

Title
Crystal Classes and Systems

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Abstract

In addition to the classification of crystals in 32 Crystal Classes divided into 6 (or 7) Crystal Systems, I propose a second further classification. The 32 Crystal Classes are rearranged in a 8x4=32 table having 8 row and 4 columns so they are constituted by eight Groups, each of them having four Classes.

This is no more a hypothesis. This is a fact, unambiguously based on physical properties.

It took me almost forty years to get here.

Aside from all the various ruminations many of which I've posted elsewhere, the final decisive step was the following:

even the second column classes ("center", bit c) share a common physical property.

This property is: "non-polar" or "non-pyro", that is, enough isotropically distributed around the center not to be pyroelectric.

No invention here, but only a rereading of what is possible for all to see, exactly written in crystallography books. Interpreted, of course.

Crystal Class And System			mnemonic symbol				
			Crystal Class	Axes	Non polar (nonpyro)	Mirror plane	Mirror & non polar
			2-bit Binary Counter	00	01	10	11
mnemonic symbol	Crystal System	3-bit Binary Counter	Bit	00	0c	m0	mc
	No axes	000	000	1	1_	m	2/m
	Binary-Axis 2	001	002	2	222	mm2	mmm
	Tetragonal low	010	040	4	4_	4mm	4/m
	Tetragonal high	011	042	422	432	4_2m	4/mmm
	Trigonal	100	300	3	3_	3m	3_2m
	Hexagonal low	101	302	6	6_	6mm	6/m
	Hexagonal high	110	340	32	622	6_m2	6/mmm
	Isometric	111	342	23	m3_	4_3m	m3m

1 - Job description

The thing is begun almost as a crossword puzzle. But basically the main reason was the following: for an engineer who works with radar, the number 32 has a single immediate meaning.

“5-bit A / D converter”.

Hence the impetus for subsequent analyzes, which seemed to be gradually confirmed by many "coincidences".

Years of varied attempts at adjustment followed , essentially empirical as can be seen in my numerous writings . Try and try again. A good quasi - final synthesis can be found in [1].

However, historically, the substantial step was undoubtedly having moved the gyroidal class 432 from cubic to tetragonal class.

I remember seeing this one night, in a dream or half asleep (see Appendix 1 and Bibliography reported there [2]).

With this, the classification found more and more well-founded clues to the existence of groups of 16, groups of 8, groups of 4.

Basically, it seemed more and more reasonable to me the subdivision of the 32 crystal classes in a 8-rows and 4-columns table, where the rows potentially represented 8 crystal systems or groups, and the columns 4 crystal classes.

The numbering appeared in 3 bits for the eight lines, with the bits having the crystallographic meaning of 3, 4, 2 corresponding to the symmetry axes A3, A4, A2.

The four columns were enumerated in 2 bits, having the crystallographic meaning "m "and "c ", corresponding to the symmetries m "mirror plane " and c "center ", centrosymmetry. See Appendix 2 and Ref [3] .

Gradually this classification did not appear to me responding to aesthetic criteria (or not only to aesthetic criteria) but linked to precise geometric motifs: the symmetries of the 32 crystal classes.

Years of successive empirical shifts of the various classes followed, to find an increasingly satisfactory arrangement.

The next substantial step was the realization (see Appendix 3) that the shift of 432 from cubic to tetragonal class was mathematically legitimate, mathematically well founded.

That is, the reason was no longer merely aesthetic, but mathematical.

This gave me more and more grounded confidence in the validity of the classification I was discovering.

In reality all things were falling into place.

Everything seemed more and more reasonable.

Two main doubts remained, relating to the meaning to be given to bit 4 and bit c. In fact, these meanings were almost clear. For bit 4 a sort of 90 ° axis, “generalized axis 4”. For bit c the meaning also appeared to be that of "generalized center of symmetry".

Meanings, so to I say, intuitively clear, but to be specified. And I couldn't define them more precisely.

It was therefore a success to have understood how bit 4 could be defined (see Appendix 4).

Bit c remained ambiguous.

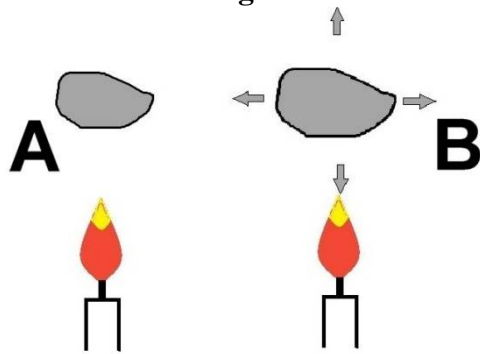
Until one day I got to the final step: I found, basically, that all 8 classes to which I had assigned the c bit actually had a common property. They enjoyed a symmetry common to all 8 classes.

This fact allowed me to explain the c bit as being caused by a very specific physical reason. No longer just intuitive or aesthetic.

What is the common property of the 8 classes?

They are all "non-pyroelectric".

What's the meaning?



A heated body (A) undergoes dilation (B).

When the body is made up of crystals belonging to a certain class called “pyroelectric”, electricity manifests itself in the body, according to certain directions. The crystal class is called in this case "pyroelectric", precisely because electricity occurs as a result of heat. If the crystal class is non-pyroelectric, the body undergoes uniform expansion, but no electricity occurs. This happens, in simple terms, because the body is sufficiently symmetrical with respect to the center. It has no type of anisotropy with respect to the center, such as to cause an electrical voltage along certain directions.

The 8 classes to which bit c belongs are precisely non-pyroelectric.

So this is what I called “a generalized center”.

The generalized center, what I called bit c, is possessed in this sense by all the 8+8 = 16 classes to which I have attributed it. Of these, 11 are centrosymmetric in the classical sense of crystallography. But all 16 are centrosymmetric in the sense specified here. Generalized center. Not pyro.

