

AN ATTEMPT AT AN ALGEBRAIC THEORY OF CRYSTAL STRUCTURE. PART 3.

David A ABOAV

29 Clements Road,  
 Chorleywood,  
 Hertfordshire, WD3 5JS, UK.

ABSTRACT

The aim of this work is to found a theory of crystal structure on the notions not of length and angle, but of number, the fundamental phenomenon involved being the patterns produced by X-rays falling on matter in the solid, or crystalline state. It is shown that some alloys of transition metals are a source of patterns complex and varied enough to enable gaps in their enumeration to be exposed by the rudiments of such a theory (Aboav, 1997, 1998).

**Key words:** crystal structure, algebraic theory, space-filling polyhedra.

INTRODUCTION

In Parts 1 & 2 (Aboav, 1997, 1998) it was shown how the topological properties of some inclusion hydrates of the 'dodecahedral series' could be classified in terms of the solutions of a simple Diophantine equation, and the result used to predict the existence of further compounds of the same type. These properties are summarized in Table 1, which shows for five of the hydrates the number of 16-, 15-, 14-, and 12-hedra (cols.2 through 5);  $N_0$ , the number of vertices (col.6);  $N_3$ , the number of polyhedra (col.7) in a unit cell of their crystal structure; and (col.8) the number  $29N_3 - 5N_0$ .  $n_0$  and  $n_3$  (cols.9 & 10) are  $N_0$  and  $N_3$  made relatively prime by the removal of their common factors.

Table 1. Topological properties of some inclusion hydrates.

hydrate	16	15	14	12	$N_0$	$N_3$	$(29N_3 - 5N_0)$	$n_0$	$n_3$
chlorine	...	...	6	2	46	8	2	23	4
chloroform	8	...	...	16	136	24	16	17	3
alkyl onium salt	...	4	4	6	80	14	6	40	7
bromine tetr.	...	4	16	10	172	30	10	86	15
bromine ortho.	4	4	4	14	148	26	14	74	13

The table shows that for each of the five unit cells listed:

- (i) the number of 12-hedra is equal to  $29N_3 - 5N_0$ , and

(ii) the numbers of 16-, 15-, 14-, & 12-hedra are multiples, or sums of multiples of their combinations  $1|0|0|2$ ,  $0|2|2|3$ , and  $0|0|3|1$ , thus:

chlorine  $2x(0|0|3|1)$ , chloroform  $8x(1|0|0|2)$ , alkyl onium salt  $2x(0|2|2|3)$ , bromine (tetr.)  $4x(0|0|3|1) + 2x(0|2|2|3)$ , & bromine (orth.)  $2x(0|2|2|3) + 4x(1|0|0|2)$ .

These two findings are, however, not independent; for, if the multiples of  $1|0|0|2$ ,  $0|2|2|3$ , and  $0|0|3|1$  are integers  $i$ ,  $j$ , and  $k$ , respectively, the number  ${}_{12}N_3$  of 12-hedra in a unit cell is given by

$${}_{12}N_3 = 2i + 3j + k ; \quad (1)$$

and, since 16-, 15-, 14-, and 12-hedra possess 28, 26, 24, and 20 vertices --- or, if they are so placed that each vertex is shared by four contiguous polyhedra, 7,  $6\frac{1}{2}$ , 6, and 5 vertices, respectively --- the number  $N_0$  of vertices of such a cell is given by

$$N_0 = 17i + 40j + 23k \quad (2)$$

and the number  $N_3$  of its constituent polyhedra by

$$N_3 = 3i + 7j + 4k ; \quad (3)$$

from which it follows that

$$\begin{aligned} 29N_3 - 5N_0 &= 2i + 3j + k \\ &= {}_{12}N_3 . \end{aligned} \quad (4)$$

This shows that, if  $N_0$  and  $N_3$  are known, the number of 12-hedra in a unit cell and consequently the *total number* ( $N_3 - {}_{12}N_3$ ) of its remaining polyhedra are also known. But the *partition* of the latter into 16-, 15-, and 14-hedra is not deducible from  $N_0$  and  $N_3$ , since the operation  $(1|-2|1|0)$  --- i.e. the replacement of two 15-hedra by a 16-hedron and a 14-hedron --- leaves  $N_0$  and  $N_3$  invariant and, since

$$(1|-2|1|0) \equiv (1|0|0|2) - (0|2|2|3) + (0|0|3|1) , \quad (5)$$

allows the numbers of different polyhedra, after the operation, to be expressible as multiples, or sums of multiples of the same combinations as before.

