

# Author

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# Title

Spherical Harmonics and Crystals

# Abstract

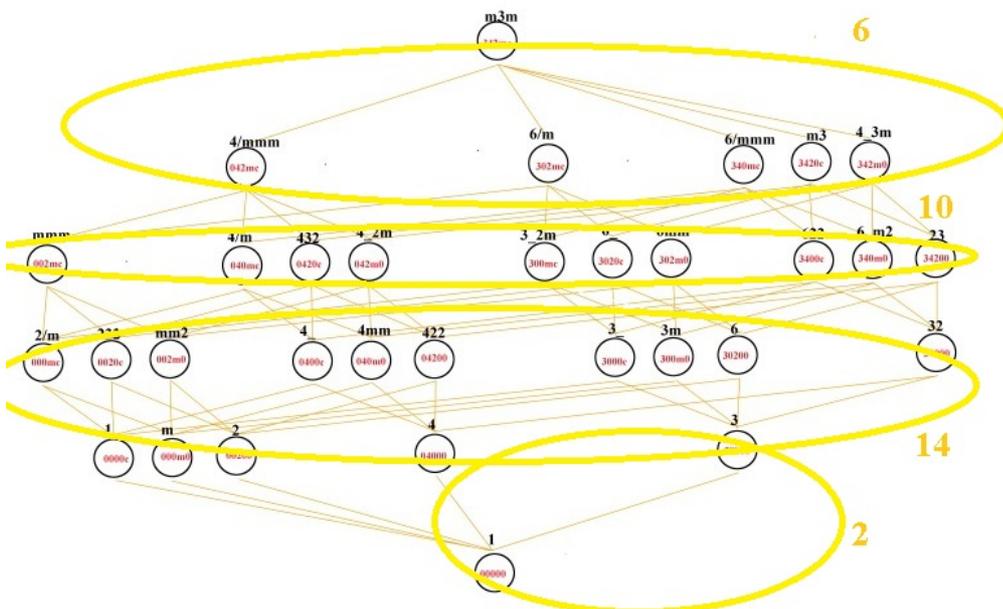
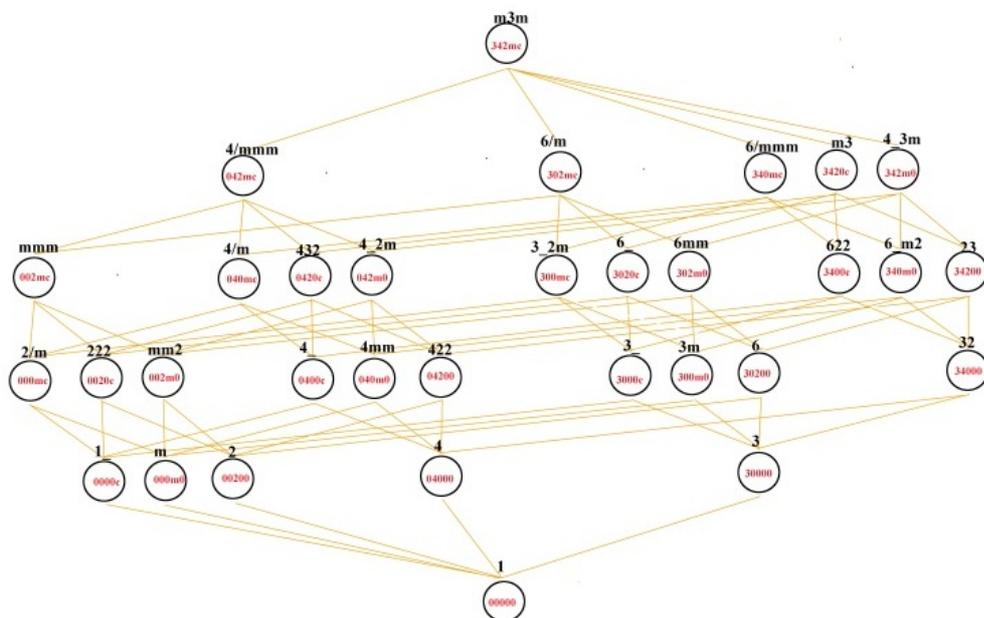
The description of Point Groups is made in crystallography, among other, with "character tables". Following my classification work entitled "5 bit 32 crystal classes" and some other curious properties I've noticed, I wanted to try to find a representation with Spherical Harmonics namely: a set of 32 Spherical Harmonics each one representing a Point Group. So the purpose of this work, in a nutshell, is to combine each of the 32 crystal classes with the corresponding Spherical Harmonic that has the same symmetry properties, in a certain sense therefore a "group description".