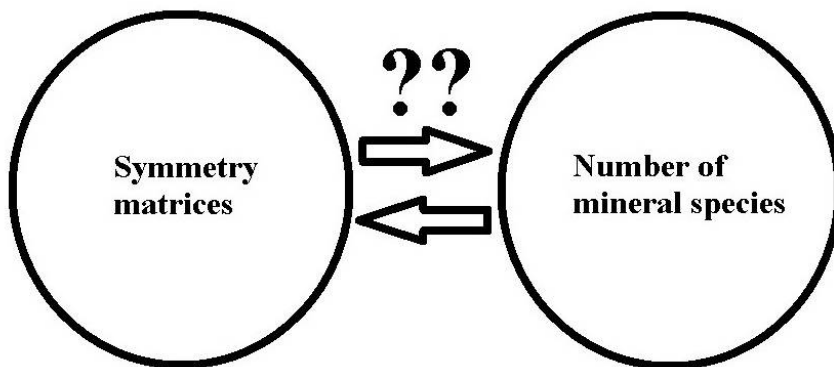
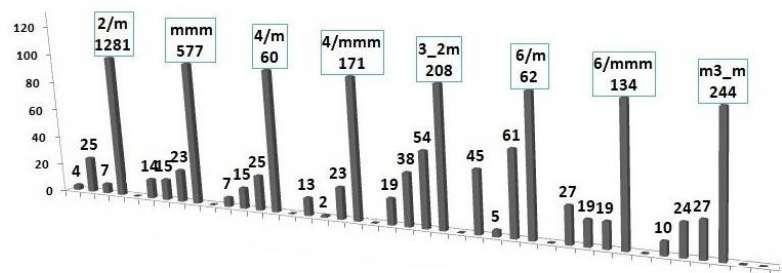
Crystal System	Enantiomorphic (axes only)	Non polar (non pyroelectric)	Mirror plane	Mirror plane & non pyro
No axes	1	1_	m	2/m
Binary-Axis 2	2	222	mm2	mmm
Tetragonal low	4	4_	4mm	4/m
Tetragonal high	422	432	4_2m	4/mmm
Trigonal	3	3_	3m	3_2m
Hexagonal low	6	6_	6mm	6/m
Hexagonal high	32	622	6_m2	6/mmm
Isometric	23	m3_	4_3m	m3m

**I consider this as the latest discovery of this long research work.
And I consider it indeed as the definitive discovery.
The missing link.**

Not only that: it broadens the horizon for new perspectives, related to symmetry and mathematics (see [5] and Appendix 5).

Either way, the fact remains that classification works. Or at least it seems to work.

1	1 ₋	m	2/m
2	222	mm2	mm m
4	4 ₋	4mm	4/m
422	432	4 ₋ 2m	4/m mm
3	3 ₋	3m	3 ₋ 2m
6	6 ₋	6mm	6/m
32	622	6 ₋ m2	6/m mm
23	m3 ₋	4 ₋ 3m	m3 ₋ m



On the left the number of symmetry matrices of the 32 ordered crystal classes $8 \times 4 = 32$, on the right the number of mineral species in each class present on planet Earth, both normalized to the value assumed in the holohedral class. The resemblance is visible.

The question is: why? Why is there this similarity? Why should symmetry matrices be related to number of mineral species on Earth?

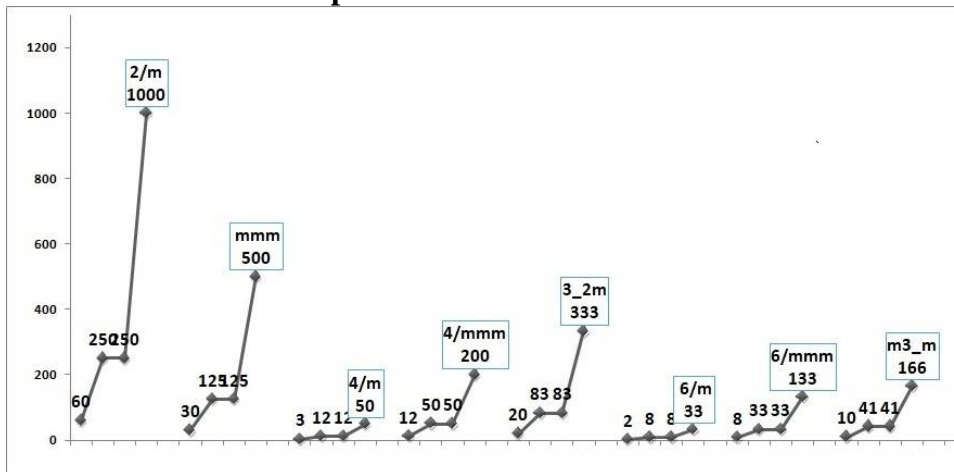
At a first glance it seems a comparison of apples and oranges or as we would say in Italy, this looks like a comparison of apples and pears.
 However, a connection may actually exist.
 An interpretation could be like this:

the number of mineral species that is formed is a function (it is also a function , or it is only a function) of the probability of being able to assemble N points respecting those symmetries, the class symmetries.

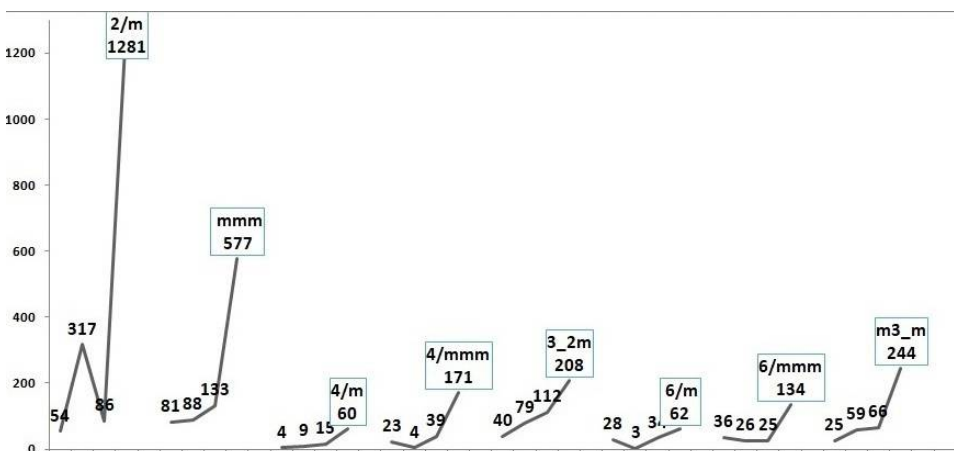
And this regardless of the type of compound (ie 1) elements, 2) sulphides, 3) halides, 4) oxides, 5) nitrates, carbonates, 6) borates, 7) sulphates, 8) phosphates, 9) silicates, 10) organic compounds) and regardless of chemistry , component chemical elements (hydrogen oxygen aluminum iron etc. etc.).

Basically, the number of species would depend on the probability of spatial conformation of the individual elements of that class and / or Configurational Entropy (“Configuration Entropy”, Wiki).

A calculation (attempt) of the probability of being able to assemble N points respecting only the class symmetries leads to this theoretical distribution of mineral species, compared with the number of mineral species on Earth. Here down:



Theoretical calculation of geometric probabilities.



Experiment . Distribution of species on Earth.

For the extended development of the calculations, I refer to Appendices 6, 7 and 8.

3 - Conclusions

I have tentatively proposed a classification of the 32 classes which seems to me to be based on very precise geometric and physical properties.