The above rule (4) does not, however, hold generally. It is a feature of 4-connected honeycombs whose polyhedral cells have pentagonal and *non-adjacent* hexagonal faces only; and many inclusion hydrates in particular (Jeffrey, 1982) have structures that do not obey it.

But there are compounds, among them alloys of the transition metals, whose structure, though differing chemically from that of the hydrates, is nevertheless governed by that rule; and the object of the investigation now to be described is to show how those compounds, too, can be classified and their existence predicted by means of the above-mentioned Diophantine equation.

**THE DIOPHANTINE EQUATION  $2^ax = 3^by + z$  .**

It has already been shown (Aboav, 1998) that the quantities  $N_0$  and  $N_3$ , and hence  $n_0$  and  $n_3$ , of Table 1 are proportional to the roots of a Diophantine equation:

$$2^ax = 3^by + z \quad (6)$$

where  $a$  and  $b$  are positive integers, and  $x$ ,  $y$ , and  $z$  odd primes or unity, with  $z$  positive or negative. To obtain agreement with experiment certain restrictions on the values of  $x$ ,  $y$ , and  $z$  had to be made, viz:

$$(i) \quad x, y < 100 ,$$

$$(ii) \quad z/2^ax < 1/100 ;$$

but the experimental facts now to be investigated suggest a change should be made both in the composition and in the limits of  $x$ ,  $y$ ,  $z$ .

As regards their composition each of these numbers was assumed to be prime (Aboav, 1997); but it will now be assumed that:

(a)  $z$  is composite,

(b) one of the two numbers  $x$   $y$  is odd prime, while the other may be odd prime or the product of two odd primes, of which one may not exceed 7.

This gives rise to five equations to be solved for  $x$  and  $y$  :

$$\left. \begin{aligned} 2^ax &= 3^by + z \\ 2^{a\underline{5}.p} &= 3^by + z \\ 2^ax &= 3^{b\underline{5}.q} + z \end{aligned} \right\} \quad (7)$$

$$\left. \begin{aligned} 2^{a\underline{7}.p} &= 3^by + z \\ 2^ax &= 3^{b\underline{7}.q} + z \end{aligned} \right\} \quad (8)$$

where  $p$  and  $q$  are odd primes. So that they may be more easily recognized, composite numbers are shown underlined.

As regards the limits imposed on  $x$  and  $y$  it will now be assumed that:

$$(iii) \quad x < 240 ; \quad y < 60 .$$

Since  $z$  is assumed composite there is no longer need to refer to its value explicitly; so that restriction (ii) may be expressed as  $1 - 3^by/2^ax < 1/100$ , or as

$$(iv) \quad 1 - 3^6n_3/2^7n_0 < 1/100$$

(Aboav, 1997, 1998); and the solutions of Eq.(6) which were formerly denoted by  $[a \ b]\{x \ y \ z\}$  may be written simply  $[a \ b]\{x \ y\}$ .

The fraction  $(1 - 3^6 n_3 / 2^7 n_0)$  will henceforth be referred to as the *comma*, and denoted by the Greek letter  $\kappa$ :

$$\kappa = 1 - 3^6 n_3 / 2^7 n_0 \quad (9)$$

so that restriction (iv) can be written

$$(v) \quad \kappa < 1/100$$

For greater clarity the comma may sometimes here be expressed as the nearest vulgar fraction with unity as numerator, as in Table 5A below.

24 solutions to Eq.(6) subject to these new conditions are shown in Table 2, which contains many of the solutions listed in Part 2 (Aboav 1998) as well as some further ones. In some cases more than one solution is shown for a given  $\{a \ b\}$ .

