 6 2)
190-i	(8 12 6)	(7 7 8)	(6 10 6)
191-a	(2 2 2)	(2 2 8)	(2 8 12)
	(2 6 14)	(8 12 6)	(6 2 18)
	(6 8 18)	(6 6 8)	(6 6 6)
191-c	(2 2 2)	(2 2 5)	(2 5 6)
	(2 3 8)	(5 6 6)	(3 8 9)
	(3 6 5)	(3 6 3)	
191-e	(8 12 6)		
191-f	(2 2 2)	(2 2 6)	(2 6 8)
	(2 4 10)	(6 8 4)	(4 2 12)
	(4 6 14)	(4 4 8)	(4 4 6)
191-h	(5 6 6)		
191-i	(6 8 4)		
191-j	(5 6 6)		
191-l	(6 10 6)	(5 6 4)	
191-n	(5 6 6)		
191-o	(6 10 6)	(5 6 4)	
191-p	(5 7 4)		
191-r	(5 7 4)		
192-l	(8 1 2)	(7 2 2)	
192-m	(7 1 1)	(6 2 1)	(6 1 2)
	(5 7 4)	(5 2 2)	
193-g	(12 6 2)	(8 6 6)	
193-j	(7 4 2)	(6 10 6)	
193-k	(10 9 12)	(5 6 6)	
193-l	(6 10 6)	(6 5 4)	(5 7 4)
	(5 6 4)		
194-c	(2 2 2)	(2 2 8)	(2 8 6)
	(2 6 8)	(8 6 6)	(6 2 6)
	(6 8 6)	(6 6 8)	(12 6 2)
	(6 6 12)	(6 12 12)	(6 6 6)
194-f	(10 9 12)	(5 6 6)	
194-h	(8 8 2)	(8 6 2)	(6 8 4)
	(6 4 2)		
194-j	(6 6 4)	(5 6 6)	
194-k	(7 7 8)	(6 10 6)	(6 8 4)
	(5 6 4)		

SG-WP	1, 4	2, 5	3, 6
194-l	(5 7 4)	(5 6 6)	
195-j	(6 7 6)	(6 1 10)	(5 8 8)
196-h	(6 4 5)		
197-f	(9 4 18)	(9 1 2)	(6 4 5)
	(6 2 2)		
198-a	(12 6 24)	(6 6 12)	(6 12 6)
198-b	(8 4 8)		
199-a	(6 12 8)	(3 9 6)	(3 6 6)
199-b	(8 4 8)	(4 6 2)	(4 2 8)
	(4 2 6)	(4 4 4)	
199-c	(9 4 18)		
200-f	(1 8 9)	(1 9 8)	(2 8 16)
200-j	(6 7 6)	(6 1 10)	
200-l	(5 5 1)		
201-h	(9 1 2)	(6 4 5)	(6 1 4)
	(5 4 1)		
202-h	(6 4 5)		
202-i	(6 7 6)	(6 1 10)	
203-g	(7 2 1)	(7 1 2)	
204-e	(1 4 12)	(5 8 1)	(4 1 9)
	(4 2 8)		
204-g	(9 1 2)	(6 4 5)	(6 1 4)
204-h	(6 4 1)	(5 9 6)	
205-c	(7 6 3)	(6 7 9)	(6 6 7)
	(6 12 8)		
205-d	(8 6 16)	(8 2 1)	
206-c	(1 3 7)	(4 1 6)	(3 2 12)
206-d	(8 6 16)	(4 4 6)	(4 8 2)
206-e	(7 1 2)	(6 2 2)	
207-k	(6 1 1)	(5 2 1)	
208-k	(1 6 2)	(3 4 2)	
208-m	(8 6 16)	(7 1 2)	(6 1 4)
	(5 4 1)		
209-j	(8 1 1)	(7 2 1)	
210-g	(2 8 16)	(4 4 2)	
210-h	(6 3 8)	(6 1 1)	(5 4 2)
	(5 1 4)		
211-i	(1 2 6)	(3 2 4)	(2 3 4)
	(4 1 4)	(2 2 5)	
211-j	(6 4 1)	(6 1 1)	(5 9 6)
	(5 1 8)	(5 1 5)	(5 1 3)
	(5 1 1)	(4 2 4)	
212-a	(6 12 6)		
212-c	(3 6 6)	(3 6 7)	(3 7 6)
	(4 12 12)	(1 3 6)	
212-d	(4 4 4)	(2 6 2)	(6 2 2)
	(4 10 8)	(4 4 4)	
212-e	(9 4 18)	(6 1 1)	(5 1 2)
214-a	(3 6 6)		
214-c	(4 4 4)		
214-e	(8 6 12)		
214-f	(4 8 2)	(2 2 5)	(2 3 4)
	(2 1 6)	(3 4 4)	
214-h	(3 4 2)	(4 2 4)	(2 4 8)
	(2 2 6)	(2 6 2)	(9 4 18)
214-i	(5 2 4)	(5 2 2)	(5 2 1)
	(5 1 1)	(4 2 2)	
215-e	(3 6 9)	(12 6 24)	
215-i	(6 7 6)	(5 8 8)	

Table 1 (continued).

