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Characteristic Lattice Complexes

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2D and 3D lattice complexes with increased self-coordination numbers T_i, $i = 1-3$, of nearest, second and third neighbors were derived for characteristic Wyckoff sets with zero or one parameters. Structure types of adsorbed atoms in 2D or elements A in 3D and A_xB_y compounds are approximated to the list of lattice complexes. Covalent bonding or electronic effects of atoms like lone electron pairs or Jahn–Teller distortion give rise to deviations from lattice complexes. Homogeneous structures A_xB_y with identical A–A or B–B self-coordination numbers T_1, T_2, T_3 of nearest, next-nearest and third neighbors are selected for different systems like magnetic ordering with $A = \oplus$ and $B = \ominus$ spin direction or crystals of organic molecules with different orientations.

1. Introduction

Some basic phenomena can be interpreted from different viewpoints. A very well-known example of the atomistic world is the simultaneous particle or wave-like character. The wave-length λ and mass m are related by the de Broglie relation ($\lambda = h/m\nu$). Other examples of different viewpoints can be found for atoms in solid matter [1]. The atoms in solid matter are characterized by rigid spheres in crystallography or as point masses interconnected by spring forces in IR spectroscopy or the Ising model [2, 3]. The crystallographic atoms are on different positions a, b, c of a space group with certain symmetry elements and parameters $x\,y\,z$. Deviations from this position are given by thermal parameters or additional contributions on electron density maps. The present article will show, that the different positions a, b, c of space groups can be approximated by characteristic lattice complexes with maximum self-coordination numbers. In the next section simple examples for educational purposes are considered for ladies A and gentlemen B sitting in 1D rows in school or an opera house. 1D ordering of elements A and B in the space groups with and without inversion center is not observed. Adsorbed atoms A on metal

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surfaces and different inorganic structures A_xB_y will follow as examples for 2D and 3D structures. The self-coordination numbers of A and B can frequently be correlated with attractive or repulsive interactions of the Ising model [2, 4]. Small numbers of nearest neighbors T_1 indicate repulsive A–A interactions, small numbers T_2 of next-nearest neighbors attractive interactions, as will be outlined for 1D ordering in the next section. The maximum Madelung factor $\mathrm{MF} = 2\ln 2$ at repulsive A–A interactions is obtained for B positions between two A positions.

2. 1D lattice complexes

The ordering of a single species A with different sizes like A = Cu atoms, macromolecules, colloidal particles, leaves or ladies can be characterized by the A–A self-coordination numbers T_i, $i = 1-3$, of nearest, next-nearest and third neighbors [2]. The ladies in a moslem school for example have $T_1 = 2$, $T_2 = 2$ and $T_3 = 2$ neighbors at distances $d = 1$, 2 and 3 between the chairs. A minimum of $n = 7$ ladies in a row is required for the 2 2 2 value of the center lady. The different T_i values of ladies close to the aisle are added to the averaged T_i values $2(n-1)/n$, $2(n-2)/n$, $2(n-3)/n$ for n ladies in a row. The 2 2 2 ordering of ladies is a homogeneous 1D structure. A second homogeneous 1D structure is found for a school desk with two ladies and a vacant place □ to the next desk. The A positions in the periodic sequence (within the commas) ,AA□,AA□, *etc*. have $T_1 = T_2 = 1$ and $T_3 = 2$ A neighbors at distances 1, 2 and 3. The 2 2 2 and 1 1 2 orderings are 1D lattice complexes, which are obtained in the same way as 2D or 3D lattice complexes [5]. The Wyckoff positions (1a) $x = 0$, (1b) $x = 1/2$ and (2c) $x, \bar{x}$ can be occupied by A in a periodic 1D ordering with lattice constant $a = 1$ and inversion center. The self-coordination numbers $T_i = 2$, $i = 1-3$, are obtained for (1a) or (1b) with distances $d = 1$, 2 and 3 between A positions. The x values of the (2c) position can vary within the asymmetric range $0 < x \leq 1/4$. The T_i values are 2 2 2 for $x = 1/4$ and 1 1 2 for all other x values. The distances between nearest neighbors $2x$ and second neighbors $1-2x$ are identical at $x = 1/4$. The same lattice complexes with distances $1-2x$, $2x$ or a between nearest, second or third neighbors, respectively, are obtained for x values in the range $1/4 < x < 1/2$. Structures with self-coordination numbers 1 1 2 (distorted structure) can be approximated to the increased 2 2 2 values by variation of x to $x = 1/4$. The vacancies □ between A positions are diminished. The 1D ordering without inversion center contains only the lattice complex with T_i values 2 2 2. The lattice complex of a second species B is translated by x. The maximum Madelung factor $\mathrm{MF} = 2\ \ln 2$ for $A = \oplus$ and $B = \ominus$ is obtained from

$$\mathrm{MF}(x) = -x[\Psi(x) + \Psi(1-x) - 2\Psi(1)],\ 0 \leq x \leq 1/2,\ \Psi(x) = \Gamma'(x)/\Gamma(x),$$
$$\Psi(1/2) = -\gamma - 2\ln 2,\ \Psi(1) = -\gamma \qquad (\gamma = \text{Euler constant})$$

for $x = 1/2$ (MF(0) = 1). The B positions are on the border of the A–A Dirichlet domain as will be outlined for 2D AB structures in Sect. 3. The A and B atoms form a chain with $T_i = 2$, $i = 1-3$ A or B atoms. The distances between A, B and □ in the 1 1 2 complex are identical for $x = 1/6$.

The homogeneous structures A_xB_y of two species like A = ladies and B = gentlemen can be derived for the two 1D lattice complexes with A–A self-coordination numbers of the minority component A and the ratio $y/x \geq 1$: ,AB, (0 2 0 ; 1), ,AABB, (1 0 1 ; 1), ,ABB, (0 0 2 ; 2), ,AB□, (0 0 2 ; 1), ,AA□BB□, (1 0 0 ; 1) and ,AB□BA□, (0 1 0 ; 1). Homogeneous structures with periodic borders in 1D are obtained for A and B on a round table like $n = 4$ people in the sequence AABB (1 0 1 ; 1) or ABAB (0 2 0 ; 1) and $T_{i+n} = T_i$ values. The T_i values of all 1D structures can be plotted in two structure maps [2]. The homogeneous structures are on the corners of a T_1 T_2 T_3 polyhedron. The corner structures with minimum or maximum T_2 values like 1 0 1 ; 1 or 0 2 0 ; 1 are obtained at attractive or repulsive A–A interactions [2]. The number of lattice complexes with different T_i, $i = 1-3$ values is increased in 2D or 3D to more than 23 or 250, as will be outlined in the present investigation for invariant or univariant solutions with some examples for homogeneous structures of elements A and compounds A_xB_y. Homogeneous 2D or 3D structures can frequently be characterized by the 1D sequences of A and B atoms like AB,AB or AABB in [100], [110] or [111] direction.