In addition, the classification seems to be linked to the geometric probability of each class, where by geometric probability I mean the probability that N elements or points have the sole constraint of respecting the symmetries of the class, in particular the rotational symmetries .

I then showed that, indeed, the statistical distribution of mineral species on planet Earth seems to correspond to these concepts.

Probably aspects to possibly investigate.

4 - Acknowledgments

I would like to thank Eckhard Hitzer for his email comment after viewing my draft work, which has served me greatly as an encouragement to continue.

To : Giuliano Bettini, hestenes@asu.edu

Dear Giuliano,

I think you are definitely onto something.

Appendix 1

The dream. The shift of 432 from cubic to tetragonal

Cubic class 432 contains only rotational symmetries. No other symmetry, "center" or "mirror". For these reasons it is called "gyroidal".

The axes of symmetry are: -

four ternary axes passing through the opposite corners of the cube, making angles between them of $109^\circ 28'$ or $70^\circ 32'$;

-three quaternary axes at 90° between them, passing through the center of opposite faces of the cube;

- six binary axes (axes 2) passing through the opposite edges of the cube.

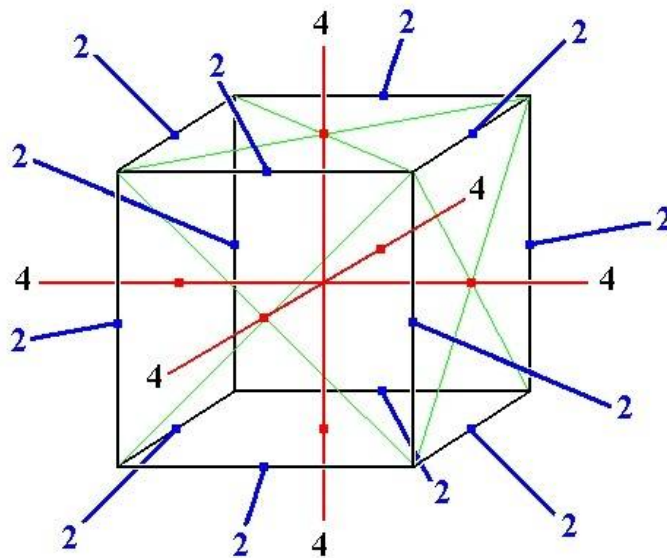


Figure 1. The ternary axes are not displayed, for the sake of clarity.

Having said that, what appeared to me in a dream or in my half-sleep was the following fact: -if in the tetragonal class 422 ($a = b$ but different from c) the "lateral" axes of symmetry A_2 become axes A_4 , then automatically the class becomes coincident with the gyroidal class.

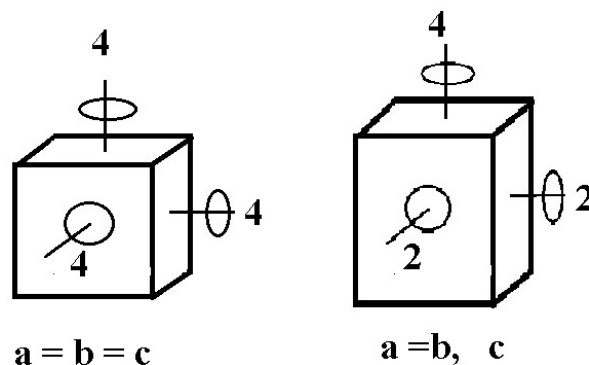


Figure 2. Cubic class 432 from cubic to tetragonal or vice versa

The reason why this banality is not usually accepted is that in crystallography the tetragonal system is defined as follows (see eg [2]) :
-one vertical axis (and only one) of symmetry 4.

If we accept the alternative definition of “a vertical axis of symmetry 4” (removing the constraint of only one), the displacement becomes legal.

On the other hand, equivalently, always in the definition of a tetragonal system, it is assumed that it must be:

$$a = b > c$$

or

$$a = b < c.$$

It is excluded that it can be $a = b = c$.

Therefore all parallelepipeds with $c < a, b$ or with $c > a, b$ are allowed, but the particular parallelepiped with $c = a, b$ is excluded.

It is clear that if all crystals with c even slightly less / greater than a, b are considered tetragonal, it is not clear why a crystal with c equal to a, b should be non-tetragonal.

The only reason would be if the crystal had a degree in crystallography.

But if the crystal does not have a degree in crystallography, he too thinks he is tetragonal.

This intuitively legitimate assumption subsequently appeared to me to be rigorous also from the mathematical point of view (see Appendix 3).

There is also another refined reason why intuition appears well placed.

One might think:

but then the cubic and tetragonal systems coincide?













This is not the case. The four remaining classes of the (true) cubic system not are characterized by axes 4.

In fact, among $23, m\bar{3}, 4_3m, m\bar{3}_m$ the first two (23 and $m\bar{3}$) does not have any axis 4.

What really characterizes the four classes of the cubic system is that they possess the ternary axes passing through the opposite corners of the cube (two are enough to generate all four).

Appendix 2.
The 32 crystal classes.

With the shift of 432 to tetragonal, the 32 classes become interpretable with two groups of 16, and subsequently with groups of 8 and 4 (Figure 3).

	 axis	 center	 m plane	 m + c
 No rotational symmetry	1 00000 0000c	1 ₋ 00001 0000c	m 00010 000m0	2/m 00011 000mc
 2	2 00100 00200	222 00101 0020c	mm2 00110 002m0	mmm 00111 002mc
 4	4 01000 04000	4 01001 0400c	4mm 01010 040m0	4/m 01011 040mc
 422	422 01100 04200	432 01101 0420c	4_2m 01110 042m0	4/mmm 01111 042mc
 3	3 10000 30000	3 ₋ 10001 3000c	3m 10010 300m0	3_2m 10011 300mc
 6	6 10100 30200	6 ₋ 10101 3020c	6mm 10110 302m0	6/m 10111 302mc
 62	62 11000 34000	622 11001 3400c	6_m2 11010 340m0	6/mmm 11011 340mc
 23	23 11100 34200	m3 ₋ 11101 3420c	4_3m 11110 342m0	m3_m 11111 342mc

16 senza bit3+altre 16 ripetute con il bit3=32

Figure 3 - The 32 classes arranged or "rearranged" in a table












The table has 8 rows and 4 columns, where the rows represent 8 groups, and the columns 4 crystal classes.

The numbering is 3-bit for the 8 lines, with the bits having the crystallographic meaning of 3, 4, 2 corresponding to the rotation axes A3, A4, A2, with some ambiguity for the meaning of bit 4.