SG-WP	1, 4	2, 5	3, 6
215-j	(4 3 5)		
216-e	(6 12 12)		
216-h	(5 2 12)		
216-i	(4 2 8)		
217-c	(3 6 14)	(9 6 8)	(6 12 8)
217-g	(9 4 18)	(8 6 16)	
217-h	(5 1 5)	(5 1 3)	
218-i	(9 4 18)	(8 6 16)	(7 1 2)
219-h	(8 1 1)	(7 2 1)	
220-a	(8 4 8)		
220-c	(8 6 12)	(5 6 3)	(3 2 12)
220-d	(1 4 4)	(5 4 2)	(4 5 4)
	(4 4 5)	(4 8 2)	
220-e	(7 2 1)	(7 1 2)	(6 2 2)
221-a	(6 12 8)		
221-c	(8 6 16)		
221-e	(4 2 8)	(5 1 8)	(1 4 9)
221-g	(3 3 4)	(6 12 8)	
221-h	(2 3 1)	(4 2 8)	
221-i	(4 2 6)	(4 4 8)	(6 7 6)
	(2 5 4)		
221-k	(4 3 5)		
221-m	(5 5 1)		
221-n	(4 3 2)		
222-i	(7 2 2)	(7 1 1)	(6 2 1)
223-c	(2 8 16)		
223-g	(2 2 4)		
223-j	(2 3 4)	(4 1 4)	(2 2 5)
223-k	(8 6 16)	(7 1 2)	(6 1 4)
223-l	(6 4 1)	(5 9 6)	(5 1 8)
224-e	(4 12 6)		
224-i	(2 2 2)	(2 3 1)	(3 6 3)
224-k	(8 6 16)	(6 1 4)	(5 4 1)
	(4 2 8)		
224-l	(5 1 5)	(5 1 3)	(4 2 4)
225-a	(12 6 24)		
225-e	(4 5 4)	(8 6 16)	
225-f	(3 3 4)	(3 6 4)	(6 6 1)
225-h	(4 2 5)	(4 3 4)	(5 2 12)
	(1 4 10)		
225-k	(6 7 6)	(4 1 4)	
225-l	(4 3 5)		
226-i	(8 1 1)	(7 2 1)	
226-j	(6 3 3)	(5 5 1)	
227-a	(4 12 12)		
227-c	(6 12 12)		
227-e	(4 6 3)	(12 6 24)	
227-f	(4 1 4)	(4 5 2)	(8 3 4)
	(4 4 6)	(4 8 8)	
227-g	(6 3 8)	(5 4 2)	(5 1 4)
227-h	(4 2 8)	(2 2 3)	
227-i	(4 3 4)		
228-g	(4 2 8)	(6 2 4)	
228-h	(8 6 16)	(6 2 2)	(6 1 4)
	(5 4 1)		
229-a	(8 6 12)		
229-b	(4 8 8)		
229-d	(4 2 8)		
229-e	(4 1 9)	(4 2 8)	(5 8 1)
	(1 12 8)		
229-f	(3 3 2)	(3 4 1)	(4 3 1)
	(1 3 9)		
229-g	(2 2 4)	(3 1 4)	(1 2 5)
229-h	(4 2 8)	(4 6 6)	(8 6 16)
	(4 6 2)	(4 2 5)	(6 1 4)
	(2 5 8)		
229-i	(2 3 2)	(4 3 2)	(2 2 4)
	(2 2 3)		
229-j	(5 1 5)	(5 1 3)	(4 2 4)
229-k	(6 4 1)	(5 9 6)	(5 1 8)
229-l	(4 4 1)	(4 3 2)	
230-b	(3 2 12)		
230-c	(4 8 2)		
230-d	(4 8 2)		
230-e	(2 3 3)	(1 4 3)	
230-f	(4 8 8)	(1 2 5)	
230-g	(3 4 4)	(2 8 16)	(6 2 2)
	(4 2 6)	(4 9 6)	(5 2 4)
	(1 6 4)		
230-h	(6 2 2)	(6 2 1)	(6 1 2)
	(6 1 1)	(5 4 2)	(5 2 2)