3. 2D lattice complexes with increased self-coordination numbers

Periodic 2D structures are usually characterized by the lattice constants a and b, the angle γ between a and b and the positional parameters x and y. Homogeneous structures of a single species A are obtained for the occupation of a single Wyckoff position. Positions with identical neighborhood like the positions of a square net with $T_1 = T_2 = T_3 = 4$ neighbors at distances 1, $\sqrt{2}$ and 2 can be described by the Wyckoff position 11-a or b (Table 1). The number of different values in a Wyckoff position is restricted to asymmetric ranges of b/a or x values in characteristic lattice complexes [5, 6]. The increased T_i values are obtained for certain ratios b/a of lattice constants, angles γ between a and b or positional parameters x and y. The T_1, T_2 or T_3 values at intermediate values are decreased. The self-coordination numbers 4 4 4 of the square net with $\gamma = 90^\circ$ between a and b axes for example vary to 4 2 2 for $60^\circ < \gamma < 90^\circ$ and reach 6 6 6 at $\gamma = 60^\circ$ (hexagonal net) in the characteristic Wyckoff position 2-a-d (Table 14.1 of Fischer and Koch [5]). The values vary further to 2 4 4, $\underline{2\ 4\ 6}$, 2 4 2, $\underline{2\ 6\ 4}$, 2 2 4, $\underline{2\ 2\ 6}$ and 2 2 2. The $\cos\gamma$ values for increased T_i values (underlined values) are given in Table 1. Identical structures are obtained at $90^\circ \pm \gamma$. The 2 2 2 values at low γ values (or γ values close to 180°) correspond to the linear chain. The formation of 1D chains from 2D structures is also observed for the characteristic Wyckoff set 6-a-d with $\gamma = 90^\circ$ and small ratios

Table 1. Self-coordination values T_1, T_2, T_3 for 2D lattice complexes of characteristic Wyckoff positions [5] with less than two parameters b/a, $\cos\gamma$ or x. The $\cos\gamma$ value of 2-a-d position is varied for the special case $a = b$. Maximum Madelung factors MF of A^+B^- with translation between A and B positions.

$\cos\gamma$ $b/a = 1$	T_i	MF	Tr. (B)
	2-a-d		
$> 17/18$	2 2 2		
$17/18$	2 2 6 (a)	1.3863	1/2 1/2
$7/8$	2 6 4	1.3863	1/2 1/2
$3/4$	2 4 6	1.3871	1/2 1/2
$3/4$	2 4 6	1.3871	1/2 0
$1/2$	6 6 6	1.5422	1/3 1/3
0	4 4 4	1.6155	1/2 1/2

b/a	T_i	MF	Tr. (B)
	6-a-d		
$< 1/3$	2 2 2		
$1/3$	2 2 4 (a)	1.3863	0 1/2
$1/2$	2 4 4	1.3863	0 1/2
$1/\sqrt{3}$	2 2 6 (b)	1.4044	1/2 1/2
1	4 4 4	1.6155	1/2 1/2

x	T_i	MF	Tr. (B)
	11-a,b		
–	4 4 4	1.6155	1/2 1/2
	11-d,e		
$1/4$	2 2 4 (b)	1.2990	1/4 0
$(2-\sqrt{2})/2$	3 1 4	1.2632	$2x - 1/2$ $1/2 - x$
$(-1+\sqrt{3})/2$	1 2 5	1.2727	1/2 1/2
	11-f		
$(-1+\sqrt{2})/2$	2 3 2	1.3717	x x
$1/4$	4 4 4	1.6155	1/4 1/4

x	T_i	MF	Tr. (B)
	12-c		
$(3-\sqrt{7})/4$	1 4 6	1.3095	1/2 1/2
$(-1+\sqrt{3})/4$	5 2 1	1.4014	$1 - 4x$ 0
$1/4$	4 4 4	1.6155	1/4 1/4
	14-d		
$1/6$	4 4 6	1.2852	1/3 2/3
	15-c		
$1/3$	6 6 6	1.5422	1/3 1/3
$(3-\sqrt{3})/3$	4 2 8	1.3199	$3x - 1$ $3x - 1$
$1/2$	4 4 6	1.2852	1/3 2/3
	17-a		
–	6 6 6	1.5422	1/3 2/3
	17-b		
–	3 6 3	1.3249	1/3 1/3
	17-c		
–	4 4 6	1.2852	1/3 2/3
	17-d		
$1/4$	2 2 2	1.1863	1/12 1/6
$2-\sqrt{3}$	2 3 1	1.2045	$x/3$ $2x/3$
$1/3$	3 6 3	1.3249	1/9 2/9
	17-e		
$(-3+2\sqrt{3})/3$	2 2 3	1.2038	x 0
$1/6$	2 4 3	1.2301	1/6 0
$(3-\sqrt{3})/6$	4 2 2	1.3271	$1 - 4x$ x
$(3-\sqrt{3})/3$	3 4 4	1.1892	$5x - 2$ $7x - 3$

b/a (or a/b). (The Wyckoff set 9-a,b with $b/a = \tan\gamma/2$ is identical with 2-a-d, $a = b$, $\cos\gamma$.) The other lattice complexes of Table 1 with the variation of the positional parameter x show a different degeneracy. The multiplicity of atoms is decreased at small or large x values. The four positions with the special x and y coordinates $x\ 0$, $\bar{x}\ 0$, $0\ x$ and $0\ \bar{x}$ of characteristic Wyckoff position 11-d,e for example decrease to one or two positions at $x = 0$ or $1/2$, respectively. Some lattice complexes like the square net (4 4 4) or the hexagonal net (6 6 6) occur in several characteristic Wyckoff positions with one variable parameter (Table 1).

Table 2. Self-coordination values T_1, T_2, T_3 of nearest, next-nearest and third A–A neighbors of adsorbed atoms A in different structure types [7] with A on top (T), bridge (B) or hollow (H) positions. The T_i values in brackets are approximate.