Obviously, classes with the rotoinversion property, such as 4₋ or 6₋, do not have the axis property, but equally obviously the axis property intervenes to define the rotoinversion. The 4 columns are enumerated in 2 bits, having the crystallographic meaning "m" and "c", always corresponding with some residual ambiguity to the symmetries m "mirror plane" and c "center", centrosymmetry.

The new enumeration then divides the 6 (or 7) crystal systems into eight groups, where each group is characterized by a characteristic position of the axes of symmetry.

On the other hand, Nature seems to agree with this classification of eight groups of four, because the statistical distribution of the point groups in the minerals present on planet Earth [3] follows precisely this trend see Figure 4.

	 axes	 center	 m plane	 m + c
No rotational symmetry	1 00000 00000	1_ 00001 0000c	m 00010 000m0	2/m 01111 000mc
 2	2 00100 00200	222 00101 0020c	mm2 00110 002m0	mmm 00111 002mc
 4	4 01000 04000	4 01001 0400c	4mm 01010 040m0	4/m 01011 040mc
 4 2	422 01100 04200	432 01101 0420c	4_2m 01110 042m0	4/mmm 01111 042mc
 3	3 10000 30000	3_ 10001 3000c	3m 10010 300m0	3_2m 10011 300mc
 3 2	6 10100 30200	6_ 10101 3020c	6mm 10110 302m0	6/m 10111 302mc
 3 2 m	32 11000 34000	622 11001 3400c	6_m2 11010 340m0	6/mmm 11011 340mc
 3 2	23 11100 34200	m3_ 11101 3420c	4_3m 11110 342m0	m3_m 11111 342mc

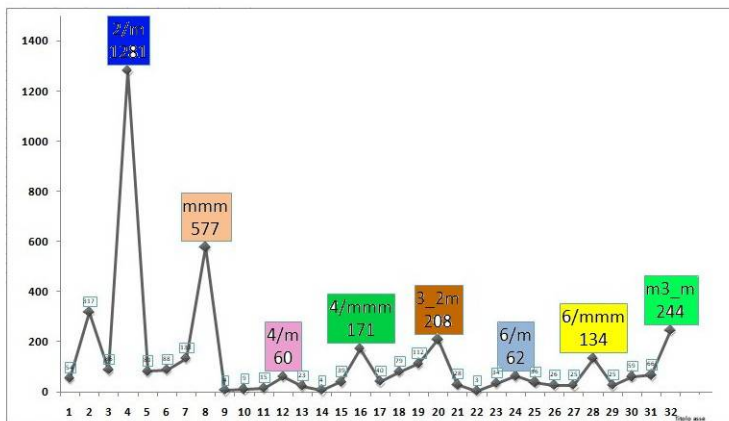


Figure 4 - Number of mineral species present in each point group

Here in color the holohedral class of each group is represented, that is the class with maximum symmetry, which coincides with the statistically most frequent class.

Evidently it appeared to me that all these "coincidences" could not be random.

Appendix 3

The 432 class as a “tetragonal” class.

In crystallography the symmetries of the 32 crystal classes or Point Groups are described by 3x3 matrices (Bilbao Crystallographic Server, [4]).

Precisely all the symmetries of a class are described by a set of matrices that represent the totality of the symmetries of the class.

This set of matrices in turn can be obtained from a limited number of basic matrices, or “generators”, which for subsequent products generate all and only the matrices of the set.

That said, it can be mathematically verified that the generators of the cubic class 432 can be obtained from “equivalent tetragonal generators”.

The proof is in Figures 5 and 6, which are obvious enough not to need explanations.

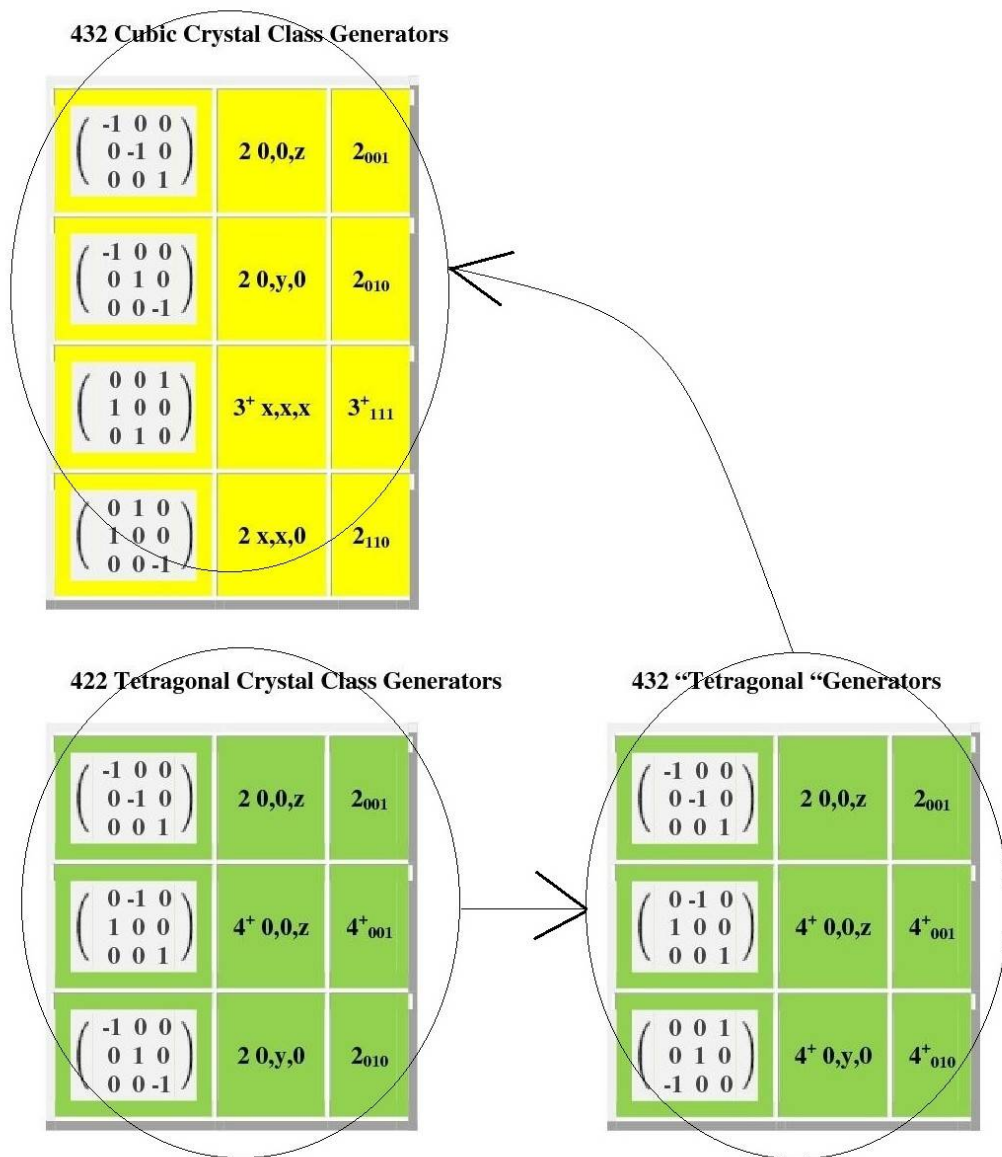


Figure 5.- Generators: how to go from 422 to 432 “tetragonal” and to 432 cubic.