Table 2. Structure types of inorganic compounds [3] with space group (SG) numbers and Wyckoff sequence (WS). The numbers of the (T_1 T_2 T_3) values of the characteristic Wyckoff positions like (4 9 6) of 230-g5 and (4 8 8) of 230-f1 positions (Table 1) are added for the x values of Ni_3Ga_4 (230-$g5'f1a$) close to the $x = 0.375$ or $x = 0$ values of (4 9 6) or (4 8 8) packings [6, 9], or equivalent positions $g5'$ as explained in the text.

Compound	SG-WS	Compound	SG-WS	Compound	SG-WS
$Cd_{0.5}Bi_{1.5}O_{2.75}$	230-*da*	$NdO_{1.5}$	229-*g3a*	$Dy_6Fe_{16}O$	229-*h5e3ca*
Ni_3Ga_4	230-*g5′f1a*	$LiCa_4B_3N_6$	229-*e3cba*	$Ag_{1.8}Au_{0.2}S$	229-*h7dcba*
W	229-*a*	$U_4Re_7Si_6$	229-*e3dca*	Tl_7Sb_2	229-*h6f3e3a*
$AuSb_3$	229-*ba*	$Ca_4Rh_3H_{12}$	229-*e2dcb*	$Li_2Zr_6MnCl_{15}$	229-*h3e2dba*
$PtHg_4$	229-*ca*	$LiBa_4Sb_3O_{12}$	229-*e3dcba*	$Th_6Br_{15}H_7$	229-*h3f1e2b*
Pt_3O_4	229-*cb*	Ru_3Sn_7	229-*f3e4d*	C	227-*a*
SF_6	229-*e2a*	$CaCu_3Ti_4O_{12}$	229-*h3cba*	NaTl	227-*ba*
$Eu(NH_3)_6$	229-*e3a*	Nb_2F_5	229-*h3e2b*	SiO_2	227-*ca*
$(NH_4)_2SrCl_4$	229-*cba*	Zr_6CoCl_{15}	229-*h3e2ba*	$MgCu_2$	227-*cb*
C	229-*f3*	Ca_3Ag_8	229-*h6e2c*	$CsNbN_2$	227-*cba*
Ag_2S	229-*dba*	$Ce_3Ni_6Si_2$	229-*h5e3c*	H_2O	227-*e1a*

Table 2 (continued).