These are among all the Spherical Harmonics the only 32 with which it is possible to create periodic structures with no gaps nor overlapping. A sort of Spherical Harmonics Restriction Theorem. Other possibly interesting connections with the s p d f sub-shells, and with spin, are to be investigated.

# Premise

All this started out by pure chance when , downstream of my works [1] [2] , I came across curious coincidences.

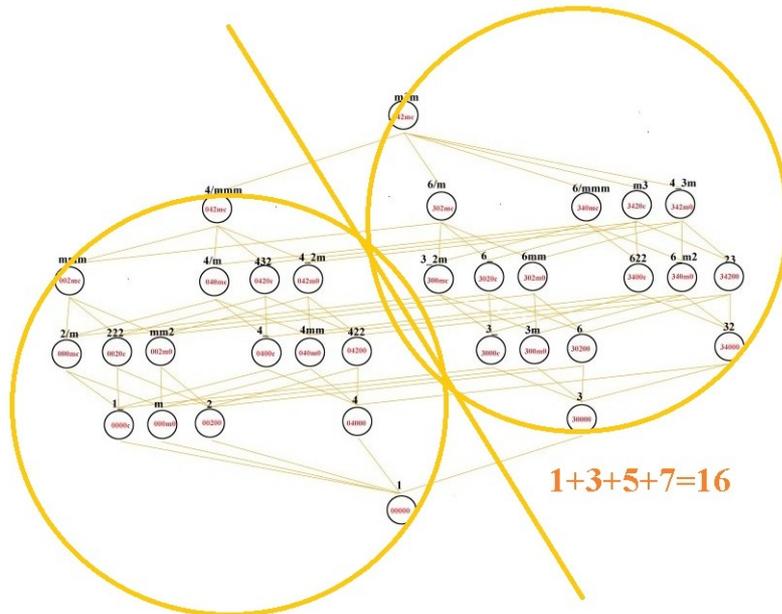
My proposed classification of the 32 crystalline classes with 5 bits suggested, on a diagram where the number of 'on' bits subsequently appears (0 in the first line, 1 in the second, ..., up to 5 in the last), a numerical analogy with the electrons in the sub shells (2, 6, 10, 14 or 1,3,5,7).



Faced with this fact, I started to think about possible hidden meanings.

Subsequently and over time I was struck by the fact that with both harmonics and the 5-bit scheme this "32" did not appear as a 32 but as a 16 + 16, repeated twice as if it were always " due of a double state of spin " .

Thinking about the analogy with electronic orbits 1 3 5 7 or 2 6 10 14 >> 32 I wondered what could be the reason for such a subdivision . And what the subdivision should be. This? Other? And with what criteria?



$16+16=32$

I would have to find, I told myself, a correspondence between these schemes.

- 0
- 1 0 1
- 2 -1 0 1 2
- 3 -2 -1 0 1 2 3

```
0000 0001 0010 0011
0100 0101 0110 0111
1000 1001 1010 1011
1100 1101 1110 1111
```

The first represents the usual subdivision of the first 16 harmonics with  $l = 0,1,2,3$  .  
 The second with the bits classifies the crystal classes in groups of four, here the first  $4 \times 4 = 16$  classes (for which evidently 4 bits are enough)

.