432 "Tetragonal" Generators

$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$2\ 0,0,z$	2_{001}
$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$4^+ 0,0,z$	4^+_{001}
$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$	$4^+ 0,y,0$	4^+_{010}

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \times \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \times \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \times \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

432 Cubic Crystal Class Generators

$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$2\ 0,0,z$	2_{001}
$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$2\ 0,y,0$	2_{010}
$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$3^+ x,x,x$	3^+_{111}
$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$2\ x,x,0$	2_{110}

Figure 6.- Generators: mathematical equivalence between 432 "tetragonal" and 432 cubic.

Appendix 4

Bit 4 as a 90 ° rotation mathematical operator

A precise mathematical meaning can be assigned to bit 4.

I say that it must be identified with the presence or absence of a "90 ° rotation" mathematical operator. In fact, in all cases where it is not present, Nature has no possibility of using a "90 degree rotation". It is only possible to generate a "one-direction" axis which can be 0 °, or 180 °, or 120 °, or 60 ° > 120 ° & 180 °

zero

two

three

or six




No rotational symmetry	monohedron no symmetry 1 C1 00000
	sphenoid 2 C2 00200
	trigonal pyramid 3 C3 30000
	hexagonal pyramid 6 C6 30200

Figure 7 - Enantiometric classes (axes only) identifying the four lines without bit 4

Conversely, when bit 4 is available, Nature acts

(and to be precise it can be said, I think, that it acts on a pre-existing symmetry 2)

-or making it become 90 °

-or rotating the axis direction by 90 °.

Basically, a 90 ° operator acts either on the rotation symmetry (which becomes 90 °) or on the spatial direction of the symmetry axis (which can no longer be arranged parallel but at 90 °).


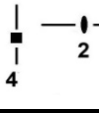
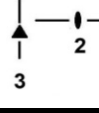
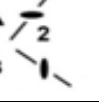
	tetragonal pyramid 4 C4 04000
	tetragonal trapezohedron 422 D4 04200
	trigonal trapezohedron 32 D3 34000
	tetartoid 23 T 34200

Figure 8 - Enantiometric classes (axes only) identifying the four lines with bit 4

So bit 4 includes (but is not limited to) the crystallographic meaning of tetragonal axis of symmetry A4.

Explicitly:

- the presence of axis (s) A4 involves bit 4;
- but bit 4 does not necessarily imply the presence of a crystallographic axis A4.

Appendix 5
Mathematical digression.

In short: this last property of pyroelectricity is evidently a geometric property, that is, linked to the symmetries of the 32 crystal classes or Point Groups.
But it is equally evidently a physical property.

In this sense, an excerpt that I quote from [5] is illuminating.

.....

1.3 Symmetry of physical properties

In determining the effect of symmetry on physical properties, there are four symmetries to be considered: (1) the symmetry of the material, (2) the symmetry of the external forces, (3) the symmetry of resulting change or displacement, and (4) the symmetry of the physical property relating displacement to external force. Here we are using the terms force and displacement in the general sense to include electric, magnetic, and thermal quantities as well as mechanical effects. All materials — whether crystalline or not — show some kind of symmetry. Single crystals have symmetry belonging to one of the 32 crystal classes (Chapter 3). Ferromagnetic, ferrimagnetic, and antiferromagnetic crystals exhibit long-range magnetic order. Additional symmetry groups involving time reversal operators are used to describe magnetic structures (Chapter 14). (and pyroelectricity too, ed)

.....

It's still:

5.5 Neumann's Principle

The most important concept in Crystal Physics is Neumann's Principle that states: "The symmetry of any physical property of a crystal must include the symmetry elements of the point group of the crystal ". The proof of Neumann's Principle is common sense.

.....

It's still:

But the reverse is not true, for the symmetry of the physical property may be much higher than that of the point group.

.....

Put simply: there are geometric symmetries (those of classical crystallography) and physical symmetries. The latter obviously include the former, and must be consistent with them, but they are more general.

Well, I believe, and in this I think I am an easy prophet, that the classification proposed by me will find its definitive mathematical arrangement through more complex symmetries, describing geometric and physical properties of crystals, and some of which properties are probably not yet sufficiently deepened.

Such are, for example, the symmetries related to pyroelectricity, as I will now try to show.

The property represented by bit c (which I have called a sort of "generalized center") is actually a geometric property, a symmetry which, however, is not pertinent to a single 3x3 matrix, the "inversion" -1 matrix, but is represented by set of all symmetry matrices (General Positions, [4]).

In this way.

The n symmetry matrices M_i of a certain class ensure that any point of the crystal is indissolubly linked to others (n-1) for a total of n points linked by symmetry.

Now for the non-Pyro classes it is verified that the sum of all n symmetry matrices is equal to zero.

$$\sum_{i=1}^n M_i = 0$$

which entails

$$\left(\sum_{i=1}^k M_i \right) + \left(\sum_{i=k+1}^n M_i \right) = 0$$

that is

$$\left(\sum_{i=1}^k M_i \right) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \left(\sum_{i=k+1}^n M_i \right)$$

This is equivalent to the following geometric property:

taken all the n points linked by symmetry, any point or sum of k points located in x, y, z has as its counterpart the sum of the remainder that is located in -x, -y, -z.

More specifically, taking half of the n points, the resultant of which is in a point with coordinates x, y, z, the sum of the remaining half points is located in -x, -y, -z.