Compound	SG-WS	Compound	SG-WS	Compound	SG-WS
Ti_2C	227-*e2c*	$Cu_4Mn_3Bi_4$	225-*f1e1′dc*	Th_3P_4	220-*c3a*
$MgAl_2O_4$	227-*e2cb*	$K_3Rh(NO_2)_6$	225-*h1e2cba*	$Au_3Y_3Sb_4$	220-*c3ba*
$LiTiO_2$	227-*e2dc*	$Mn_6Bi(PO_4)O_8$	225-*f1f3′dba*	Pu_2C_3	220-*d2′c2*
$HTaWO_6$	227-*f3c*	$RuAl_{0.67}Sn_6O_8$	225-*f3′f2′e2ca*	La_4GeC_4	220-*d2′c2a*
$Fe_{3.7}O_4$	227-*e2dca*	KY_3F_{10}	225-*i3f1e2c*	$Li_{0.64}Pt_3O_4$	218-*e3da*
$Al_2(OH)_3F_3{\cdot}H_2O$	227-*f3cb*	Th_6Mn_{23}	225-*f2f3′e1′da*	Ag_3PO_4	218-*e2da*
$ThZr_2H_7$	227-*f5cba*	$Mg_3Ni_{20}B_6$	225-*h3f1′e1′ca*	SiF_4	217-*c2a*
$AgSbO_3$	227-*f4dc*	$Zr_6Zn_{23}Si$	225-*f2f3′e1′dba*	Li_5B_4	217-*c1c2′*
$KTaWO_6{\cdot}H_2O$	227-*f3dc*	$Sc_{11}Ir_4$	225-*f1f3′e1′dba*	Tl_3VS_4	217-*c2ba*
As_2O_3	227-*f3e2*	$KCo[Co(CN)_6]{\cdot}10H_2O$	225-*f3e1e2e1′cba*	Ta_2O	217-*c1c3ba*
Al_2O_3	227-*e1e2da*	$Zr_9Co_7In_{14}$	225-*i3f2e1cba*	ZnS	216-*ca*
$Ca_2Nb_2O_7$	227-*f3′dca*	$K_{19}Pb_8O_4(OH)_3$	225-*h3f3′e1e1′ba*	MgAgAs	216-*cba*
SbO_2	227-*f4dcba*	$Nb_3Cl_6(OH)(H_2O)_7$	225-*h3f2e1e1′c*	Li_2AgSb	216-*dcba*
Mn_3Ni_2Si	227-*f3′e2c*	$Na_{14}Ba_{14}CaN_6$	225-*f1f3′e1e1′da*	$KClO_4$	216-*e1ba*
$TlNb_2O_5F$	227-*f3e1′c*	$Ni_{20}AlB_{14}$	225-*h3f3f2′e1′a*	Cu I	216-*e1′ca*
Na_8SnSb_4	227-*f4′e2ca*	$Ca_{11}Ga_7$	225-*h3f3f2′e1′ba*	Be_5Au	216-*e1″ca*
W_6Fe_6C	227-*f3′e2cb*	$Y_6Mn_{23}H_{8.3}$	225-*f1f3f2′e1dba*	$ZnSO_4$	216-*e1ca*
$Cu_2Cr_2Te_4$	227-*f5e2cb*	$Ni_{20}Al_3B_{9.75}$	225-*h3f1′e1e2e1′ca*	$Na_{1.67}AlSiO_{4.33}$	216-*e1dcba*
$Tl_2Nb_2O_{6.07}$	227-*f3′e1da*	$Rb_5Tc_6S_{14}$	225-*h4f3f1′e1e1′ca*	$K_9(C_{70})$	216-*e1e1′da*
$CuIn_2Se_3$ I	227-*f5e2cba*	$K_7Mo_6Se_8(CN)_6(H_2O)_8$	225-*h4f3f1′e1e2e1′ca*	$Ba_2Cu_2WYO_{5.67}$	216-*f2dcba*
W_4Co_2C	227-*f3′e2dc*	$Th_6Mn_{23}H_{16}$	225-*h1f2f3′f1′e1′da*	Cu_2Se	216-*e1e1′dca*
$Sm_2Mo_2O_7$	227-*f4e2dc*	$Th_6Mn_{23}H_{16.2}$	225-*i1f1f3f2′e1dba*	MoSBr	216-*e1e1′e1″*
$Zn_4Nb_8C_3$	227-*f3e2dca*	Cu_2O	224-*ba*	Be_4TeO_7	216-*f2e1′ca*
$Pd_{3.5}Te$	227-*f5e2dca*	$Ag_2O_{2.5}$	224-*db*	Mo_4GaS_8	216-*e1e1′e1″a*
$K_{1.17}Bi_{2.33}O_{5.87}(H_2O)$	227-*f3′e1dca*	H_2O	224-*e1a*	$CsMgAsO_4(H_2O)_6$	216-*f1′e1cba*
Al_2O_3	227-*f4′e2e1′c*	$Si(CN_2)_2$	224-*e1ba*	$Cu_2Al_4O_7$	216-*f2e1′dca*
$AgPb_2Cl_3(OH)F$	227-*f4e2e1′c*	H_2O	224-*g2e1*	$Co_{2.95}O_4$	216-*e1e1′e1″da*
$Tl_{1.5}Ta_{1.5}W_{0.5}O_6$	227-*f3′e2e1d*	Cr_3Si	223-*ca*	$Cu_2Fe(CN)_6$	216-*f1f1′cba*
