STANDARD REPRESENTATION OF INORGANIC STRUCTURES BASED ON SIMPLE AND ON LOOSE PACKINGS (*)

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ABSTRACT — The standard representation recently proposed by the author, and applied in detail to structures based on cubic and hexagonal closest packings, has been extended to inorganic structures based on simple and on loose packings. This standard representation clearly shows that these structures have a much simpler atomic organization and are more interrelated than could be imagined using conventional ways of structure representation.

INTRODUCTION

A certain uniformity in the representation of inorganic crystal structures is necessary in order to facilitate their relationship. However, each author represents inorganic structures, even the simplest ones, in several different ways, either considering the linkage between atoms within the unit cell, or the linkage between atomic polyhedra, or the packing of atoms with different sizes, or again the projection of atoms in a certain plane of the unit cell. It is this situation that originated a proposal by the author for a standard representation of layered inorganic structures [1] inspired on the condensed models' technique [2]. The application of this standard method to the representation of crystalline structures based on cubic and on hexagonal closest packings gave rise to very simple descriptions of these structures and of interesting relationships among them [1]. The aim of this work

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is to extend this standard representation to structures based on other types of close packings, in particular on simple and on loose packings.

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The standard representation of inorganic layered structures consists on the representation of the constructive layers [3], or of their subdivisions, in which the structure can be sliced and the way they stack together. The constructive layers correspond to the transparent sheets of the condensed models and, to represent the kind of layers and their stacking, we only need to consider that part of the condensed model which is included within the unit cell and draw it in perspective (Fig. 1).

Close packed structures, either closest, loose, or simple, normally admit more than one layer description. For instance in the cubic closest packing there are seven possible layer descriptions: four perpendicular to the triad axes, and three perpendicular to the tetrad axes. What is important is to find out the simplest layer description for each structure. This is called the «proper layer description», and the standard representation is the one which corresponds to the proper layer description.

The conventions used in the standard representation are the following. In close packed structures without interstitial atoms the packing atoms are represented by small circles. In structures with interstitial atoms these are represented by small circles and the unoccupied interstices by small squares (a widely used symbol for vacancies); the packing atoms are represented by dots, because it is the configuration of the interstitial atoms i.e., the «distribution pattern» [2] which changes and which it is important to emphasize, the packing being well defined, and identical for a particular group of structures.

The so called loose-packings [4] are less dense close packings and are obtained by stacking closest packed layers not over the holes (as in the densest way) but over valleys, that is, with one atom touching only two atoms of the layer below. These packings are designated by *Tb*, *Tv*, *Td* (*T* for the triangular closest packed