It is a question of reconciling this

-0  
 -1 0 1  
 -2 -1 0 1 2  
 -3 -2 -1 0 1 2 3

	<b>m=-3</b>	<b>m=-2</b>	<b>m=-1</b>	<b>m=0</b>	<b>m=+1</b>	<b>m=+2</b>	<b>m=+3</b>
<b>l=0</b>							
<b>l=1</b>							
<b>l=2</b>							
<b>l=3</b>							

with (for example) this

0000 0001 0010 0011  
 0100 0101 0110 0111  
 1000 1001 1010 1011  
 1100 1101 1110 1111

1	1_	m	2/m
2	222	mm	mmm
4	4_	4mm	4/m
422	432	4_2m	4/mmm
3	3_	3m	3_2/m
6	6_	6mm	6/m
32	622	6_m2	6/mmm
23	m3	4_3m	m3m

where here one of the groups in green is to be moved to blue.

But again, what subdivision, and why?

Leaving aside numerous other arguments and speculations, it became clear to me that in any case the examination of Spherical Harmonics was going into greater detail. It also appeared to me that the problem could be stated in more limited but clearer terms:

find a one-to-one correspondence, if any, between the Spherical Harmonics and the 32 Crystallographic Point Groups.

Such as?

Simple. Based on the imposition that, one by one, enjoyed the same symmetries.

# Names of Spherical Harmonics

The harmonics, Complex Spherical Harmonics, and the real and imaginary parts 'Real Harmonics', are defined and partly tabulated in various places eg. Wiki etc. [3] [4].

Premise: since with Word I can put the indices  $l, m$  only horizontally, then I use the writing  $(l, m)$  only for the real harmonics, and then when I write  $Y(l, m)$  I refer to the real harmonics.

Symmetry  $m$   
summarize  
my plane

Matrix ...  
$$\begin{matrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{matrix}$$

Meaning : plane  $m$  perpendicular to the  $y$  axis .

Vertical plane  $xz$  perpendicular to  $y$ , then in the drawing, on the  $xy$  plane, it appears as an axis  $x$ .

The symmetry  $m$  is conventionally understood as symmetry with respect to this axis and therefore precisely respect to a change of the  $y$  coordinate.

How can we study the symmetries of Spherical Harmonics? (I repeat: real) .

Premise

These, the real spherical harmonics, are defined by the complex and are indexes  $l, m$ , written  $Y(l, m)$

They are practically the real and imaginary parts of the complex .

In this way:

The  $Y(l, +m)$  are the Re part

The  $Y(l, -m)$  are the Im part.

Now to clarify this happens: the Spherical Harmonics complex, whether they are indexes  $(l, +m)$  or  $(l, -m)$ , have the same real part. And instead they have an imaginary part Im with the opposite sign. So when it is said that the real Spherical Harmonics  $Y(l, m)$  correspond to the real and imaginary part of the complex what is meant? Means:

real part of  $(l, +m)$

and also

imaginary part of  $(l, +m)$ .

Having said that, since the  $Y(l, -m)$  always start with the  $\sin(\phi)$  that is, with  $y = \sin(\phi)$  it follows that they are odd with  $y$  .

Namely

they change sign from  $+$  to  $-$  when  $y$  changes from  $+$  to  $-$  and therefore they cannot be  $m$ -symmetric.

The  $m$  symmetrical are the  $Y(l, +m)$ , the real parts Re.

Which in the graphs appear to be even across the  $x$ -axis.

Links to graphs and formulas in [3] [4] .