$Li_{13}In_3$	227-*f5e2dcba*	Nb_3SnH	223-*dca*	$Cu_2Fe(CN)_6(H_2O)_{0.5}$	216-*f1f1′dcba*
Ti_2NiH	227-*f3′e2dcba*	Pt_3O_4	223-*ec*	$Hg_5In_2Se_8$	216-*g2e1e1″ba*
Cu	225-*a*	$NaPt_3O_4$	223-*eca*	$Yb_{0.88}S$	216-*g2f2dcba*
NaCl	225-*ba*	$AuNb_3H_{2.9}$	223-*i4dca*	$Ag_{3.2}Hg_{2.4}SiSe_6$	216-*f2e1e1′e1″a*
CaF_2	225-*ca*	Po	221-*a*	$Zr_2C_{1.2}H_{0.8}$	216-*g2f2e1dba*
BiF_3	225-*cba*	CsCl	221-*ba*	$Cr_4Al_{13}Si_4$	216-*g1′f1′e1e1′a*
K(CN)	225-*e1′a*	Cu_3Au	221-*ca*	$Ru_4Pb_4O_{13}$	216-*g1′f1′e1e1″a*
$CuPt_7$	225-*dba*	ReO_3	221-*da*	$Ca_3Er_3Ge_2BO_{13}$	216-*f2e1e1′e1″dcba*
$NaSbF_6$	225-*e1ba*	$CaTiO_3$	221-*dba*	$Mn_5Ni_2Bi_4$	216-*g1′f1′e1e1′ba*
$Cu_{1.8}S$	225-*e1′ca*	NbO	221-*dc*	$Bi_{1.6}Y_{0.4}Sn_2O_7$	216-*g1′f1′e1e1″ca*
K_2PtCl_6	225-*e2ca*	U_4S_3	221-*dca*	$Mo_3Ni_2P_{1.18}$	216-*g1′f1e1e1′e1″a*
$NaBaLiNiF_6$	225-*dcba*	$Ga(CN)_3$	221-*e3a*	$Na_{11}Ca_{6.5}P_8$	216-*g2′f1e1e1′e1″dca*
$(NH_4)_3FeF_6$	225-*e1cba*	TiC_2	221-*f1a*	$AuTa_5S$	216-*g1f1e1e1′e1″e1‴*
$BaBiO_3$	225-*e2cba*	CaB_6	221-*f2a*	Fe_4C	215-*e2a*
HCl	225-*h3a*	Mo_3N_2	221-*dcba*	$(NH_4)Br$	215-*e1ba*
UB_{12}	225-*i3a*	CsN_3	221-*e1ba*	Cu_3AsS_4	215-*e2ca*
$CdCo_{0.67}(CN)_4$	225-*e1e1′ba*	$(NH_4)Br$	221-*g1ba*	Cu_3VS_4	215-*e2da*
$NaNb_{1.25}F_6$	225-*e1dba*	$K_{0.9}Li_{0.1}TaO_3$	221-*e3cba*	$K_3(SO_4)F$	215-*e1cba*
Cs_2MoOBr_5	225-*e1e2ca*	$CsHgCl_3$	221-*e3dba*	$AgB(CN)_4$	215-*e1e2ba*
$RuCl_2N_2(NH_3)_5$	225-*e1e1′ca*	$K_3(SO_4)F$	221-*g1cba*	$Li_8Al_3Si_5$	215-*e2e2′dcba*
Mg_6MnO_8	225-*e2dca*	$Pd_{0.75}H$	221-*h2ba*	Ag_3AuTe_2	214-*f1′e1′a*
$Cs_2LiCo(CN)_6$	225-*e1e1′cba*	YF_3	221-*g2dca*	Ca_3PI_3	214-*h6′g6a*
$CrFe_7C_{0.45}$	225-*e2dcba*	$Fe_{13}Ge_3$	221-*g2dcba*	$SrSi_2$	213-*c3a*
$TlPd_3O_4$	225-*f3dba*	$(NH_4)_3SnF_7$	221-*g1e2cba*	Mn	213-*d3c3*
Cu_3SbS_4	225-*f2dc*	$Ba_8Y_3Pt_4O_{17.5}$	221-*h2g2e1dca*	Mo_3Al_2C	213-*d3c3a*
Co_9S_8	225-*f2′e2ca*	$Ce_8Pd_{24}Sb$	221-*h2g2f1e2a*	Si	206-*c2*
$PtGa_2In_6O_8$	225-*f3′e2ca*	$Sr_8Rh_5H_{23}$	221-*h1g2f1e1dba*	H_2S	205-*a*
$Na_6(SO_4)_2ClF$	225-*f3e1cba*	$Ta_{1.08}O$	221-*h2g2f1e1dcba*	FeS_2 (SiO_2)	205-*c1′a*
$AgPF_6$	225-*h2e1ba*	$K_9U_6BiO_{24}$	221-*h2g2f2e1dcba*	CO_2	205-*c1a*
$Ba_2Ni(NO_2)_6$	225-*h1e2ca*	$Na_2Nb_7Cl_8F_{13}$	221-*j3h1f1e1ca*	CuCl	205-*c1c1′*
$Ag_6Hg(NO_3)O_8$	225-*f3e1′dba*	Ga	220-*a*	$Na_{9.7}C_{60}$	202-*f1cba*