Table 2. Solutions of Eq.(6) subject to restrictions (iii) and (iv)

	b = 4	b = 5	b = 6	b = 7
a	{ x y }	{ x y }	{ x y }	{ x y }
5	{43 17}	{53 7}	<b>{23 1}</b>	---
6	{29 23}	{19 5}	<b>{149 13}</b>	{103 3}
7	<b>{7 11}</b> --- ---	{59 31} {89 47} {101 53}	<b>{17 3}</b> {97 17} {131 23}	--- --- ---
8	{13 41} ---	{41 43} ---	<b>{37 13}</b> <b>{151 53}</b>	<b>{43 5}</b> ---
9	<b>{3 19}</b>	{11 23}	{67 47}	{47 11}
10	---	---	<b>{5 7}</b>	---

13 solutions of Eq.(7) and 7 solutions of Eq.(8) are shown in Tables 3 & 4, respectively. In Tables (2), (3) & (4) numbers that describe a known crystal structure (*v. infra*) are shown in **bold type**.

These tables, to which more solutions subject to the same restrictions can be added, are not meant to be complete. The 44 solutions here chosen are gathered together in Table 5A, in which are listed, after a serial number (col.1) a solution (col.2) and its corresponding values of  $n_0$  and  $n_3$  (cols.3 & 4). Column 5 lists the comma,  $\kappa$ ; cols.6 & 7, the numbers  $60(1 + n_3/n_0)$  and  $2(1 + n_0/n_3)$  to 3 decimal places; and col.9, the integer  $29n_3 - 5n_0$ .

Table 3. Solutions of Eq.(7) subject to restrictions (iii) and (iv)

	b = 5	b = 6	b = 7	b = 8	b = 9
a	{ x y }	{ x y }	{ x y }	{ x y }	{ x y }
5	---	---	{ <u>5.41</u> 3}	---	---
6	---	---	---	---	---
7	{ <u>5.11</u> 29} {67 <u>5.7</u> }	{ <u>5.47</u> 41} ---	---	{ <u>5.31</u> 3} ---	---
8	{ <u>5.7</u> 37} ---	{71 <u>5.5</u> } {157 <u>5.11</u> }	{ <u>5.29</u> 17} ---	---	---
9	{31 <u>5.13</u> }	---	{107 <u>5.5</u> }	---	{ <u>5.23</u> 3}
10	{13 <u>5.11</u> }	---	---	---	---

Table 4. Solutions of Eq.(8) subject to restrictions (iii) and (iv)

	b = 4	b = 5	b = 6	b = 7	b = 8
a	{ x y }	{ x y }	{ x y }	{ x y }	{ x y }
3	---	{ <u>7.13</u> 3}	---	---	---
4	---	---	---	---	---
5	---	---	---	---	---
6	---	---	{ <u>7.31</u> 19}	---	---
7	{31 <u>7.7</u> }	---	---	---	---
8	---	{73 <u>7.11</u> }	---	---	{ <u>7.11</u> 3}
9	---	---	---	{ <u>7.19</u> 31}	---
10	---	---	---	{ <u>7.7</u> 23}	---

THE CRYSTAL: THE PICTURES OF HAÜY (1784), AND OF FEDOROV (1890).

The numbers listed in Table 5A, which are solutions of a Diophantine equation or numbers derived from them, are dimensionless and hence *scale-free*. It is proposed next to compare them with some other numbers which, since they depend on a physical process and necessitate measurements of length and angle, are *scale-dependent*.

Table 5A. Solutions to Eqs (6),(7), &amp; (8), and some related numbers.