T_1 T_2 T_3	substrate	structure type	adsorbate
6 6 6	Al (111)	(1×1)	O on T
	Cu (111)	(1×1)	Ni on H
	Ni (111)	$(\sqrt{3} \times \sqrt{3})$ R30°	CO on B
	Ir (111)	$(\sqrt{3} \times \sqrt{3})$ R30°	S on H
	Rh (111)	$(\sqrt{3} \times \sqrt{3})$ R30°	CO on T
	Ni (111)	(2×2)	S on H
	Cu (111)	(2×2)	Cs on T
(6 6 6)	Rh (111)	(2×2)	3 CO on T or B
	Pd (100)	$(2\sqrt{2} \times \sqrt{2})$ R45°	2 CO on B
	Rh (110)	$C(2 \times 2)$	S on H
	Ir (110)	$C(2 \times 2)$	O on B
	Ir (110)	(2×2)	2 S on H
4 4 4	Ni (100)	(1×1)	Cu on H
	Ni (100)	$C(2 \times 2)$	Se on H
	Ni (100)	(2×2)	2 C on H
	Ni (100)	(2×2)	O on H
(4 4 4)	Pt (111)	$C(4 \times 2)$	2 CO on T or B
3 6 3	Ni (111)	(2×2)	2 H on H
(2 2 6)	Ag (110)	(2×1)	O on B
	Ni (110)	(2×2)	S on H
2 2 4	Ta (100)	(1×3)	O on H

The adsorbed atoms A of many surface structures are ordered in a hexagonal or square net with self-coordination numbers T_1, T_2, T_3 of nearest, next-nearest and third A–A neighbors 6 6 6 or 4 4 4 (Table 2). This is obviously related to the hexagonal or square net of the substrate atoms of most structures. Some structures with (6 6 6) or (4 4 4) values in brackets show that the hexagonal or square net of adsorbed atoms is approximated for other symmetries of substrate atoms (Table 2). A hexagonal net can also be found in incommensurate structures (like Ag (111) Xe) [7] or the 2D ordering of macromolecules or colloids without specific bonding to the Ag, water or glass surface. The honeycomb net with T_i values 3 6 3 is observed for H atoms on Ni (111). The O atoms on Ag (110) with $b/a \approx 0.71$ or the S atoms on Ni (110) with $b/a \approx 0.62$ are close to the lattice complex 2 2 6 (b) of characteristic Wyckoff position 6-a-d at $b/a = 1/\sqrt{3}$ (Table 1). The 2 2 4 values at $b/a = 1/3$ are obtained for O atoms on Ta (100).

The hexagonal net (6 6 6) and square net (4 4 4) of adsorbed atoms correspond to circle packings with maximum density [2, 8]. The density is decreased in the 3 6 3, 2 2 6 or 2 2 4 lattice complexes.

The 2D Ni (100) $C(2 \times 2)$ Na / $C(2 \times 2)$ S structure [7] with two square nets (4 4 4) of Na and S atoms at translation $1/2$ $1/2$ (maximum distance between A and B atoms) has the 2D ordering with maximum Madelung factor (Table 1). The Madelung factor is decreased from 1.6155 to 1.3789 in Ni (100) (2×2) Na / (2×2) S with translation 1/2 0 of the square nets. The maximum MF value for the combination of lattice complexes is obtained at different translations of B atoms. The B positions are such that a maximum number of them lies on the border of the A–A Dirichlet domain. The A and B atoms form lattice complexes like a square or honeycomb net of A and B atoms in Wyckoff position 11-a,b or 17-a. There are two groups of 2D lattice complexes with space groups 10–12 (square) or 13–17 (hexagonal). The lattice complexes of the same space group can be combined without distortion. The MF values of homogeneous structures with identical potential surfaces like 0 4 4 ; 1 and 2 2 0 ; 1b of the 4 4 4 (square) net [2] are related:

$$\mathrm{MF}(4\,4\,4 \mid 0\,4\,4\,;1) = 2\,\mathrm{MF}(4\,4\,4 \mid 2\,2\,0\,;1\mathrm{b})\ (= 1.6155),$$

$$\mathrm{MF}(3\,6\,3 \mid 0\,6\,0\,;1) = 3\,\mathrm{MF}(4\,4\,6 \mid 2\,0\,0\,;2)\ (= 1.5422),$$

$$\mathrm{MF}(3\,6\,3 \mid 0\,6\,0\,;1) = 6/5\,\mathrm{MF}(4\,4\,6 \mid 0\,4\,0\,;2),$$

$$\mathrm{MF}(3\,6\,3 \mid 0\,6\,0\,;1) = 1/2\,\mathrm{MF}(\mathrm{A} = 6\,6\,6,\ \mathrm{B} = 3\,6\,3).$$

The last example shows a relation between MF values of an AB and AB_2 structure (with A and B at Wyckoff positions 17-ab).

Rod-like molecules with rotational freedom (calamitic liquid crystals) are frequently ordered in two dimensions [9]. A hexagonal net (6 6 6) is observed for liquid crystals in hexatic B, smectic I, F, L or crystal B, J and G phases. The tilt of molecule axes in smectic I/crystal J or smectic F/crystal G phases is directed towards the top or bridge position of the hexagonal net. The two-dimensional ordering of crystal E, K or H phases is approximated by the (2 2 6), (2 6 4) or (2 4 6) complexes of Wyckoff letter 2-a-d with two orientations A and B (instead of two species). AB structures are also observed in smectic C_{alt}, C_d, C_1 or C_2 phases. Non-rotating molecules can be analyzed by different directions A, B, C, *etc.* of the molecules depending on the symmetry elements of the space group [2]. The center atom of a molecule in the general Wyckoff position with coordinates $x\,y\,z$ has T_1, T_2, T_3 first, second and third neighbors. 2D tiles similar to Dirichlet domains are obtained, if the lines between A or B positions are intersected midway by vertical lines (vertical planes in 3D structures). The other atoms of the molecule are in these domains with different orientation A, B, C, D depending on the symmetry. The A, B, C, D sequences of molecules frequently form 1D rows in different directions. The ≈ 60 000 entries of the Cambridge Structure Database with a single molecule in the triclinic unit cell $P1$ have the same orientation in linear A_∞ chains (2 2 2) in [100], [010] and [001] directions [2,10]. The third neighbors (T_3) form A_∞ rows in [110] direction of the triclinic unit cell of layered compounds. AB sequences are formed in compounds crystallizing in $P\bar{1}$ [10]. This alignment of molecules with 180° rotation of the B position can be compared to antiferromagnetic ordering in magnetic compounds. The orientations A, B, C and D are observed in most organic molecules with frequently occurring space groups like *Pc*, *Cc*, *C*2, $P2_1$ (AB) or $C2/c$, $P2_1/c$, $P2_12_12_1$, $Pca2_1$ and $Pna2_1$ (ABCD) [11, 12]. Centrosymmetric molecules with space groups $C2/c$ or $P2_1/c$ have two different orientations A and B. The minimum values 1 1 1 are obtained in the oblique (monoclinic) space group *p*2 (2*e*). Symmetrical molecules like C_6Cl_6 or rotating α-N_2 with the center of the molecule in the special Wyckoff position $x = y = z = 0$ form the 6 6 6 packing with increased density. The stacking of the Dirichlet domains of molecules without ionic or hydrogen bridge bonding can be compared with the formation of stone walls without cement. The Dirichlet domains of space groups with mirror planes will deteriorate. These space groups are very rare for organic molecules [11, 12].