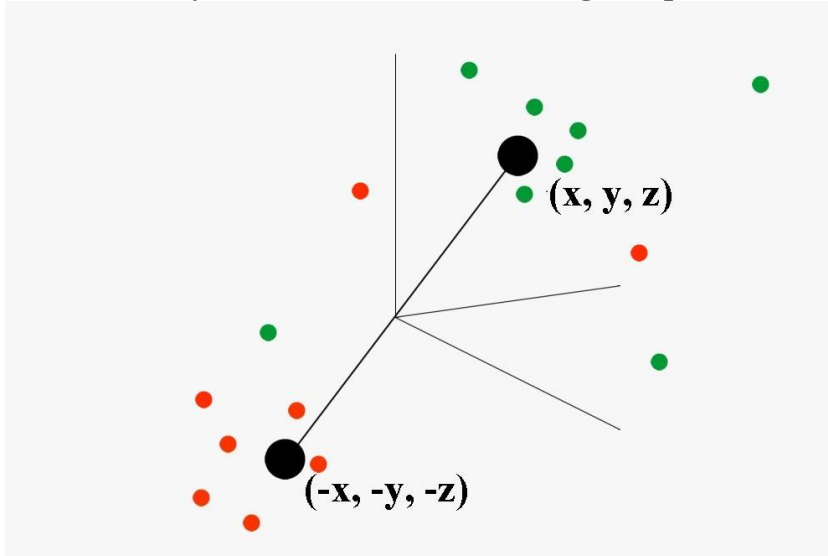


Figure 9 - Centrosymmetric cluster of points

So the problem to have centrosymmetric clusters of points is trivially solved for all classes that have n zero-sum symmetry matrices. This is a "generalized centrosymmetry".

Please note that this result is automatic for all truly centrosymmetric crystals, because the matrix (-1) appears among the symmetry matrices M_i , so that all matrices appear with a double sign and cancel each other out.

Appendix 6

With simple hypotheses, I try to establish a connection between the symmetry matrices and the number of mineral species that are formed.

6.1 – Relative frequency of each of the 8 group

Premise.

Without mathematically boring, I affirm without justification that an examination and reorganization of the Generators of the various groups show the following:

for each of the 8 groups the sequence 00 (axes only) 0c (center) m0 (mirror) mc (center + mirror) is confirmed .

That said, let's proceed.

From [4] , Wyckoff Position (max) is the maximum number of points connected in symmetry, and coincides with the number of symmetry matrices (General Positions).

It is therefore the number of points necessarily connected by symmetry in each of the 32 Classes and is summarized here following the order of the 8-row and 4-column table :

1 2 2 4

2 4 4 8

4 4 8 8

8 24 8 16

3 6 6 12

6 6 12 12

6 12 12 24

12 24 24 48

The first column concerns the Classes with "axes only", and indicates the number of points necessarily connected by the symmetries that the axes impose (here indicated in black).

1 1 1_ m 2/m

2 2 222 mm2 mmm

4 4 4_ 4mm 4/m

8 422 432 4_2m 4/mmm

3 3 3_ 3m 3_2m

6 6 6_ 6mm 6/m

6 32 622 6_m2 6/mmm

12 23 m3_ 4_3m m3_m

I can now draw the number of mineral species that are formed.

I take and compose the N chemical elements available (hydrogen silicon aluminum iron or gold etc.) and package them .

In composing them, that is, to compose each group, each of them must respect the symmetries that the axes impose. Therefore, in the construction of each group, the elements must first of all position themselves respecting the 1 2 4 8 3 6 6 12 positions that are obliged, as required by the General Positions of the generators of the group (i.e. the symmetries imposed by the axes). For example in group **1 1_ m 2/m** one can start from 1 element taken anyway, because it is not linked to others by any symmetry. In group **2 222 mm2 mmm** the elements must respect in pairs obliged reciprocal positions. In group **3 3_ 3m 3_2m** there are forced triplets. Etc.

So neglecting precise calculations, combinatorics , etc. , to estimate the number of possible compounds (starting from X elements available), I have the following situation:
for example I can form the second group starting from X / 2 pairs , because with X elements I form X / 2 pairs;

I can form the fifth group starting from X / 3 triplets , because with X elements I form X / 3 triplets;

instead the first group with X elements involves X different cases.

Etc.

It follows that the compounds of 1 are more numerous than those of 2 etc etc.

Therefore the number of compounds that can be formed for the various groups lies in the following ratios:

$$1000/1 = 1000$$

$$1000/2 = 500$$

$$1000/4 = 250$$

$$1000/8 = 125$$

$$1000/3 = 333$$

$$1000/6 = 167$$

$$1000/6 = 167$$

$$1000/12 = 83$$

How do the four classes 00, 0c, m0, mc of each group behave?

6.2 - Number of minerals in each class of each group

Given the points connected by symmetry in each class of each group , I assume that the compounds are made in the following manner.

I elaborate.

With "axes only" let x the number of points connected by symmetry.

Let's try to understand, starting from the symmetries "axes only", which and how many are the symmetries introduced by bit c and then from bit m, and then by bits mc.

This number, starting from x, if the center symmetry is introduced, will become 2x (because the " connected " points will double).

Likewise, again starting from x "axes only", the number will become 2x if the symmetry m plane is introduced (intuitively, because the points will double).

If then, from 0c center symmetry and 2x connected points, we introduce the further m plane symmetry , we can assume that the 2x points double and become 4x.

Similarly from m0 plane symmetry and 2x connected points, if we introduce the further center symmetry , we can assume that the 2x points double and become 4x.

So

the intuitively predictable number of bonds or connected points or symmetries will be like:

x 2x 2x 4x

To draw the number of mineral species I assume this number proportional to the square 1 4 4 16 of the bonds x 2x 2x 4x. From here the number of minerals that are formed in each class of each group , which is in the relative frequency

6 25 25 100 .

Overall I have the following number of mineral species:

1000/1 = 1000 60 250 250 1000

1000/2 = 500 30 125 125 500

1000/4 = 250 15 62 62 250

1000/8 = 125 8 31 31 125

1000/3 = 333 20 83 83 333

1000/6 = 167 10 42 42 167

1000/6 = 167 10 42 42 167

1000/12 = 83 5 21 21 83

6.3 - Graph of the number of mineral species

The final result is the following graph.