No.	$\{a\ b\}\{x\ y\}$	$n_0\ n_3$	$\kappa$	$60(1+n_3/n_0)$	$2(1+n_0/n_3)$	$29n_3-5n_0$
1	{5 6}{23 1}	23 4	1/104	70·435	13·500	1
2	{7 5}{67 <u>5.7</u> }	201 35	1/121	70·448	13·486	10
3	{7 8}{ <u>5.31</u> 3}	155 27	1/126	70·452	13·481	8
4	{9 5}{11 23}	132 23	1/131	70·455	13·478	7
5	{8 7}{43 5}	86 15	1/151	70·465	13·466	5
	" "	" "	1/151	70·465	13·466	5
6	{7 6}{ <u>5.47</u> 41}	235 41	1/157	70·468	13·463	14
7	{6 6}{149 13}	149 26	1/162	70·470	13·462	9
8	{7 4}{7 11}	63 11	1/179	70·476	13·455	4
9	{9 5}{31 <u>5.13</u> }	372 65	1/206	70·484	13·446	25
10	{6 7}{103 3}	103 18	1/213	70·485	13·444	7
11	{8 5}{41 43}	246 43	1/223	70·488	13·442	17
12	{9 7}{ <u>7.19</u> 31}	532 93	1/228	70·489	13·441	37
13	{7 5}{101 53}	303 53	1/264	70·495	13·434	22
14	{10 6}{5 7}	40 7	1/301	70·500	13·428	3
	" "	" "	1/301	70·500	13·428	3
	" "	" "	1/301	70·500	13·428	3
15	{6 6}{ <u>7.31</u> 19}	217 38	1/375	70·507	13·421	17
16	{7 5}{59 31}	177 31	1/397	70·508	13·419	14
17	{8 6}{157 <u>5.11</u> }	314 55	1/414	70·510	13·418	25
18	{8 4}{13 41}	234 41	1/476	70·513	13·415	19
19	{9 7}{107 <u>5.5</u> }	428 75	1/503	70·514	13·413	35
20	{7 6}{97 17}	97 17	1/540	70·515	13·412	8
21	{8 8}{ <u>7.11</u> 3}	154 27	1/680	70·519	13·407	13
22	{9 6}{67 47}	268 47	1/837	70·522	13·404	23
23	{6 5}{19 5}	57 10	1/1216	70·526	13·400	5
24	{8 6}{151 53}	302 53	1/2035	70·530	13·396	27
25	{9 7}{47 11}	188 33	1/3438	70·532	13·394	17
26	{7 6}{131 23}	131 23	1/16,768	70·534	13·391	12
27	{5 7}{ <u>5.41</u> 3}	205 36	-1/6562	70·537	13·389	19
28	{7 4}{31 <u>7.7</u> }	279 49	-1/3968	70·538	13·388	26
29	{8 6}{37 13}	74 13	-1/1894	70·540	13·385	7
	" "	" "	-1/1894	70·540	13·385	7
	" "	" "	-1/1894	70·540	13·385	7
	" "	" "	-1/1894	70·540	13·385	7
30	{5 4}{43 17}	387 68	-1/1376	70·543	13·382	37
31	{7 5}{ <u>5.11</u> 29}	165 29	-1/1006	70·546	13·379	16
32	{8 5}{73 <u>7.11</u> }	438 77	-1/813	70·548	13·377	43
33	{3 5}{ <u>7.13</u> 3}	91 16	-1/728	70·549	13·375	9
34	{8 7}{ <u>5.29</u> 17}	290 51	-1/629	70·552	13·373	29
35	{9 4}{3 19}	108 19	-1/512	70·556	13·368	11
36	{10 7}{ <u>7.7</u> 23}	392 69	-1/401	70·561	13·362	41
37	{7 5}{89 47}	267 47	-1/393	70·562	13·362	28
38	{8 6}{71 <u>5.5</u> }	142 25	-1/371	70·563	13·360	15
39	{9 9}{ <u>5.23</u> 3}	460 81	-1/348	70·565	13·358	49
40	{5 5}{53 7}	159 28	-1/339	70·566	13·357	17
41	{8 5}{ <u>5.7</u> 37}	210 37	-1/289	70·571	13·351	23
42	{6 4}{29 23}	261 46	-1/265	70·575	13·348	29
43	{10 5}{13 <u>5.11</u> }	312 55	-1/251	70·577	13·345	35
44	{7 6}{17 3}	17 3	-1/198	70·588	13·333	2

Table 5B. Crystal structure of some 't.c.p.' alloys (Shoemaker &amp; Shoemaker, 1986).