4. 3D lattice complexes with increased T_i values

The self-coordination numbers T_1, T_2, T_3 of 3D lattice complexes with zero or one parameters could be determined in a similar way as outlined for 2D structures [13] (Table 3). The cubic lattice complexes with variable *x* can degenerate at certain *x* values as was outlined for 2D complexes. The tetragonal or hexagonal lattice complexes of space groups 75–194 degenerate to 2D lattice complexes like 4 4 4 (square net), 6 6 6 (hexagonal net), 4 4 6 (kagomé net), 3 6 3 (honeycomb net) or the 1D sequence 2 2 2 for small or large ratios of lattice constants c/a.

Most of the lattice complexes with $4 \leq T_1 \leq 12$ are homogeneous sphere packings [8, 13]. The nearest neighbors of layered structures or unstable sphere packings are on the meridian or one hemisphere. Layered structures and structures with $T_1 < 4$ are usually formed at attractive A–A interactions like covalent bonding in Cl_2 ($T_1 = 1$), sulfur chains ($T_1 = 2$) or graphite ($T_1 = 3$). Straight chains of A positions are rod packings [14].

Structures of the Inorganic Crystal Structure Database (ICSD) [15], standardized structure types (TYPIX) [16] or alloys [17] with one or two Wyckoff positions are analyzed for T_i values (Table 4), if the positions of atoms can be approximated by the lattice complex with maximum T_i values.

Some elements like Cu (12 6 24), W (8 6 12) or diamond (4 12 12) have the structure of undistorted lattice complexes. The same applies for homogeneous structures A_xB_y with identical neighborhood of A and B atoms like NaCl (12 6 24), CsCl (6 12 8) or NaTl (4 12 12). The electron configurations of the atoms are either spherical like Na and Cl or in accordance with the symmetry of the lattice complex like the sp^3 electron configuration of C atoms with $T_1 = 4$ C–C bonds. Most lattice complexes however are distorted. Several reasons for the distortions can be recognized:

Jahn–Teller distortion: The Co^{2+} atoms of CoO (12 6 24) have a non-spherical d^7 electron configuration with different bond length in *c* direction and $c/a = 0.99$ of the tetragonally distorted NaCl structure.

Table 3. Self-coordination values T_1, T_2, T_3 for 3D lattice complexes of characteristic Wyckoff positions [5] with less than two parameters c/a or x in space groups 75–194 or 195–230, respectively including invariant cubic lattice complexes (second origin of space groups).

c/a	T_i
123-a-d	
	2 2 2
$1/3$	2 2 6
$1/2$	2 6 8
$1/\sqrt{3}$	2 4 10
1	6 12 8
$\sqrt{2}$	4 6 8
2	4 4 6
	4 4 4
139-a,b	
	2 2 2
$\sqrt{2/35}$	2 2 10
$\sqrt{2/15}$	2 10 8
$1/2$	2 8 6
$\sqrt{2/3}$	10 4 8
1	8 6 12
$\sqrt{2}$	12 6 24
$\sqrt{6}$	4 12 20
$\sqrt{14}$	4 4 12
	4 4 4
141-a,b	
	2 2 2
$2/\sqrt{143}$	2 2 6
$2/\sqrt{63}$	2 6 4
$2/\sqrt{55}$	2 4 6
$2/\sqrt{15}$	6 4 8
$2/\sqrt{7}$	4 6 8
$\sqrt{2/3}$	4 4 10
$2/\sqrt{5}$	4 12 2
$\sqrt{2}$	4 12 12
2	4 4 16
$\sqrt{12}$	8 12 4
	4 4 4
141-c,d	
	2 2 2
$\sqrt{2/143}$	2 2 6
$\sqrt{2/63}$	2 6 4
$\sqrt{2/55}$	2 4 6
$\sqrt{2/15}$	6 4 2
$\sqrt{2}/3$	4 2 6
$1/2$	4 4 4
$\sqrt{2/7}$	4 2 6
$\sqrt{2}$	6 12 12
$\sqrt{6}$	2 4 12
	2 4 4
166-a,b	
	2 2 2
$\sqrt{3/80}$	2 2 8
$\sqrt{3/35}$	2 8 6
$\sqrt{3/32}$	2 6 8
$\sqrt{3/8}$	8 6 12
$\sqrt{3/5}$	6 8 6
1	6 6 8
$\sqrt{3/2}$	6 12 8
$\sqrt{3}$	6 6 12
$\sqrt{6}$	12 6 24
$\sqrt{15}$	6 6 12
$\sqrt{24}$	6 12 12
	6 6 6
166-d,e	
	2 2 2
$\sqrt{3/320}$	2 2 6
$\sqrt{3/140}$	2 6 4
$\sqrt{3/128}$	2 4 6
$\sqrt{3/32}$	6 4 8
$\sqrt{3/20}$	4 6 4
$1/2$	4 4 6
$\sqrt{6}/4$	4 8 8
$\sqrt{3}/2$	4 4 10
$\sqrt{6}/2$	8 6 16
$\sqrt{15}/2$	4 4 10
$\sqrt{33}/2$	4 4 10
	4 4 6
180/181-c,d	
	2 2 2
$3/\sqrt{320}$	2 2 6
$3/\sqrt{140}$	2 6 4
$3/\sqrt{128}$	2 4 6
$3/\sqrt{32}$	6 4 4
$3/\sqrt{20}$	4 6 4
$3\sqrt{6}/8$	4 4 6
$3\sqrt{2}/4$	4 4 4
$3\sqrt{3}/4$	4 4 10
$3/2$	4 10 4
$3\sqrt{3}/2$	10 4 8
$9/2$	6 4 10
$3\sqrt{11}/2$	6 10 4
$3\sqrt{15}/2$	6 6 10
	6 6 6
191-a,b	
	2 2 2
$1/3$	2 2 8
$1/2$	2 8 12
$1/\sqrt{3}$	2 6 14
1	8 12 6
$\sqrt{2}$	6 2 18
$\sqrt{3}$	6 8 18
2	6 6 8
	6 6 6
191-c,d	
	2 2 2
$1/\sqrt{27}$	2 2 5
$1/\sqrt{12}$	2 5 6
$1/3$	2 3 8
$1/\sqrt{3}$	5 6 6
1	3 8 9
$2/\sqrt{3}$	3 6 5
	3 6 3
191-f,g	
	2 2 2
$1/6$	2 2 6
$1/4$	2 6 8
$1/\sqrt{12}$	2 4 10
$1/2$	6 8 4
$\sqrt{2}/2$	4 2 12
$\sqrt{3}/2$	4 6 14
1	4 4 8
	4 4 6
194-c,d	
	2 2 2
$2/\sqrt{105}$	2 2 8
$2/\sqrt{45}$	2 8 6
$2/\sqrt{21}$	2 6 8
$2/3$	8 6 6
$\sqrt{6}/3$	6 2 6
1	6 8 6
$4/3$	6 6 8
$\sqrt{8/3}$	12 6 2
$\sqrt{20/3}$	6 6 12
$\sqrt{32/3}$	6 12 12
	6 6 6