**Example:**

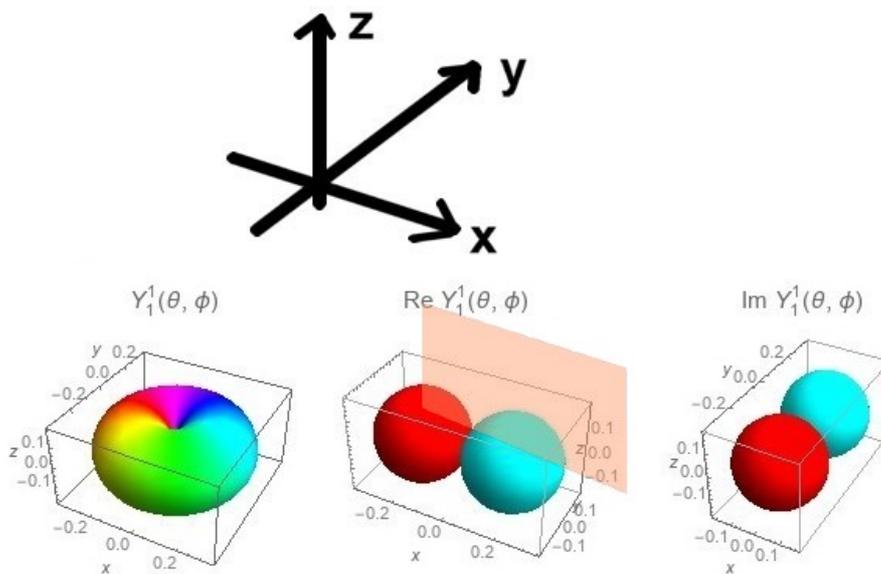
Y (1,1) even with respect to the x axis

Formula

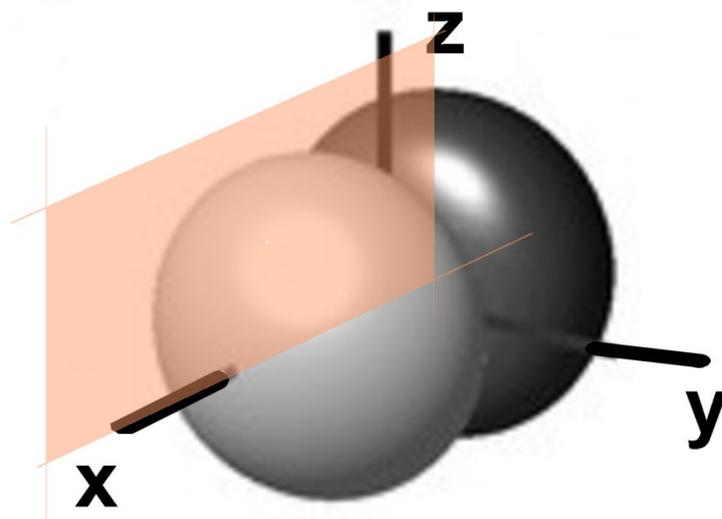
$$Y_{1,1} = p_x = \sqrt{\frac{1}{2}} (Y_1^{-1} - Y_1^1) = \sqrt{\frac{3}{4\pi}} \cdot \frac{x}{r}$$

(with a change of y it does not change sign).

Graph



Of course the axes are sometimes drawn differently, each one draws the axes as they like and of course does not say which way. Here I 'strengthened' the x axis to make it see better. I also drew the symmetry plane myself.