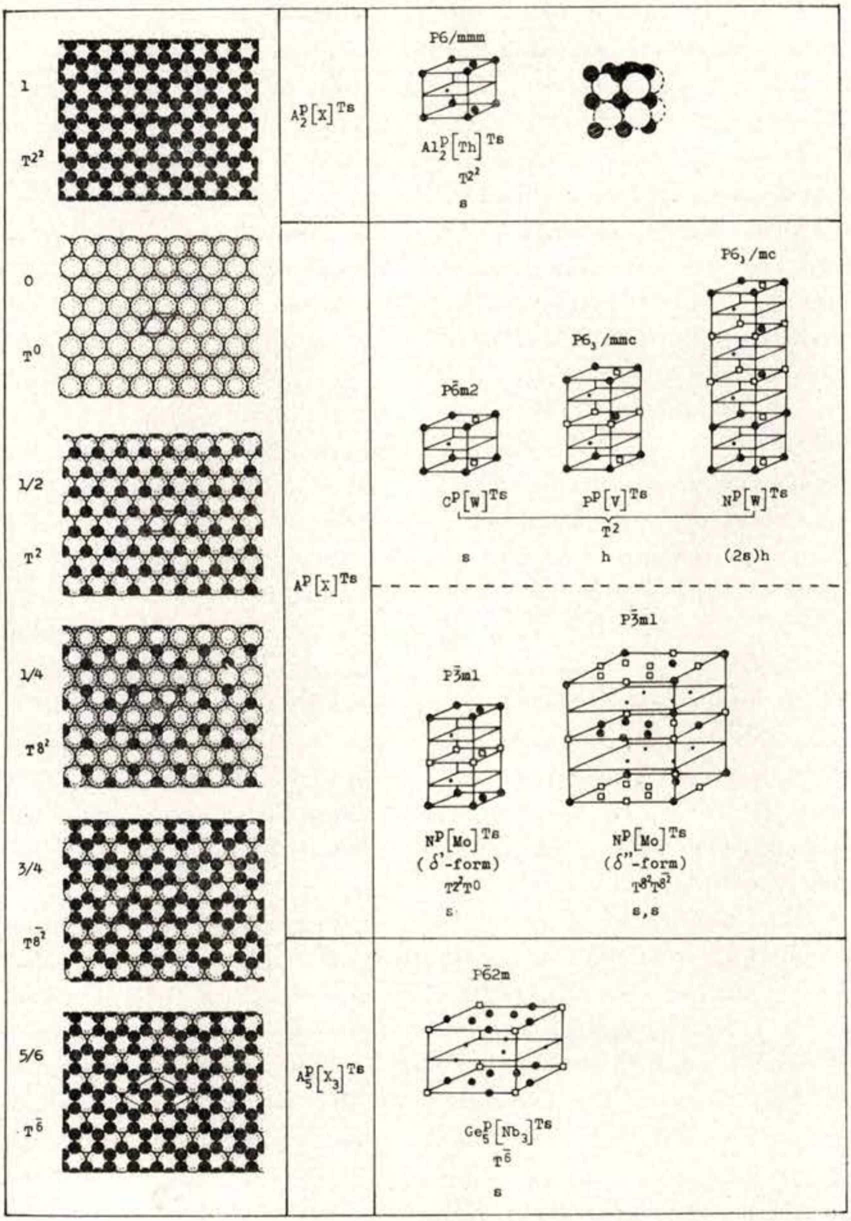

Fig. 1 — Standard representation of inorganic structure types of general formula $A^{p}_{m}\left[X_{n}\right]^{Ts}$ (*Ts* means simple hexagonal packing, and *p* triangular prismatic coordination).

layer, and *b*, *v* and *d* for the different kinds of stacking sequences). Similar modes of stacking can be found in structures based on square layers of atoms (Q) and in the body-centered cubic packing, if the rhombic layers (B) parallel to (110) planes are considered. Therefore all these packings are included under the same designation of loose packings [5].

The simple packings are the well known simple hexagonal and the simple cubic packings represented respectively by *Ts* and *Qs* (*s* for the stacking sequence which corresponds to the juxtaposition of the layers with one atom touching only one atom of the layer below).

Before applying the standard representation to the structures based on simple and on loose packings we have determined their proper layer description, and we have restricted our work to structures of binary compounds. The result is shown on Chart I.

The standard representation has then been applied to all these structures, but here only one family is presented (Fig. 1). We have chosen the structures corresponding to the general formula $A_m^p [X_n]^{Ts}$, that is, based on the simple hexagonal packing Ts of the larger atoms *X*, with interstitial smaller atoms *A*, having triangular prismatic coordination *p*. Because the plane of the interstitial atoms does not coincide with the plane of the packing atoms, we have subdivided the constructive layers into two different levels, in order to achieve a more exact representation (Fig. 1).

The distribution pattern of either the packing atoms in minor proportion, or of the interstitial atoms, is symbolized by a capital letter indicating the shape of the plane unit cell of their patterns, using *T* for hexagonal (triangular net), *Q* for square (quadrangular net) and *R* for rectangular or oblique shape. An upper symbol indicates the occupancy of the atoms in the possible sites within this unit cell, for instance $T^{8^{2}}$ means a proportion of 2/8 (2/8 = 1/4 but the eight expresses the multiplicity of the unit cell); in the particular cases of 1/2, 1/3, 1/4 ... the number one is omitted, for reasons of simplicity, and consenquently T^2, for example, corresponds to a proportion 1/2; T^0 corresponds to zero occupancy. Another simplification is used when a certain distribution pattern is complementary to a simpler one, e.g.,