Lone electron pairs: The neighborhood of Tl^+ atoms in TlF with $c/a = 1.14$ of the same structure type is non-spherical with a lone electron pair. A different tetragonal distortion with $c/a' = 1.05$ is found in the high pressure modification of GeP. (The a' value of the lattice complex is different from the a value of the hexagonal cell.) Trigonally distorted NaCl structures with $c/a = 2.57$ or

Table 3. continued.

x	T_i
198-a	
0	12 6 24
$(3-\sqrt{5})/8$	6 6 12
$1/8$	6 12 6
199-a	
0	6 12 8
$1/16$	3 9 6
$1/8$	3 6 6
199-b	
$-1/8$	8 4 8
$(3-\sqrt{13})/8$	4 6 2
0	4 2 8
$(3-\sqrt{5})/8$	4 2 6
$1/8$	4 4 4
200-f,g	
$(5-\sqrt{21})/4$	1 8 9
$(3-\sqrt{5})/4$	1 9 8
$1/4$	2 8 16
204-e	
$1/8$	1 4 12
$(-1+\sqrt{3})/4$	5 8 1
$(3-\sqrt{5})/4$	4 1 9
$1/4$	4 2 8
205-c	
$(-1+\sqrt{5})/8$	7 6 3
$(-1+\sqrt{3})/4$	6 7 9
$(-3+\sqrt{15})/4$	6 6 7
$1/4$	6 12 8
206-c	
$(3-\sqrt{5})/8$	1 3 7
$(-1+\sqrt{2})/4$	4 1 6
$1/8$	3 2 12
206-d	
0	8 6 16
$(3-\sqrt{5})/8$	4 4 6
$1/8$	4 8 2
208-k,l	
$(3-\sqrt{8})/4$	1 6 2
$(-3+\sqrt{12})/4$	3 4 2
210-g	
0	2 8 16
$(3-\sqrt{8})/8$	4 4 2
211-i	
$(3-\sqrt{5})/8$	1 2 6
$(-1+\sqrt{2})/4$	3 2 4
$(-3+\sqrt{12})/4$	2 3 4
$1/8$	4 1 4
$\sqrt{3}/12$	2 2 5
212/213-a,b	
–	6 12 6
212-c	
$-1/8$	3 6 6
$(1-\sqrt{2})/4$	3 6 7
$(5-\sqrt{30})/8$	3 7 6
0	4 12 12
$< 1/8$	1 3 6
212-d	
0	4 4 4
$5/24$	2 6 2
$(-1+\sqrt{33})/16$	6 2 2
$3/8$	4 10 8
$1/2$	4 4 4
214-a,b	
–	3 6 6
214-c,d	
–	4 4 4
214-e	
0	8 6 12
214-f	
$-1/8$	4 8 2
$(1-\sqrt{3})/8$	2 2 5
$(2-\sqrt{5})/4$	2 3 4
$-1/24$	2 1 6
0	3 4 4
214-h	
$(-3+\sqrt{12})/8$	3 4 2
$(-1+\sqrt{8})/8$	4 2 4
$1/4$	2 4 8
$(-1+\sqrt{33})/16$	2 2 6
$(1+\sqrt{17})/16$	2 6 2
$3/8$	9 4 18
215-e	
$(2-\sqrt{2})/4$	3 6 9
$1/4$	12 6 24
216-e	
$1/8$	6 12 12
217-c	
$(2-\sqrt{2})/8$	3 6 14
$3/16$	9 6 8
$1/4$	6 12 8
220-a,b	
–	8 4 8
220-c	
0	8 6 12
$(2-\sqrt{2})/16$	5 6 3
$1/8$	3 2 12
220-d	
0	1 4 4
$(-3+\sqrt{11})/8$	5 4 2
$(-1+\sqrt{2})/4$	4 5 4
$(-2+\sqrt{6})/4$	4 4 5
$1/8$	4 8 2
221-a,b	
–	6 12 8
221-c,d	
–	8 6 16
221-e	
$1/4$	4 2 8
$(2-\sqrt{2})/2$	5 1 8
$(-1+\sqrt{3})/2$	1 4 9
221-g	
$(-1+\sqrt{3})/4$	3 3 4
$1/4$	6 12 8
221-h	
$(-1+\sqrt{2})/2$	2 3 1
$1/4$	4 2 8
221-i	
$(-2+\sqrt{6})/2$	4 2 6
$1/4$	4 4 8
$(2-\sqrt{2})/2$	6 7 6
$1/3$	2 5 4
223-c,d	
–	2 8 16
223-g,h	
$1/8$	2 2 4

Table 3. continued.

x	T_i
223-j	
$(-3+\sqrt{12})/4$	2 3 4
$(3-\sqrt{6})/4$	4 1 4
$(-2+\sqrt{7})/4$	2 2 5
224-e	
$(-2+\sqrt{6})/4$	4 12 6
224-i,j	
1/8	2 2 2
$(2-\sqrt{3})/2$	2 3 1
1/6	3 6 3
225-a,b	
–	12 6 24
225-e	
$(-1+\sqrt{2})/2$	4 5 4
1/4	8 6 16
225-f	
$(-2+\sqrt{6})/4$	3 3 4
1/8	3 6 4
$(2-\sqrt{2})/4$	6 6 1
225-h,i	
$(2-\sqrt{3})/2$	4 2 5
$(2-\sqrt{2})/4$	4 3 4
1/6	5 2 12
$(3-\sqrt{5})/4$	1 4 10
227-a,b	
–	4 12 12
227-c,d	
–	6 12 12
227-e	
$(-2+\sqrt{6})/8$	4 6 3
1/4	12 6 24
227-f	
$> 1/8$	4 1 4
$(-1+\sqrt{10})/8$	4 5 2
5/16	8 3 4
$(-1+\sqrt{14})/8$	4 4 6
3/8	4 8 8
227-h	
1/8	4 2 8
1/6	2 2 3
228-g	
1/8	4 2 8
1/6	6 2 4
229-a	
–	8 6 12
229-b	
–	4 8 8
229-d	
–	4 2 8
229-e	
$(2-\sqrt{2})/4$	4 1 9
1/4	4 2 8
$(2-\sqrt{2})/2$	5 8 1
3/8	1 12 8
229-f	
1/8	3 3 2
$(3-\sqrt{6})/4$	3 4 1
$(3-\sqrt{3})/8$	4 3 1
3/16	1 3 9
229-g	
1/8	2 2 4
$(2-\sqrt{2})/4$	3 1 4
$(-1+\sqrt{3})/4$	1 2 5
229-h	
3/16	4 2 8
$(4-\sqrt{10})/4$	4 6 6
1/4	8 6 16
$(2-\sqrt{2})/2$	4 6 2
1/3	4 2 5
$\sqrt{8}/8$	6 1 4
$(4-\sqrt{6})/4$	2 5 8
229-i	
1/12	2 3 2
$(-1+\sqrt{2})/4$	4 3 2
1/8	2 2 4
$(2-\sqrt{2})/4$	2 2 3
230-b	
–	3 2 12
230-c	
–	4 8 2
230-d	
–	4 8 2
230-e	
1/16	2 3 3
$(-1+\sqrt{7})/16$	1 4 3
230-f	
0	4 8 8
$(-3+\sqrt{11})/8$	1 2 5
230-g	
$(-3+\sqrt{12})/8$	3 4 4
1/4	2 8 16
$(4-\sqrt{3})/8$	6 2 2
$(1+\sqrt{17})/16$	4 2 6
3/8	4 9 6
$(8-\sqrt{23})/8$	5 2 4
5/12	1 6 4