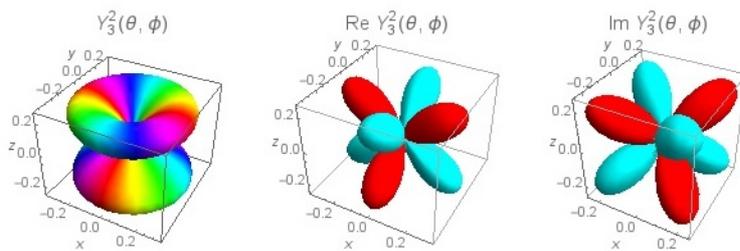
**Another example:**

**Y (3,2)**

**Formula**

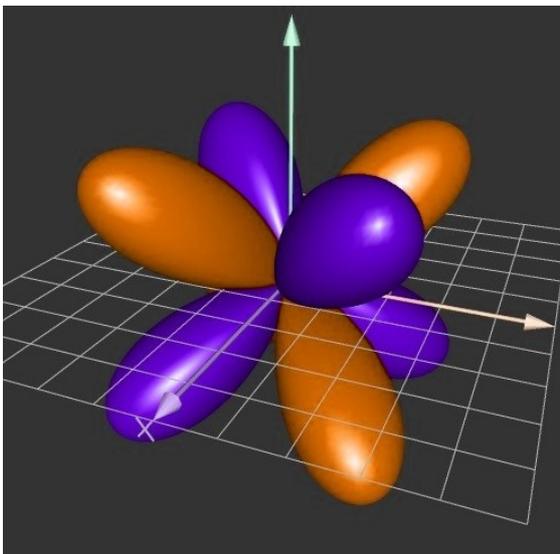
$$Y_{3,2} = f_{z(x^2-y^2)} = \sqrt{\frac{1}{2}} (Y_3^{-2} + Y_3^2) = \frac{1}{4} \sqrt{\frac{105}{\pi}} \cdot \frac{(x^2 - y^2) z}{r^3}$$

**Graph**



**This author puts the 'x-axis (almost) parallel to the sheet.**

**Instead this other author puts the x-axis coming out of the sheet. .... Here is the harmonic Y (3, -2). As you can see, it is odd compared to a change of the y coordinate.**



# Formulas and symmetries of harmonics and groups

Now I try to start a grid search. With logic 1 3 5 7.  
And these will be the 16 groups from which to start

1	1_	m	2/m
2	222	mm	mmm
4	4_	4mm	4/m
422	432	4_2m	4/mmm
3	3_	3m	3_2/m
6	6_	6mm	6/m
32	622	6_m2	6/mmm
23	m3	4_3m	m3m

with one of the groups in green to be moved in blue.

The Spherical Harmonics, for each type of rotation example A3, have here in the table 4 point groups or crystal classes if you prefer. There must be 4 groups with  $m = 3$ . Therefore they must or may be 3.3 and 3, -3 and then 4.3 and 4, -3. And continuing along this path, there are two more at each step, 5.3 and 5, -3, then 6.3 and 6, -3 etc. The same applies to every other rotation. So let's try. Formulas from <http://www.quanty.eu/QuantyDocsu2.php>

$$3,3 \ x(x^2 - 3y^2)$$

$$3,-3 \ y(y^2 - 3x^2)$$

e

$$4,3 \ xz$$

$$4,-3 \ yz(y^2 - 3x^2)$$

Y(5,3) e Y(5,-3) give:

$$5,3 \ x(x^2 - 3y^2)(x^2 + y^2 - 8z^2)$$

$$5,-3 \ y(y^2 - 3x^2)(x^2 + y^2 - 8z^2)$$

But I immediately observe that these, in terms of symmetries, will give the same result of respectively 3.3 and 3, -3.

It is worth trying also with the A4 rotation.

$$4,4 \ (x^4 - 6x^2y^2 + y^4)$$

$$4,-4 \ xy(x - y)(x + y)$$

then

$$5,4 \ z(x^4 - 6x^2y^2 + y^4)$$

$$5,-4 \ xyz(x - y)(x + y)$$

And finally

$$6,4 \ (x^4 - 6x^2y^2 + y^4)(x^2 + y^2 - 10z^2)$$

$$6,-4 \ xy(x - y)(x + y)(x^2 + y^2 - 10z^2)$$

Also here 6,4 and 6, -4 reproduce the symmetries of, respectively 4,4 and 4, -4.

**I also enter the A2 rotation**

**2,2**  $(x - y)(x + y)$

**and**

**2,-2**  $xy$

**then**

**3,2**  $z(x - y)(x + y)$

**and**

**3,-2**  $xyz$

**and finally**

**4,2**  $(x - y)(x + y)(x^2 + y^2 - 6z^2)$

**e**

**4,-2**  $xy(x^2 + y^2 - 6z^2)$

**Again, 4,2 e 4,-2 look like repetitions.**

**I also write four A1 rotations.**

**1,1**  $x$

**and**

**1,-1**  $y$

**then**

**2,1**  $xz$

**and**

**2,-1**  $yz$

**then**

**3,1**  $x(x^2 + y^2 - 4z^2)$

**and**

**3,-1**  $y(x^2 + y^2 - 4z^2)$

**As usual, two apparently useless groups.**

Then we notice other strange 'symmetrical' behaviors so to speak, for example A3 reproposes certain behaviors of A1, and so does A4 with A2. Oh well.