Table 2 (continued).

Compound	SG-WS	Compound	SG-WS	Compound	SG-WS
$W(W_{0.42}Al_{5.58})Ge$	200-$f3ba$	$Ba_3Fe_2Cl_2O_5$	199-$b2'b4''a2a1'a3'$	ZrSO	198-$a2a2''a2''''$
$RbHg(NO_2)_3$	200-$f3dba$	CO	198-$a2'a1'$	$KAlOCl_2$	198-$a1a1'a1''$
$Na_{0.28}Co_{0.74}Pt_6O_8$	200-$i2f3a$	FeSi	198-$a2a3'$	SrBr(OH)	198-$a2a3a2'''a2''''$
UCo	199-$a2a2''$	PdF_2	198-$a1a2''a2''''$	$NiGa_4$	197-$e4d4c2c2'$
$Hg_3S_2Cl_2$	199-$b2'a1a1'$	NiSbS	198-$a1a3'a3''$		

Table 3. Combinations of Wyckoff positions (SG-WS) to a packing of a characteristic Wyckoff position (WP).

SG-WS	SG-WP	SG-WS	SG-WP
230-$g5b$	221-a	191-$b8a8$	191-$a5$
230-$f1a$	221-a	191-$b5a5$	191-$a3$
230-dc	223-c	187-$d5a5$	194-$c7$
229-$e2dc$	225-a	180-$d11c11$	166-$d9$
229-$e2d$	221-c	180-$d5c5$	180-$c4$
229-ba	221-a	166-$e10d10$	229-b
227-dc	225-a	166-$e5d5$	166-$d4$
227-ba	229-a	166-$b12a12$	225-a
225-ba	221-a	166-$b10a10$	221-a
223-dc	229-d	166-$b5a5$	166-$a4$
221-dc	229-b	141-$d10c10$	139-$a8$
221-ca	225-a	141-$d9c9$	225-a
221-ba	229-a	141-$d7c7$	139-$a4$
220-ba	230-d	141-$b10a10$	221-a
216-$e1e1''$	225-a	141-$b9a9$	229-a
216-$dcba$	229-a	139-$b7a7$	221-a
216-ca	227-a	139-$b5a5$	123-$a4$
216-ba	221-a	123-$d6a6$	225-a
214-$h6a$	225-a	123-$d5a5$	229-a
214-dc	230-c	123-$d3a3$	139-$a4$
214-ba	230-b	123-$c6a6$	123-$a7$
212-$d4b$	227-c	123-$c5a5$	123-$a6$
212-ba	214-a	123-$b7a7$	221-a
194-$d5c5$	191-$c4$	123-$b5a5$	123-$a3$
191-$g8f8$	191-$f5$	107-$a7a7'$	221-a
191-$g5f5$	123-$a3$	82-$c7a7$	227-a
191-$d7c7$	191-$c5$	82-$c5a5$	141-$a7$
191-$b11a11$	139-$a8$		

the present investigation. The number 1 or 8 is added to the Wyckoff position. A layered structure with alternating square net layers for example corresponds to the 123-$a8$ position. A slightly deformed primitive cubic packing can be found for 123-$a5$ at lattice constants close to $c/a = 1$. The primitive cubic packing with T_i values (6 12 8) is the fifth packing in 123-a position (Table 1). The same applies for other Wyckoff positions like 75-a, 79-b, 83-c, *etc.* [7] with the same sequences of T_i values as the characteristic Wyckoff position 123-a.

The present analysis of cubic structures with less than two parameters [3] demonstrates the preference of few combinations as is outlined by few examples. The atoms of the characteristic Wyckoff position 198-a (position (4a) $x\,x\,x$ of space group number 198, $P2_13$) for example form an fcc sphere packing with T_i values (12 6 24) at $x = 0$, and two packings with T_i values (6 6 12) at $x = (3-\sqrt{5})/8$ and (6 12 6) at $x = 0.125$. The asymmetric range of x values is $0 \le x \le 1/8$. The fcc packings at $x = 0$, 0.25, 0.5 and 0.75 are characterized as 198-$a1$, $a1'$, $a1''$ or $a1'''$, respectively. The $KAlOCl_2$ structure with Cl, O and K + Al atoms in 198-a positions (oxygen atoms with an occupancy 0.5) at $x = 0$, 0.25 and 0.48 is characterized by 198-$a1a1'a1''$ (Table 2). The NiSbS (ullmannite) structure with Ni, Sb and S atoms in 198-a positions at $x \approx 0.02$, 0.37 and 0.62 gets the symbol 198-$a1a3'a3''$. The $a3'$ and $a3''$ positions correspond to the sphere packing (6 12 6) at $x = 3/8$ and 5/8. FeSi (fersilicite) with Si and Fe in 198-a position at $x \approx 0.09$ and 0.39 is characterized by 198-$a2a3'$. The $a3$ position at $x \approx 1/8$ is not occupied.