$[X_mY_n]^{Tb/v/d}$			$A_m^p[X_n]^{Ts}$			$A_m^{p/o}[X_n]^{Tc/h/s}$		
Pr.l.d.	St.	Str. type	Pr.l.d.	St.	Str. type	Pr.l.d.	St.	Str. type
T^1	b	$[Pa]^{Tb}$	T^1	s	$[InSn_4]^{Ts}$	$T^{3^2}T^0$	h	$Cu^p[Ba]^{(2Ts)h}$
T^1	d	$[Pu]^{Td}$	T^{2^2}	s	$Al_2^p[Th]^{Ts}$	T^2T^0	c	$Mo^p[S_2]^{(2Ts)c}$
R^2	b_y	$[CuTi]^{Tb}$	T^2	s	$C^p[W]^{Ts}$	T^2T^0	h	$Mo^p[S_2]^{(2Ts)h}$
T^3	b	$[MoSi_2]^{Tb}$	T^2	h	$P^p[V]^{Ts}$	T^2T^0	s	$Nb^p[S_2]^{(2Ts)h}$
T^3	v	$[CrSi_2]^{Tv}$	T^2	(2s)h	$N^p[W]^{Ts}$	T^2T^0	(3h)s	$Nb^p[Se_2]^{(2Ts)ch}$
T^3	d	$[TiSi_2]^{Td}$	$T^{2^2}T^0$	s	$N^p[Mo]^{Ts}$ (δ'-form)	T^1T^0	c	$N^o[W_2]^{(2Ts)c}$
R^{16^4}	b_y	$[Nb_3Au_2]^{Tb}$	$T^{6^2}T^{6^{\bar{2}}}$	s, s	$N^p[Mo]^{Ts}$ (δ''-form)	$T^{\bar{3}}T^0$	s	$Al^o[(OH)_3]^{(2Ts)h}$ Gibbsite
			$T^{\bar{4}}$	s	$Ge_5^p[Yb_3]^{Ts}$	$T^{\bar{3}}T^0$	s	$Al^o[(OH)_3]^{(4Th)s}$ Nordstrandite
						$T^2T^2T^0$	(2s)h	$N_2^{\bar{3}}[W_3]^{(3Ts)h}$

$A_q^{o/t}[X_mY_n]^{Bb}$								
Pr.l.d.	St.	Str. type	Pr.l.d.	St.	Str. type	Pr.l.d.	St.	Str. type
Q^1	f	$[W]^{Bb}$	Q^{9^4}	f	$[V_4Zn_5]^{Bb}$	Q^6	b	$D^t[Ta_2]^{Bb}$
Q^2	d	$[NaTl]^{Bb}$	$T^1(4T^0)T^1(3T^0)$	h	$[Pb_2Li_7]^{Bb}$	$\tilde{Q}^{6^3}$	fr	$H_3^t[U]^{Bb}$
Q^1Q^0	s	$[LiHg]^{Bb}$	$R^{11^3}(110)$	b_y	$[Pb_3Li_8]^{Bb}$	$\tilde{Q}^{6^2}Q^4$	s, s	$Ni_3^t[S_2]^{Bb}$
$Q^1Q^1Q^0Q^0$	f	$[CuTi]^{Bb}$	Q^3Q^0	s	$B^o[Ta_2]^{Bb}$	Q^8	d	$Th^t[Cl_4]^{Bb}$
$Q^1Q^0Q^0$	f	$[AlCr_2]^{Bb}$	$Q^{12}Q^0$	f.	$N^o[Fe_4]^{Bb}$	$R^4R^{4^2}(110)$	f, s	$D_3^t[Ta_4]^{Bb}$
Q^2Q^0	f	$[BiFe_3]^{Bb}$						