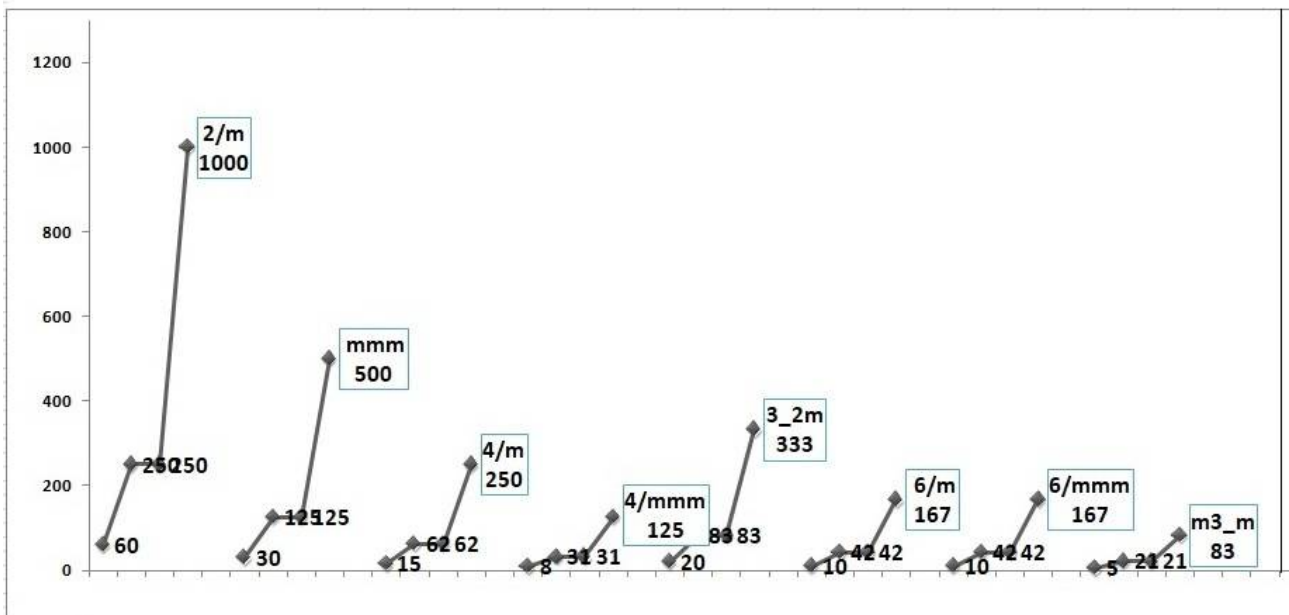


Figure 10 - Plot of mineral species under the previous assumptions

In comparison the terrestrial mineral species.

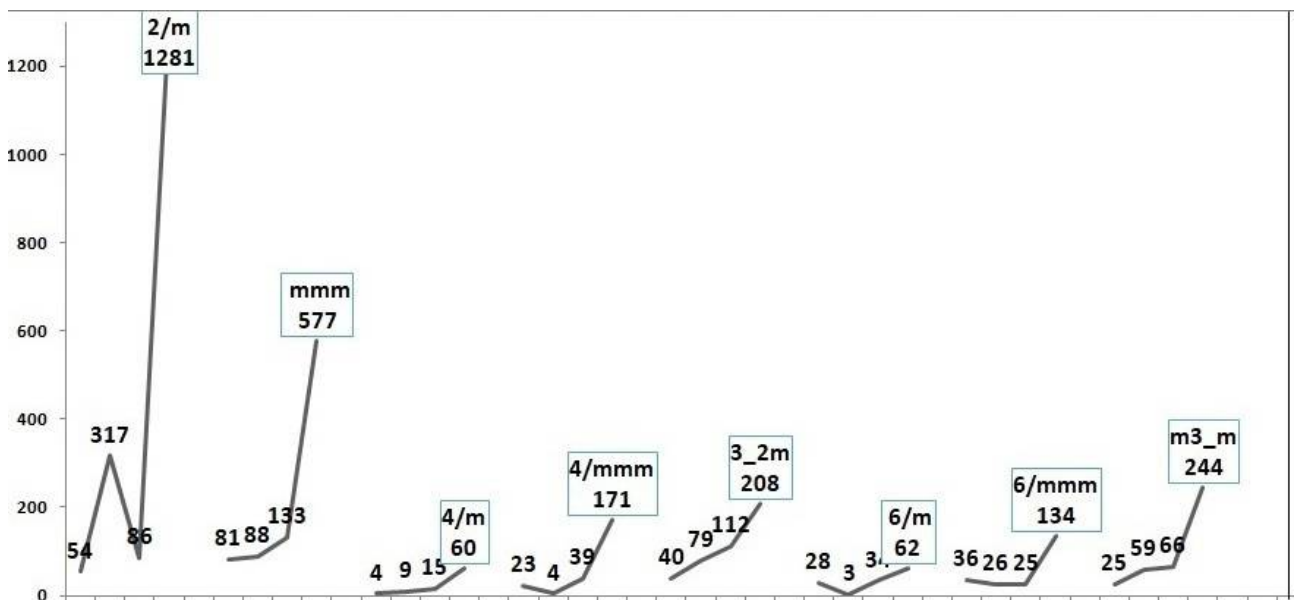


Figure 11 - Number of mineral species currently known on Planet Earth.

Appendix 7

The assumptions of the previous Appendix allow to build an interesting model, but with some oddities, for example the trend is decreasing proceeding from classes 6/m and 6/mmm to m3_m. But I would like to reiterate, if necessary, that at this moment I am not able to calculate the probabilities of each class and the link, if any, between the symmetry matrices and the probabilities of each class. I can try to make different hypotheses .

I start from the following observation (Appendix 6 , paragraph 6.1):

" in the construction of each group, the elements must first of all position themselves respecting the 1 2 4 8 3 6 6 12 positions that are obliged, as required by the General Positions of the generators of the group (i.e. the symmetries imposed by the axes)".

The symmetries imposed by the axes can be simplified as in figure 12 in which I make the following hypotheses :

1-in the Tetragonal Low & High groups an axis 4 is imposed and I can form $1000/4 = 250$ compounds in all;

2-in the Hexagonal Low & High groups an axis 6 is imposed and I can form a total of $1000/6 = 166$ compounds;

2-in the Isometric group (which can be characterized with $A3 + A2$, see Appendix 8 for those who do not believe it) 6 points are imposed and I can form a total of $1000/6 = 166$ compounds.






Group	Common Axes	P probability
No axes	No rotational symmetry	A1 $1000/1 = 1000$
Binary-Axis 2		A2 $1000/2 = 500$
Tetragonal low		A4 $1000/4 = 250$
Tetragonal high		
Trigonal		A3 $1000/3 = 333$
Hexagonal low		A6 $1000/6 = 166$
Hexagonal high		
Isometric		$A3 + A2$ $1000/6 = 166$

Figure 12 - Symmetries and probabilities imposed by the axes .

To divide the 250 mineral species between 4/m and 4/mmm I observe that in 4/m the symmetry matrices are 8 while in 4/mmm they are 16 [4] . This doubling is compatible with the introduction of bit 2, which reasonably doubles the number of connected points from 1 to 2. The number of mineral species I assume that it is distributed proportionally to the square , 1:4, and therefore the mineral species become 50 in 4/m and 200 in 4/mmm. Similarly, to divide the 166 mineral species between 6/m and 6/mmm I observe that in 6/m the symmetry matrices are 12 while in 6/mmm they are 24 [4] . Reasoning as in the previous case, the 166 mineral species are divided in the ratio 1: 4 and become 33 and 133.

All the remaining assumptions are the same as in Appendix 6.