The Wyckoff position 216-e ($x\,x\,x$) with the asymmetric range $0 < x \le 1/8$ contains only the (6 12 12) packing at $x = 1/8$ (216-$e1$) and equivalent positions at $x = 3/8$ ($e1'$), $x = 5/8$ ($e1''$) and $x = 7/8$ ($e1'''$). The $x = 0.125$ or 0.12 values of $KClO_4$ (216-$e1ba$), $ZnSO_4$ (216-$e1ca$) or $Na_{1.67}AlSiO_{4.33}$ (216-$e1dcba$) correspond to a (6 12 12) packing ($e1$) in addition to NaCl (216-ba or 225-ba), ZnS (216-ca), LiMgPdSn (216-$dcba$) or NaTl $\widehat{=}$ (LiMg)(PdSn) structures. The atoms of the invariant positions can be combined to the primitive cubic packing of Po (221-a), the diamond structure (227-a) or bcc W (229-a) (Table 3). The S, Mo and Br atoms of MoSBr (216-$e1e1'e1''$) have the $x \approx 0.12$, 0.35 and 0.62 values close to 1/8, 3/8 and 5/8, respectively. The fcc sphere packing (225-a) is obtained for the combination of S and Br atoms (216-$e1e1''$) (Table 3). The PrI_2 structure with $x \approx 0.11$, 0.36 and 0.63 corresponds to the same structure type. This structure, which was determined later than the MoSBr structure, is not listed in Table 2. The same applies for the Ti_2Ni, CdNi, Nb_5Ni and $NaAg_3S_2$ structures [3] of the Mn_3Ni_2Si structure type (227-$f3'e2c$) or the W_3Fe_3C, Ti_3NiAl_2C and $BaCd_2Cl_6 \cdot 5H_2O$ structures of the W_4Co_2C struc-

ture type (227-$f3'e2dc$). The (8 3 4) and (12 6 24) sphere packings $f3$ and $e2$ are also observed in As_2O_3 or Sb_2O_3 (227-$f3e2$) or W_6Fe_6C (227-$f3'e2cb$). The sphere packings are added to the $MgCu_2$ Laves phase (227-*cb*) or spinel $MgAl_2O_4$ (227-*e2cb*). The numbers of structure types could be reduced further for consideration of the structures with the longest sequence of Wyckoff letters like Ti_2NiH (227-$f3'e2dcba$) or $Ca_3Er_3Ge_2BO_{13}$ (216-$f2e1e1'e1''dcba$) and omitting the first 14 structures of space group 216 with shorter sequences from ZnS (216-*ca*) to Mo_4GaS_8 (216-$e1e1'e1''a$) for example.

An extended Table 3 with all possible combinations would allow a numerical analysis of crystal structures like the pc, diamond, bcc and fcc packings of 216-*ba*, 216-*ca*, 216-*dcba* and 216-$e1e1''$. The repulsive or attractive interactions of K, Cl, Zn, S, Na, Al, Si, S and Br atoms in $KClO_4$ (216-$e1ba$), $ZnSO_4$ (216-$e1ca$), $Na_{1.67}AlSiO_{4.33}$ (216-$e1dcba$) or MoSBr (216-$e1e1'e1''$) can be analyzed by structure maps [17, 18]. The determination of combinations (Table 3) is also necessary for the analysis of the habit of minerals.