No.	Compound	a(Å)	b(Å)	c(Å)	$\beta(^{\circ})$	N	$\langle\theta\rangle$	$\langle CN\rangle$	$x_{calc}$
1	Cr <sub>3</sub> Si	(4.564)				8	70.435	13.500	1.00
2									
3									
4									
5	Cr <sub>46</sub> Fe <sub>54</sub>	(8.800		4.544)		30	70.465	13.466	4.98
	H complex	(4.5	17.5	4.5)		30	70.465	13.466	4.98
6	K complex	...	...	...	...	82	...	13.46	...
7	F complex	...	...	...	...	52	...	13.46	...
8	J complex	...	...	...	...	22	...	13.45	...
9									
10									
11									
12	Mn <sub>81.5</sub> Si <sub>18.5</sub>	(16.992	28.63	4.656)		186	70.489	13.441	37.11
13									
14	Zr <sub>4</sub> Al <sub>3</sub>	(5.433		5.390)		7	70.500	13.428	3.00
	Mo <sub>12</sub> Cr <sub>18</sub> Ni <sub>40</sub>	(9.070	16.983	4.752)		56	70.500	13.428	6.04
	MoNi	(9.108	9.108	8.852)		56	70.500	13.428	6.04
15									
16									
17	Mn <sub>77</sub> Fe <sub>4</sub> Si <sub>19</sub>	(13.362	11.645	8.734	90.5)	220	70.510	13.418	25.14
18									
19									
20									
21									
22									
23									
24	Mo <sub>31</sub> Cr <sub>18</sub> Co <sub>51</sub>	(10.903		19.342)		159	70.530	13.396	26.93
25									
26									
27									
28									
29	Mo <sub>6</sub> Co <sub>7</sub>	(4.762		25.615)		39	70.540	13.385	6.96
	K <sub>7</sub> Cs <sub>6</sub>	(9.078		32.950)		26	70.540	13.385	6.96
	W <sub>6</sub> (Fe, Si) <sub>7</sub>	(9.283	7.817	4.755)		26	70.540	13.385	6.96
	Nb <sub>48</sub> Ni <sub>39</sub> Al <sub>13</sub>	(9.303	16.266	4.933)		52	70.540	13.385	6.96
30									
31									
32									
33									
34									
35	V <sub>41</sub> Ni <sub>36</sub> Si <sub>23</sub>	(13.462	23.381	8.940	100.3)	228	70.556	13.369	10.94
36									
37									
38	V <sub>2</sub> (CoSi) <sub>3</sub>	(17.17	4.66	7.55	99.2)	50	70.563	13.360	14.92
39	Mg <sub>32</sub> (Zn, Al) <sub>39</sub>	(14.16)				162	70.565	13.358	48.75
40									
41	Mn <sub>45</sub> Co <sub>40</sub> Si <sub>15</sub>	(15.42	12.3	4.74)		74	70.571	13.351	22.90
42									
43	Mg <sub>4</sub> Zn <sub>7</sub>	(25.96	5.24	14.28	102.5)	110	70.577	13.345	34.89
44	MgZn <sub>2</sub> (MgCu <sub>2</sub> )	(5.16[7.08]		8.50)		12[24]	70.588	13.333	2.00

The physical process referred to is the scattering of X-rays by matter in the crystalline state. The characteristic pattern of spots this produces on a photographic plate is thought of as originating in a microscopic structure possessed by the crystal. This postulated structure is pictured macroscopically in at least two ways. In the first way, associated with the name of Haüy (1784), the crystal is pictured as a regular array of particles, or 'atoms', located in a space of three dimensions: in the second, that of Fedorov (1890), the space is pictured as divided into contiguous, congruent polyhedral regions, or *stereohedra*. The two representations are equivalent, the one being the 'dual' of the other; but Fedorov's has for us the advantage that, in emphasizing a topological feature of crystal structure, it facilitates the eventual passage to an algebraic theory.

Fedorov's stereohedron is topologically equivalent to the *Voronoi polyhedron* (Okabe et al., 1992) generated by a point at its centre; and in some cases, as in the truncated octahedron of Fig.1, may also be congruent to it. Hence, where only a topological feature of a crystal is in question, Voronoi's figure can be used in place of Fedorov's. The number of faces of the Voronoi polyhedron is also known as the *coordination number*, CN, of the atom at its centre.