I also enter the A6 rotation.

$$6,6 (x^6 - 15x^4y^2 + 15x^2y^4 - y^6)$$

and

$$6,-6 xy(3x^4 - 10x^2y^2 + 3y^4)$$

Then I should go on with Y (7,6) etc. but I do not have the data.  
But I suppose, by symmetry, that they are of the type:

$$7,6 z(\dots)$$

and

$$7,-6 xyz(\dots)$$

with the parenthesis ....invariant for symmetries 2,3, m, c.

Then, it seems for symmetry reasons, I also suppose that 8.6 and 8, -6 reproduce the symmetries of 6.6 and 6, -6.

Let's go on.

Let's move on to the symmetries of the groups and then to the comparison with the Spherical Harmonics .

We summarize the symmetries of the groups . Generators from [5] .

Hermann Mauguin	5 bit symbols	Generators	Generators modificati	Real Harmonics Y(l,m)
1	00000			
1_	0000c	c	c	
m	000m0	my	my	
2/m	000mc	2y,c	my,c	
2	00200	2y	2z	
222	0020c	2z, 2y	2z, 2y	
mm2	002m0	2z, my	2z, my	
mmm	002mc	2z, 2y, c	2z, my, c	
4	04000	4z	4z	
4_	0400c	4z_	(4z&c)	
4mm	040m0	4z, my	4z, my	
4/m	040mc	4z, c	4z, my,c	
422	04200	2y, 4z	4z, 2y	
432	0420c	2z, 2y, 3111,2110	4z, 2y, 4y	
4_2m	042m0	4_, 2y	(4z&c), 2y, m110	
4/mmm	042mc	2y, 4z, c	4z, 2y, m110, c	
3	30000	3z	3z	
3_	3000c	3z, c	3z, c	
3m	300m0	3z, m110	3z, m110	
3_2/m	300mc	3z, 2(1-10), c	3z, m1-10, c	
6	30200	3z, 2z	3z, 2z	
6_	3020c	mz, 3z	((3z, 2z) &c)	
6mm	302m0	3z, 2z, m110	3z, 2z, m110	
6/m	302mc	3, 2z, c	3z, 2z, m001, c	
32	34000	3z, 2(1-10)	3z, 2(1-10)	
622	3400c	3z, 2z, 2(110)	3z, 2(1-10), 2z	
6_m2	340mc	3z, mz, m110	3z,2(1-10), m110	
6/mmm	340mc	3z, 2z, m(110),c	3z,2(1-10), m110, c	
23	34200	2z, 2y, 3111	2z, 2y, 3111	
m3	3420c	2z, 2y, 3111,c	2z, 2y, 3111,c	
4_3m	342m0	2z, 2y, 3111,m(1-10)	2z, 2y, 3111,m(1-10)	
m3m	342mc	2z, 2y, 3111,2110,c	2z, 2y, 3111, m(1-10),c	

I try the A3 rotations. I try to make an attempt to see if with the Spherical Harmonics I can represent the 4 groups of the following table(hypothesis ...). To adequately represent the symmetries of the groups ('generators') I would say that I can use the matrices here in the table .

Note that with the planes of symmetry we are distant from the rules of crystallography but I believe that the my plane suffices.

Hermann Mauguin	5 bit symbols	Generators	Generators modificati	Matrici
3	30000	3z	3z	3z
3 <sub>-</sub>	3000c	3z, c	3z, c	..... 3z... -1 0 0 0 -1 0 .... 0 0 -1
3m	300m0	3z, m110	3z, my	1 0 0 3z...0 -1 0 0 0 1 ... ....
3 <sub>2</sub> /m	300mc	3z, 2(1-10), c	3z, my, c	1 0 0 3z...0 -1 0 0 0 1 ... -1 0 0 .... 0 -1 0 0 0 -1 ....

These are therefore the symmetry matrices that represent the groups above.