2.50 instead of 2.45 are found in GeTe or BiO with lone electron pairs of Ge^{2+} or Bi^{2+}.

Non-invariant sphere packings: The $c/a = 0.539$ of Sn or $c/a = 0.831$ of Pa are close to $c/a = 0.516$ of the (6 4 8) or to $c/a = 0.817$ of the (10 4 8) sphere packing. The same applies for $x = 0.1667$ or $x = 0.1003$ values of C or γ-Si in the (4 3 1) or (4 1 6) sphere packings with $x = 0.1585$ or 0.1036 values. The

Table 4a. Self-coordination values T_1, T_2, T_3 of A and B atoms in A or A_xB_y structure types with one or two characteristic Wyckoff positions [5] of Table 3. The T_i values in brackets are approximated in the experimental structures.

A	B	A_xB_y	SG-WS	A	B	A_xB_y	SG-WS
12 6 24	–	Cu	225-a	8 6 12	–	W	229-a
(12 6 24)	–	(Al,Zn)	166-a	8 6 12	6 12 8	Pt Hg_4	229-ac
(12 6 24)	–	In	139-a	8 6 12	(4 12 6)	Si F_4	208-ag
(12 6 24)	–	N_2	198-a	8 6 12	2 8 16	Si Cr_3	223-ac
12 6 24	12 6 24	Zn S	216-ac	8 4 8	–	Ga	220-a
12 6 24	12 6 24	Na Cl	225-ab	8 4 8	(5 6 3)	Eu_3 S_4	220-ac
(12 6 24)	(12 6 24)	Co O	139-ba	8 4 8	(3 2 12)	Th_3 P_4	220-ac
(12 6 24)	(12 6 24)	Ge Te	160-aa	(8 3 4)	6 12 12	F_3 Fe	227-fc
(12 6 24)	(12 6 24)	Ge P	107-aa	(7 6 3)	–	N_2	205-c
12 6 24	8 6 12	O Cu_2	224-ab	(6 12 12)	(6 12 12)	Pt Cu	166-ba
(12 6 24)	(8 3 4)	As_2 O_3	227-ef	6 12 12	4 12 12	Cu_2 Mg	227-cb
12 6 24	(7 6 3)	Fe S_2	205-ac	6 12 12	4 12 12	O_2 Si	227-ca
12 6 24	(7 6 3)	C O_2	205-ac	6 12 8	–	Po	221-a
(12 6 24)	6 12 12	Ti_2 C	227-ec	6 12 8	6 12 8	Cs Cl	221-ab
12 6 24	6 12 8	Ca F_2	225-ac	(6 12 8)	(6 12 8)	Ti Cu	123-da
(12 6 24)	6 12 8	Fe_4 C	215-ea	6 12 8	(5 1 8)	Ca B_6	221-af
(12 6 24)	(6 12 8)	Pt S	131-ce	6 12 8	4 8 8	O_4 Pt_3	229-cb
(12 6 24)	(6 12 8)	Th H_2	139-ad	6 12 8	2 8 16	O_4 Pt_3	223-ec
(12 6 24)	(6 6 12)	N_2	198-aa	(6 12 8)	(2 4 10)	Hg_2 Pt	123-ea
(12 6 24)	(6 6 12)	C O	198-aa	6 12 6	(3 7 6)	Sr Si_2	213-ac
12 6 24	(5 2 12)	U B_{12}	225-ai	(6 8 18)	(6 8 18)	Li Rh	187-da
12 6 24	(4 12 6)	C O_2	201-be	(6 8 18)	(6 6 12)	Nd	194-ac
12 6 24	(4 12 6)	Ca C_2	201-be	(6 6 12)	–	Hg	166-a
12 6 24	4 8 8	Ag_2 O_3	224-bd	(6 6 12)	(6 6 12)	Fe Si	198-aa
12 6 24	(2 2 4)	P H_3	208-bi	(6 6 12)	(6 6 12)	Hg In	166-ab
(12 6 2)	–	Mg	194-c	(6 6 12)	(6 6 12)	B N	194-cd
(12 6 2)	(12 6 2)	C	186-bb	(6 6 12)	(6 2 18)	C	194-cb
(12 6 2)	(12 6 2)	Zn S	186-bb	(6 6 8)	–	Po	166-a
(12 6 2)	(8 12 6)	S Fe	194-ca	(6 6 8)	(2 6 14)	As Ni	194-ca
(12 6 2)	(2 6 14)	S Co	194-ca	(6 4 8)	–	Sn	141-b
(10 4 8)	–	Pa	139-a	(6 2 2)	(3 7 6)	β-Mn	213-dc
(9 6 8)	8 6 12	F_4 Si	217-ca	(5 6 6)	(2 6 14)	Hg_2 U	191-da
(9 6 8)	(3 6 14)	Li B	217-cc	(5 6 6)	(2 6 14)	Ti	191-da
(8 12 6)	–	(Sn,Hg)	191-a	(5 6 3)	(5 4 2)	Pu_2 C_3	220-cd
(8 12 6)	(8 12 6)	W C	187-ad	4 12 12	–	C	227-a
(8 12 6)	(3 8 9)	Mo B_2	191-ad	4 12 12	4 12 12	Na Tl	227-ab
(8 12 6)	(3 6 5)	Al B_2	191-ad	(4 6 8)	(4 6 8)	Cu Au	123-ad
(8 12 4)	(8 12 4)	Nb P	141-ab	(4 4 16)	(4 4 16)	U Pb	141-ab
(8 12 4)	(8 12 4)	Nb As	109-aa	(4 4 6)	(4 4 6)	Pd O	75-ab
8 6 16	8 6 16	Nb O	221-cd	(4 3 1)	–	C	229-f
8 6 16	6 12 8	Cu_3 Au	221-ca	(4 1 6)	–	Si	206-c
8 6 16	6 12 8	O_3 Re	221-da	(3 9 6)	(3 9 6)	U Co	199-aa
(8 6 16)	(6 12 8)	F_3 Ti	166-da				

Table 4b. The same as Table 4a for $A_xB_yC_z$.