$A_m^{p/sq}[X_n]^{Qd}$			$A_m^{cb/sq}[X_n]^{Qs}$			$A_q^{p/\ /sq}[X_mY_n]^{Qf/b/s}$		
Pr.l.d.	'St.	Str. type	Pr.l.d.	St.	Str. type	Pr.l.d.	St.	Str. type
$\tilde{Q}^{2^2}$	d	$Si_2^p[Th]^{Qd}$	Q^1	s	$[Po]^{Qs}$	Q^1	(2b)f	$[Ga]^{(2Qb)f}$
Q^1	d	$As^p[Nb]^{Qd}$	Q^2	f	$[KF]^{Qs}$	$Q^2Q^2Q^0$	f	$[AsFe_2]^{(3Qf)s}$
Q^1	d	$P^{sq}[Nb]^{Qd}$	Q^1	s	$Cs^{cb}[Cl]^{Qs}$	$Q^2Q^2Q^0$	(2s)f	$[SbLa_2]^{(3Qf)s}$
			Q^2	f	$Ca^{cb}[F_2]^{Qs}$	$Q^1Q^0Q^0$	s	$[CuGa_2]^{(3Qf)s}$
			Q^2	s	$Pt^{cb}[Hg_2]^{Qs}$	$Q^2Q^2Q^0Q^0$	(2f)b	$[AsMn_3]^{(4Qf)s}$
			Q^1Q^0	s	$Fe^{cb}[Si_2]^{Qs}$	Q^1	(2b)f	$Tl^s[I]^{(2Qb)f}$
			$T^1T^0T^0$	c	$U^{cb}[O_3]^{Qs}$	$\tilde{Q}^{2^2}Q^0$	b	$B^p[Ni]^{(2Qb)f}$
			$T^1T^0T^0$	h	$Ni_2^{cb}[Al_3]^{Qs}$	$\tilde{Q}^{2^2}Q^0$	br	$B^p[Mo]^{(2Qb)f}$
			Q^4	f	$Pt^{cb}[Hg_4]^{Qs}$	Q^2Q^0	f	$Pd^{sq}[Cl_2]^{(2Qb)f}$
			$Q^{\bar{4}}$	f	$Pt_3^{cb}[O_4]^{Qs}$	$\tilde{Q}^{2^2}\tilde{Q}^{2^2}Q^0$	d	$B_4^p[Cr_3]^{(3Qb)f}$
			Q^2	f	$Pt^{sq}[S]^{Qs}$			

Chart I — Proper layer description of structure types of binary compounds based on simple and on loose packings. Notice the simplicity of the layer description of most of these structure types.

instead of T^{3^2} we use $T^{\bar{3}}$, the bar meaning the complementary proportion of 1/3. The sequence of the distribution patterns of either the packing atoms in minor proportion or of interstitial atoms, is indicated by a small letter. When two letters are used, like *br*, this corresponds to a composed operation, that is, a translation *b* followed by a rotation *r* of 90° [6]. The translations (projected vectors) and/or rotations indicating the sequences of the *T*, *Q* and *R* types of the distribution patterns mentioned in Chart I and on Fig. 1 are shown in Fig. 2.

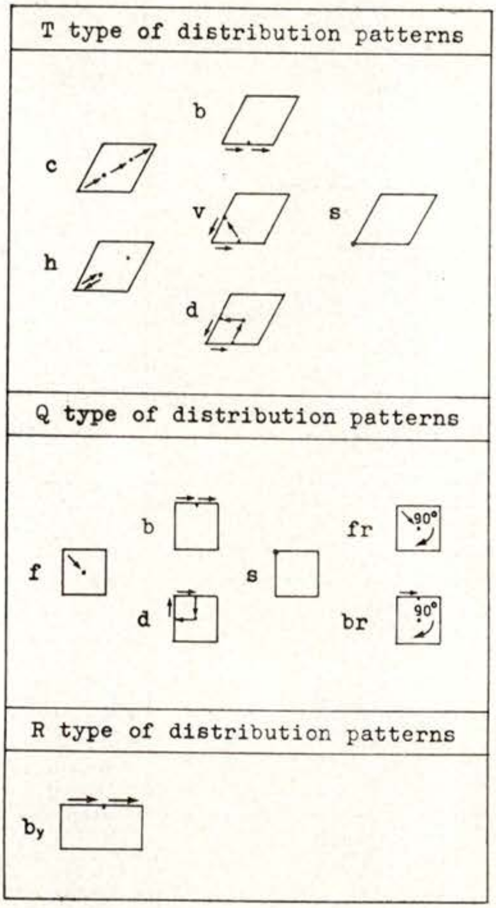

Fig. 2 — Translations (projected vectors) and/or rotations indicating the sequences for the *T*, *Q* or *R* type of distribution patterns mentioned in Fig. 1 and Chart I.

As happened with the closest packed structures [1] we can conclude from Chart I that most of the structures show a very simple proper layer description, based on simple and symmetrical layers, like T^1, T^0, T^2, Q^1, Q^0, Q^2, … . It is also remarkable that a few types of sequence of the distribution patterns (Fig. 2) are adopted by several different structure types (Chart I) and that these sequences are practically the same as those observed for the structures based on closest packings [1] and for the inorganic structures in general [7]. The standard representation clearly shows that structures have a much simpler atomic organization and are more interrelated than could have been imagined using the conventional ways of structure representation found in the literature.

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