The morphological lattice of single crystals can have another symmetry than the structural lattice [19–22]. Octahedral or rhombododecahedral crystals of NaCl are expected from the structural lattice. Planes with low $h\ k\ l$ values and a high density of atom positions like the $\{1\ 1\ 1\}$ planes of octahedra or the Dirichlet domain with $\{1\ 1\ 0\}$ planes of the lattice point P = Na or Cl are derived from Bravais' or Wulff's theory [21–25]. The observed cubic form can be related to the Dirichlet domain of a primitive cubic packing (6 12 8) with $T_1 = 6\ \{1\ 0\ 0\}$ planes of P = Na = Cl as morphological lattice. The cleavage rhombohedron with P = Ca = C of the $CaCO_3$ (calcite) structure is another well-known example [23]. The analogous analysis of structures like the $KClO_4$, $ZnSO_4$, $Na_{1.67}AlSiO_{4.33}$ or MoSBr structures reduces each structure to two packings. These packings are sphere, layer or rod packings [26]. The Dirichlet domain of (6 12 12) or (6 12 8) (cubic crystals like NaCl) would be expected for $KClO_4$ depending on the dominance of oxygen or K + Cl atoms. Plate-like crystals are observed for MoS_2 (molybdenite), Te_2SBi_2 (tetradymite), Fe_2O_3 (hematite), $FeTiO_3$ (ilmenite), $PbCO_3$ (cerussite) or C (graphite) with (6 6 6), (6 6 12), (4 3 6), (6 6 8) or (3 6 3) layered packings of atoms, rod-like crystals for NiS (millerite), $Pb(CO_3)$ (cerussite) or TiO_2 (rutile) with rod-like packings (2 2 12), (2 6 14) or (2 8 6). $Pb(CO_3)$ is an example with different plate- or rod-like habit of crystals, depending on the dominance of Pb–Pb or (CO_3)–(CO_3) interactions. The A = Pb or B = carbon atoms of CO_3 groups have an increased density in layers or rods. The Dirichlet domains of sphere packings should have planes with low $h\ k\ l$ values and high densities of atoms like the $\{100\}$ planes of the primitive cubic packing (6 12 8) or $\{1000\}$ and $\{0001\}$ planes of the primitive hexagonal packing ((8 12 6) like the Fe atoms in FeS, pyrrhotite). The $\{110\}$ planes of the Dirichlet domain of the (12 6 24) lattice complex as an example have a lower density than the $\{111\}$ planes of octahedra in F centered cubic structures. Octahedral crystals are frequently observed for compounds with (12 6 24) lattice complexes like NaCl, $Fe(S_2)$, CaF_2, As_2O_3, $K_2(SiF_6)$, $MgAl_2O_4$ or $CuFeS_2$. The rhombododecahedron as Dirichlet domain of Mn atoms with (12 6 24) lattice complex, however, has dense planes in Mn_2O_3 (bixbyite) with a cubic I centered cell ($h+k+l=2n$).

Conclusion

The analysis of inorganic structures as combinations of frameworks in invariant cubic structures [27–33] can also be applied to structure types with one or more parameters. Standardized structure types of the Landolt-Börnstein compilation of inorganic compounds [3] with less than two parameters were analyzed for lattice complexes with increased self-coordination numbers ($T_1\ T_2\ T_3$) of nearest, second and third neighbors. Numerical calculations similar to trial-and-error or least-squares refinement calculations with n runs are necessary to find the nearest set of increased T_i values in standardized structures with n parameters x, y, z, c/a, $\cos\gamma$, *etc.*

The 1128 Wyckoff positions of the 230 space groups are reduced to 402 lattice complexes with a characteristic Wyckoff position at maximum symmetry [7]. Sequences 1, 2, 3, *etc.* of lattice complexes with increased ($T_1\ T_2\ T_3$) values were determined for most of the characteristic Wyckoff positions (Table 1). About 500 different ($T_1\ T_2\ T_3$) values are estimated as the total number. The determination of all possible combinations like the combination of the invariant ($T_1\ T_2\ T_3$) values [32] would give a very large number. The Wyckoff letters of characteristic lattice complexes like the (1*a*) position of space group number 123 (123-*a*) and equivalent positions 75-*a*, 79-*b*, 83-*c*, *etc.* [7] get the number 5 (123-*a*5) for structures close to a primi-

tive cubic packing with T_i values (6 12 8), which is the fifth value in Table 1. Some parameters like the c/a values close to $c/a = 1$ for the primitive cubic packing are more frequent than other values [4, 5]. The present analysis suggests a similar relation for x values in characteristic lattice complexes like the (8 3 4) or (12 6 24) sphere packings 227-f3 or 227-e2 at $x = 5/16$ or 0.25 (Table 2). Combinations of Wyckoff positions like the combination of the Na and Cl position in NaCl (225-*ba*) to the primitive cubic packing of Na and Cl atoms with T_i values (6 12 8) and the characteristic Wyckoff position 221-*a* (Table 3) are useful for the determination of the crystal habit (cubes of NaCl crystals) and the repulsive Na–Na or Cl–Cl interactions in structure maps [17, 18, 22].

An increased number of (T_1 T_2 T_3) values of characteristic Wyckoff positions with increased numbers of variables is necessary for an extended analysis of structure types. Structures of organic molecules with low symmetry [34] could be analyzed for the center of gravity similar as N_2 or CO_2 (205-*a*). A new (T_1 T_2 T_3) set like 1-*a*6 is characterized by the lowest values of parameters x, y, z, $\cos\alpha$, *etc.* compared to 1-$a6'$ *etc.* with increased values.

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