A	B	C	$A_xB_yC_z$	SG-WS
12 6 24	12 6 24	12 6 24	Mg Ag As	216-abc
12 6 24	12 6 24	8 6 16	Cu Pt Pt_6	225-abd
12 6 24	12 6 24	(6 12 12)	Mg Sn Cu_4	216-ace
12 6 24	12 6 24	6 12 8	Al Mn Cu_2	225-abc
(12 6 24)	(12 6 24)	(4 6 8)	V Sn Rh_2	139-abd
12 6 24	(8 6 16)	6 12 8	Pt Cl_6 K_2	225-aec
(12 6 24)	8 6 16	6 12 8	S_4 Cu_3 As	215-eca
(12 6 24)	8 6 16	6 12 8	S_4 Cu_3 V	215-eda
(12 6 24)	(8 3 4)	6 12 12	Ni_2 Mn_3 Si	227-efc
(12 6 24)	6 12 12	6 12 12	O_2 Li Ti	227-edc
(12 6 24)	6 12 12	4 12 12	O_4 Al_2 Mg	227-ecb
(12 6 24)	(6 12 8)	(6 12 8)	C Y Co	131-cfa
(12 6 24)	(6 12 6)	(6 6 12)	Ni Sb S	198-aaa
(12 6 2)	(12 6 2)	(8 12 6)	Ga Ge Li	186-bba
(12 6 2)	(12 6 2)	(8 12 6)	Be Si Zr	194-cda
(9 6 8)	(9 6 8)	4 8 8	Pt_4 Ge_4 Na_3	217-ccb
(9 6 8)	8 6 12	4 8 8	S_4 V Tl_3	217-cab
(8 12 6)	(8 12 6)	(8 12 6)	Li Ba Si	187-eda
(8 12 6)	(8 12 6)	(3 8 9)	N Li Li_2	191-abc
(8 12 6)	(4 6 14)	(3 8 9)	Sn Co_3 Sn_2	191-afd
(8 12 6)	(4 6 14)	(3 8 9)	Ca Cu_3 Cu_2	191-agc
(8 12 4)	(8 12 4)	(8 12 4)	La Pt Si	109-aaa
8 6 16	8 6 16	6 12 8	S_3 U_3 U	221-dca
8 6 16	6 12 8	6 12 8	O_3 Ca Ti	221-dba
8 6 12	6 12 8	2 8 16	Na O_4 Pt_3	223-aec
8 6 12	(4 9 6)	(4 8 8)	Ga Ni_3 Ga_3	230-agf
8 4 8	8 4 8	(3 2 12)	Ca_3 U_3 S_4	220-abc
(6 12 12)	(6 12 12)	(6 12 12)	Mo S S	160-aaa
(6 12 12)	(6 12 12)	(6 8 18)	Cd I I	186-bba
(6 12 12)	(6 12 12)	(6 2 18)	K As Sn	186-bba
(6 12 8)	(6 12 8)	(4 6 8)	Sr Pb Pb_2	123-ace
6 12 8	6 12 8	(2 8 16)	W Ge Al_6	200-abf
6 12 8	(5 8 1)	(4 2 5)	Si_2 Ce_3 Ni_6	229-ceh
6 12 8	(6 1 4)	(4 2 8)	Ag_2 Ag_6 Ca_3	229-che
(6 12 8)	(2 4 10)	(2 4 10)	U_2 U (U,Mo)	123-eac
6 12 6	(6 2 2)	(3 7 6)	C Mo_3 Al_2	213-adc
(6 8 18)	(6 8 18)	(6 8 18)	Ni Ni H	156-abc
(6 8 4)	(5 6 6)	(2 6 14)	Co_3 B_2 Ce	191-gca
(6 6 12)	(6 6 12)	(6 6 12)	Zr S O	198-aaa
(6 6 12)	(6 6 12)	(6 2 18)	Cd Cl (OH)	186-bba
(6 6 8)	(6 6 8)	(2 6 14)	In Ni Ni	194-cda
(5 6 6)	(4 2 12)	(2 6 14)	Ni_2 Al_3 Pr	191-cga
(4 12 20)	(4 12 20)	(4 6 8)	Ti Al Al_2	139-abd
(4 6 8)	(4 6 8)	(4 6 8)	Fe Ni N	123-cba
(4 3 1)	4 2 8	(1 12 8)	Sn_4 Sn_3 Ir_3	229-fde

$x = 0.31125$ or 0.2976 values of oxygen atoms in Sb_2O_3 or As_2O_3 are close to $x' = 0.3125$ of the undistorted (8 3 4) packing.

Covalent A–A bonding: The structure of pyrite (FeS_2) with $T_i = 12\ 6\ 24$ of Fe atoms contains S–S dumb-bells with covalent bonding between S atoms. The same applies for the peroxides like CdO_2 with $x' = 0.09$ of the same structure type (identical lattice complexes for $0 \pm x$ or $1/2 \pm x'$). The $x' \approx 0.16$ value of SiO_2 and PdF_2 without O–O or F–F bonding is close to $x = (-1 + \sqrt{5})/8$ of the lattice complex with T_i values 7 6 3 (Table 3). The O atoms in CO_2 with $x \approx 0.12$ contain a C atom in the center of the dumb-bell (linear O=C=O molecules).

Combinations of packings: The invariant cubic F and T lattice complexes [5] with T_i values (12 6 24) and (6 12 12) occur in different space groups 225 and 227. The $x = 0.245$ value of Ti atoms in the Ti_2C structure ($CdCl_2$ anti-structure type) is close to $x = 1/4$ of the (12 6 24) packing. The cubic F and P (primitive cubic lattice with T_i values 6 12 8) lattice complexes of space groups 225 and 221 are combined in the ratio 1 : 2 in the invariant CaF_2 structure. The combination in the ratios 4 : 1 or 1 : 1 in Fe_4C or PtS is not possible in an invariant structure. The $x = 0.265$ value of Fe atoms in Fe_4C is close to $x = 1/4$ of the undistorted lattice.