Figure 1 shows part of the structure of a body-centred cubic crystal pictured in each of the above two ways. The black dots represent the sites of Haüy's atoms; while the stereohedron of Fedorov, or Voronoi polyhedron, is shown as a truncated octahedron surrounding an atom at the centre of the cube.

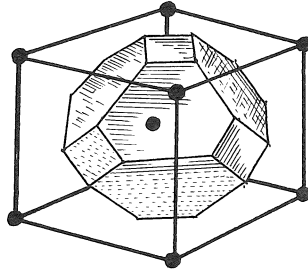


Fig.1. Structure of body-centred cubic crystal.

In this case the stereohedra, like the polyhedral compartments of the crystal structures so far investigated (Aboav, 1997), form a 4-connected honeycomb; but in other structures, like for example the face-centred cubic lattice, they may be  $n$ -connected, with  $n > 4$ . That the algebraic theory now put forward may nevertheless be valid for these cases, too, may be seen from the following considerations.

Figure 2a shows a Voronoi diagram in two dimensions only: it is a periodic tessellation of 3-connected Voronoi polygons whose generating points, here represented as black dots, form a 'dual' tessellation of parallelograms. With the angle  $\beta$  of a parallelogram equal to  $75^\circ$ , as in the figure, the side AB of the Voronoi polygon is roughly 4mm long; and with  $\beta$  increased to  $85^\circ$  (Fig.2b) it diminishes to about 1mm.

As  $\beta$  approaches a rightangle there comes a stage where AB can no longer be distinguished from a point, and 4 instead of 3 sides of the Voronoi polygon, which now looks like a rectangle, appear to meet at the vertex A. (Fig.2c). The figure



may then be regarded either as a 4-connected, or as a 'degenerate' 3-connected tessellation of polygons. A degenerate figure often appears when its generating points are regularly spaced (Okabe et al., 1992), the concepts of 'symmetry' and 'degeneracy' going hand in hand.

Since the notion of degeneracy applies equally to honeycombs of polyhedra in a space of 3 dimensions, every such honeycomb can in principle be regarded as 4-connected (Okabe et al., 1992), thus enabling the proposed algebraic theory of crystal structure (Aboav, 1997), which invokes a geometrical property of 4-connected honeycombs, to be applied more generally.

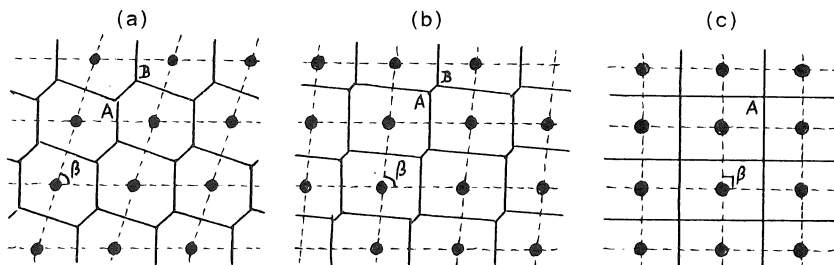


Fig.2. Periodic tessellations of Voronoi polygons in 2 dimensions.

We end this section by indicating briefly how the rudiments of such a theory may predict for some transition metals the topological structure of a number of alloys as yet unidentified.

#### 'TETRAHEDRALLY CLOSE-PACKED' ALLOYS

The alloys of some transition metals, the so called 'tetrahedrally close-packed', or t.c.p. alloys, display a crystal structure of wide variety and complexity, which as we have seen may be described in terms either of the neighbouring atoms of a central atom, or of the space-filling packing of polyhedra. Shoemaker and Shoemaker (1986), used both these representations to express, for some 20 alloys of this type, metrical and topological features of their structure, of which some are reproduced in Table 5B

In col.1 of that table is shown an ordinal number, to help align its entries with those of Table 5A. The formula of each alloy is given in col.2, and its lattice constants in cols.3 through 6.  $N$ , the number of Voronoi polyhedra in its unit cell, is shown in col.7;  $\langle\theta\rangle$ , the average dihedral angle of the tetrahedral interstices formed by the atoms of the alloy, in col.8; and  $\langle CN\rangle$ , the average coordination number of those atoms, in col.9. An approximate value,  $x_{calc}$ , of the number of dodecahedral Voronoi polyhedra per unit cell, deduced by the above authors from the values of  $\langle\theta\rangle$ , is given in col.10; and equivalent data (Rivier & Aste, 1996) for 3 alloys discovered after the publication of their results are added to the table, in italics, at positions 6, 7, and 8.