Overall I have the following number of mineral species:

1000/1 = 1000 60 250 250 1000

1000/2 = 500 30 125 125 500

1000/4 = 250 | 50 3 12 12 50
 | 200 12 50 50 200

1000/3 = 333 20 83 83 333

1000/6 = 166 | 33 2 8 8 33
 | 133 8 33 33 133

1000/6 = 166 10 41 41 166

from which the graph:

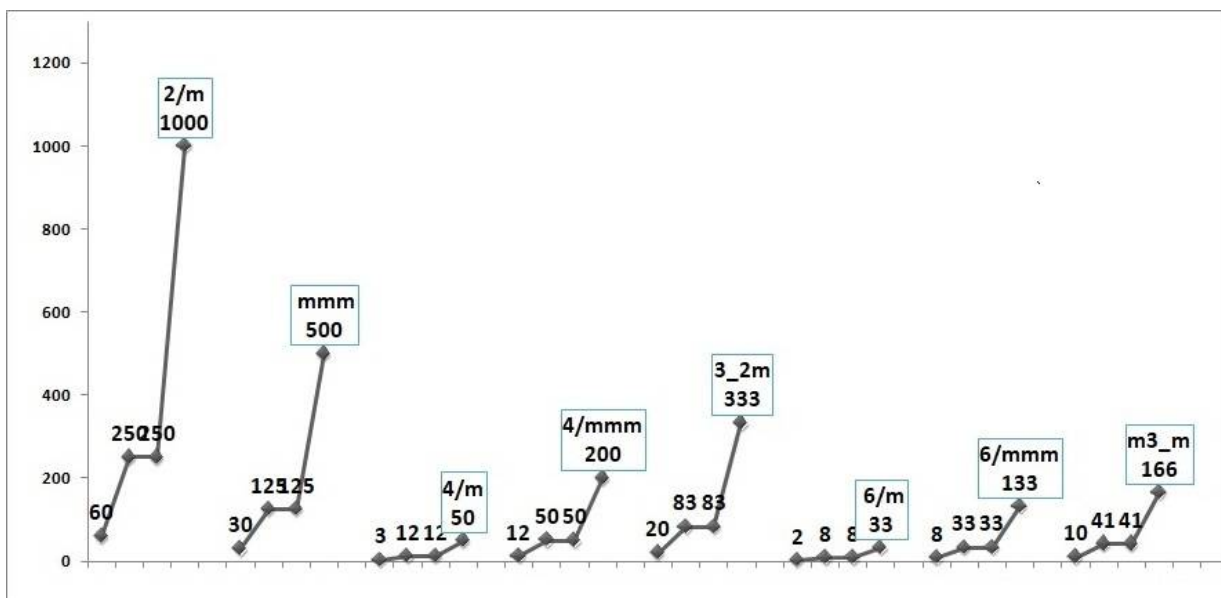


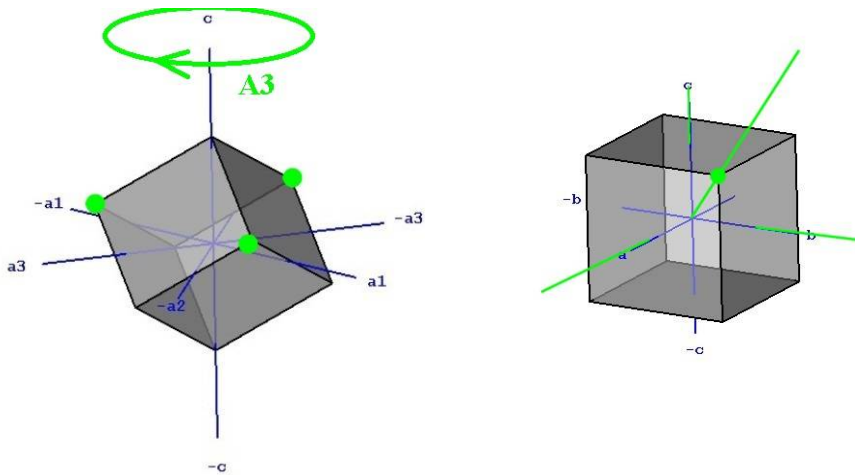
Figure 13 - Plot of mineral species under the previous assumptions.

Appendix 8
On the Generators of the Isometric Group.

The rotational symmetries of the Isometric group are not usually a single axis A3 and a single axis A2, because the generators are not chosen in this way [4], nor is the reference system chosen in this way. But I can try to look at the facts beyond convention, and the facts are:

can a single axis A3 and a single axis A2 suffice?

First of all, I can think of Isometrics in an (unusual) trigonal reference (Hexagonal Axes)



Seen in the “cubic” reference (Cartesian Orthogonal) let $3x, x, x$ and (for example) $20, y, 0$ the appropriate matrices A3 and A2.

So these:

1)

$$3x, x, x = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

2)

$$20, y, 0 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

I can multiply them together as follows:

$$(3x, x, x)X(20, y, 0) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = (3x, -x, -x)$$

$$(3x, x, x)X(3x, x, x) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = (3^{(-)}x, x, x)$$

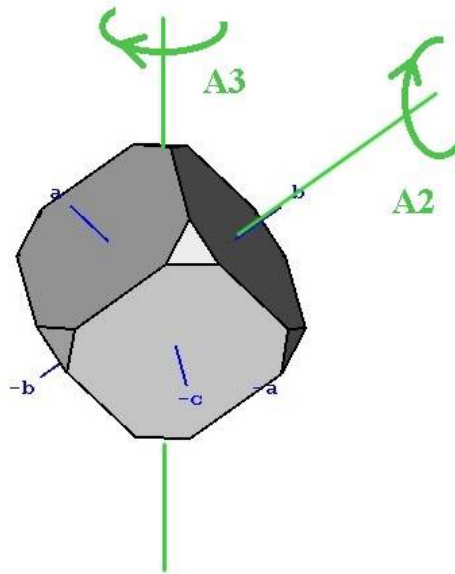
$$(3x, -x, -x)X(3^{(-)}x, x, x) = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \mathbf{20,0,z}$$

As you can see, with them you can make various products and you get 20,0,z. (Note: 3 means A3, while 3 ^ (-) means A3 in the opposite sense).

So actually 3x, x, x and 20, y, 0 are enough to have all the generators of the "axes only" class 23, which are as foreseen by Bilbao 3x, x, x 20, y, 0 20,0, z. For subsequent introduction of the symmetries c, m and then mc we arrive at the holohedry m3_m.

So actually the holohedry m3_m and the whole Isometric group can be characterized simply with two suitably directed rotations A3 and A2, plus the symmetries m and c.

The appropriate rotations are these:



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