Combinations of distorted packings: The $c/a = 1.41$ and $c/a' = 2$ values of undistorted F and P complexes in PtS are different. The $c/a = 1.758$ value of PtS is intermediate. The same applies for the combination of the hcp sphere packing (12 6 2) with $c/a = 1.633$ and two primitive hexagonal packings ph′ (8 12 6) with $c'/a = 2$ in SV with $c/a = 1.73$ or SFe with $c/a = 1.69$. A different complex (2 6 14) at $c/a = 1.155$ is approximated for metal atoms with decreased $c/a = 1.548$ (SNi) or 1.525 (SCr). The (6 6 8) packing with $c/a = 1.33$ is approximated for Se, As or Sb atoms in SeNi ($c/a = 1.46$), AsNi (1.39) or SbNi (1.31). The formation of the (2 6 14) chain of Ni atoms with $T_1 = 2$ nearest neighbors in c direction is probably related with attractive Ni–Ni interactions.

Combinations of three or more packings: Compounds with three or more Wyckoff positions (Table 4) are frequently related with binary compounds. The three compounds $PtCl_6K_2$, S_4Cu_3As and S_4Cu_3V with the (12 6 24), (8 6 16) and (6 12 8) packings of A, B and C atoms for example are related to CaF_2 or Fe_4C with (12 6 24) and (6 12 8) packings in the ratio 1 : 2 or 4 : 1 and to Cu_3Au or O_3Re with (8 6 16) and (6 12 8) packings in the ratio 3 : 1. The B and C atoms of Cu_3Au and S_4Cu_3As or O_3Re and S_4Cu_3V have the translations 1/2 1/2 0 or 1/2 0 0.

Colloids and micelles: Colloidal particles can crystallize in (12 6 24) (fcc-), (10 4 8) (bct-), (8 12 6) (bcc-), (2 8 4) (sft-) or (2 2 8) (bco-colloids) packings [18]. Binary mixtures of colloidal particles with different sizes were observed in (8 12 6) (3 6 5) AlB_2, (6 12 8) (6 12 8) (6 2 4) $NaZnZn_{12}$, (8 12 6)

(4 6 14) (3 8 9) $CaCu_3Cu_2$ or (6 12 12) (4 12 12) Cu_2Mg structures (Table 4) [19]. The $NaZn_{13}$ and $CaCu_5$ structures are examples of different neighborhoods of B particles. Different packings were also observed for micelles [20] in Wyckoff positions 225-a (12 6 24), 229-a (8 6 12), 223-ac (8 6 12 and 2 8 16) or 227-da (6 12 12 and 4 12 12).

5. Surfaces of cylinders or spheres

Some circle packings with high density like 6 6 6 or 4 4 4 can be related to the ordering of leaves (phyllotaxis) [21, 22]. This can be shown, if the packing within the periodic boundary lines [2] is rolled to a cylinder around the stem of the plant. Whorles with $\nu = 6$ leaves for example can be compared with the table of $\nu = 6$ ladies A (Sect. 1). The ordering is periodic within a short section of the stem. The A positions show the directions of leaves. The formation of single spirals ($\nu = 1$) with an angle $\beta \approx 360^\circ/\tau^2 \approx 138^\circ$ ($\tau = (1+\sqrt{5})/2$) [22] can be described by a distorted (4 4 4) packing of $n = 2$ rhombs with angle $\gamma \approx 99^\circ$ and the inclination angle α. Other spirals like the α-helix ($n = 3$) or a double helix ($\nu = 2$) with $\nu n = 10$ or 12 base pairs are obtained at variation of n and γ:

$$\nu\beta = \frac{360(n - \cos\gamma)}{n^2 - 2n\cos\gamma + 1}, \qquad \tan\alpha = \frac{\sin\gamma}{n - \cos\gamma}, \qquad \text{rise} = \sin\alpha, \tag{1}$$

$$n\beta = 360\cos\gamma \quad (\alpha = 0), \qquad \text{rise} = \sin\gamma. \tag{2}$$

A pairwise spiral is also obtained for $n = 2$ rhombs with $\alpha = 0^\circ$ and different β values at varied angles γ of the rhombs (Eq. 2). A double helix with $\nu = 2$ leaves at the same height of the stem is observed for the stinging nettle as example. The spiral growth in the 6 6 6 or 4 4 4 packing is observed for about 80% of the plants [21, 22]. The density of leaves is decreased in the 3 6 3 honeycomb or 4 4 6 kagomé net on the cylinder surface. 33% or 25% of the positions of the hexagonal net (6 6 6) are vacant.

Other structures can be considered as circle packings on the surface of a sphere (Platonic or Archimedean solids) [2]. The highest density of homogeneous solids is obtained for the icosahedron with T_i values 5 5 1 of the $T_1 + T_2 + T_3 + 1 = 12$ vertices v in alloys or polyoxomolybdates. The density is increased for viruses with $T_1 = 5$ or $T_1 = 6$ values of capsomeres protecting the virus genome. The capsomeres of the tobacco mosaic virus form a single spiral ($\nu = 1$) with $n = 17$ rhombs. The β values of the helices in cholesteric liquid crystals increase at increased temperatures [9].

The curved eyes of many insects like flies, bees or dragon-flies contain many facet eyes in a hexagonal net with a honeycomb frame [23]. The muscle of the fly (*bombylius major*) has a hyperbolic surface with a hexagonal net of bundles of myosin molecules and a kagomé net of actin molecules.

6. Conclusion

All 2D or 3D structures can be characterized by lattice complexes with increased self-coordination numbers of nearest, second and third A–A neighbors $T_i, i = 1-3$, if the values for more than one parameter c/a, cos γ or x (Tables 1 and 3) are available. The homogeneous A_xB_y structures are characterized by two lattice complexes for A and B positions. The same applies for two directions A and B for the ordering of magnetic moments or the ordering of organic molecules [2]. The lattice complexes for organic molecules with more than one parameter are not yet determined. Curved surfaces like the surfaces of cylinders or spheres are analyzed by $T_i, i = 1-3$ values for phyllotaxis or the ordering of capsomeres of viruses.

Most homogeneous structures with identical T_i values of A and B can be related with different interactions. Pauling's rule of parsimony is obeyed for the homogeneous structures with identical neighborhood: *The number of essentially different kinds of constituents in a crystal tends to be small* [24]. The AB, AABB or ABB sequences of the linear row are observed for most homogeneous 2D and 3D structures [2]. Most structures of the 5 5 5 or 5 2 1 nets are not homogeneous. A structure with $T_1 = 5$ neighbors cannot be divided in equal parts because of the absence of a five-fold symmetry operation. The honeycomb (3 6 3), square (4 4 4) and hexagonal (6 6 6) nets are examples with $T_1 = 3$-, 4- or 6-fold symmetries. $T_1 = 5$-fold symmetry is obtained in the icosahedron (5 5 1). Inhomogeneous 1D structures are essential for DNA sequences, music notes or letters of languages [25].

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