The table shows, first, that for each of its 20 values of  $\langle CN\rangle$  there is a value of  $2(1 + n_0/n_3)$  in Table 5A to equal it; and that, if such pairs of numbers are placed in alignment,  $\langle\theta\rangle$  is seen to equal the corresponding value of  $60(1 + n_3/n_0)$ ;

$N$ , to equal a small integral multiple of the corresponding value of  $n_3$ ; and the nearest whole number to  $x_{\text{calc}}$ , to equal the corresponding value of  $29n_3 - 5n_0$ ;

secondly that, when the entries of the tables are aligned in that way, gaps appear in those of Table 5B, that is, there are entries in Table 5A to which there is nothing to correspond in Table 5B;

and thirdly that, if to these alloys are added the above three subsequently identified ones, they are found to fill gaps in Table 5B, that is, the same kind of correspondence is found to exist between their data and numbers in Table 5A as was found for the alloys of Shoemaker & Shoemaker.

This last fact indicates that the most recent enumeration of tetrahedrally close-packed alloys (Rivier & Aste, 1996) may not be complete, and that further compounds of that type may eventually be found to fill some, if not all of the remaining gaps in Table 5B. Eq.(6) leads to values of  $N$ ,  $\langle \Theta \rangle$ , and  $\langle CN \rangle$  and  ${}_{12}N_3$  (a multiple of the nearest integer to  $x_{\text{calc}}$ ) that indicate structures to be expected, of which the most likely to turn up are those with the smallest values of  $n_3$ : Nos.10, 20, 23, and 33 of Tables 5A & B.

Shoemaker & Shoemaker also determined the partition of  $N$  into the numbers of constituent 16-, 15-, 14-, and 12-hedra (not shown here); but Table 5A has nothing to correspond to this partition since, as we have seen, its solutions furnish the numbers  $N_0$  and  $N_3$  (and hence  $n_0$  and  $n_3$ ) only; nor has it any numbers to correspond to the crystal's symmetry, or to its lattice constants (Table 5B). These omissions indicate that the proposed algebraic theory is, as yet, powerless to describe some of the most characteristic properties of a crystal.

Nevertheless, since the theory, even as it now stands, enables some crystals to be classified and topological features of their structure to be quantitatively predicted, it cannot be dismissed as a useless numerical exercise. On the contrary, if as a result of this investigation a tetrahedrally close-packed alloy of the transition metals is found to possess one of the predicted structures, there will be all the more reason to seek, as Einstein envisaged (Aboav, 1997) and as is here attempted, a description of Nature grounded on a purely numerical axiomatic framework.

*(to be continued)*

## REFERENCES

- Aboav DA. An attempt at an algebraic theory of crystal structure. *Acta Stereologica*. Part 1, 1997: 16; 41-53. Part 2, 1998: 17;
- Fedorov E. Cited in Vainshtein BK. *Fundamentals of Crystals*, 2nd. edn. Springer Verlag, Berlin, 1994. p.149.
- Haüy R-J. *Essai d'une théorie sur la structure des cristaux*. Paris, 1784.
- Jeffrey GA. Hydrate inclusion compounds. In: *Inclusion compounds*. Academic Press, 1984: 1; 135-186.
- Okabe A, Boots B, Sugihara K. *Spatial tessellations: concepts and applications of Voronoi diagrams*. Wiley, Chichester, 1992: p.68.
- Rivier N, Aste T. *Organized packing*. Forma, 1996: 11; 223-231.
- Shoemaker DP, Shoemaker CB. The relative number of atomic coordination types in tetrahedrally close packed metal structures. *Acta Cryst.*, 1986: B46; 3-11.