Let's try the symmetries of Spherical Harmonics now . m=3. Note that the A3 symmetry is certainly respected for all Spherical Harmonics , since there appears exp (+/- i3phi).

First try.

Harmonic Y (3,3).

$$3,3 x(x^2 - 3y^2)$$

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
Asse/assi di rotazione	Rotazione A3	X	
x,y,z > x,-y,z	Piano xz di simmetria lungo l'asse x	X	
x, y, z > -x, -y, -z	inversione risp. centro		X

$$3, -3 y(y^2 - 3x^2)$$

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
Asse/assi di rotazione	Rotazione A3	X	
$x, y, z > x, -y, z$	Piano xz di simmetria lungo l'asse x		X
$x, y, z > -x, -y, -z$	inversione risp. centro		X

$$4, 3 xz$$

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
Asse/assi di rotazione	Rotazione A3		
$x, y, z > x, -y, z$	Piano xz di simmetria lungo l'asse x	X	
$x, y, z > -x, -y, -z$	inversione risp. centro	X	

$$4, -3 yz(y^2 - 3x^2)$$

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
Asse/assi di rotazione	Rotazione A3	X	
$x, y, z > x, -y, z$	Piano xz di simmetria lungo l'asse x		X
$x, y, z > -x, -y, -z$	inversione risp. centro	X	

Interesting. It seems that we are in the simple rules of my paper "5 bit etc ...".

00 0c m0 mc .

Now let's try the situation with axis 2. That is these crystal classes:

Hermann Mauguin	5 bit symbols	Generators	Generators modificati
2	00200	2y	2z
222	0020c	2z, 2y	2z, 2y
mm2	002m0	2z, my	2z, my
mmm	002mc	2z, 2y, c	2z, my, c

$$2,2 (x - y)(x + y)$$

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
Asse/assi di rotazione	Rotazione A2	X	
$x,y,z > x,-y,z$	Piano xz di simmetria lungo l'asse x	X	
$x, y, z > -x, -y, -z$	inversione risp. centro	X	

$$2,-2 xy$$

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
Asse/assi di rotazione	Rotazione A2	X	
$x,y,z > x,-y,z$	Piano xz di simmetria lungo l'asse x		X
$x, y, z > -x, -y, -z$	inversione risp. centro	X	

$$3,2 z(x - y)(x + y)$$

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
Asse/assi di rotazione	Rotazione A2	X	
$x,y,z > x,-y,z$	Piano xz di simmetria lungo l'asse x	X	
$x, y, z > -x, -y, -z$	inversione risp. centro		X

$$3,-2 xyz$$

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
Asse/assi di rotazione	Rotazione A2	X	
$x,y,z > x,-y,z$	Piano xz di simmetria lungo l'asse x		X
$x, y, z > -x, -y, -z$	inversione risp. centro		X

Again the motif 00 0c m0 mc is repeated .

Go on.

In order not to bore too much, the rest of the analysis I reported in the Appendix.

## Summary of results

For the moment we have a series of Y (l, m) harmonics that have been examined with respect to following symmetries (whether possessed or not):

axes / m / c.

Precisely

- rotation axis according to z : 1 2 3 4 6

$$\begin{matrix} 1 & 0 & 0 \\ \dots & & \end{matrix}$$

-my symmetry ... 0 -1 0

$$\begin{matrix} 0 & 0 & 1 \\ \dots & & \end{matrix}$$

- c symmetry, inversion ... -1 0 0  
0 -1 0  
0 0 -1

I summarize the results below, following the scheme 00 0c m0 mc.

Axis 3

$$3,3 \ x(x^2 - 3y^2) \ m0$$

$$3,-3 \ y(y^2 - 3x^2) \ 00$$

$$4,3 \ xz \ mc$$

$$4,-3 \ yz(y^2 - 3x^2) \ 0c$$

Axis 2

$$2,2 \ (x - y)(x + y) \ mc$$

$$2,-2 \ xy \ 0c$$

$$3,2 \ z(x - y)(x + y) \ m0$$

$$3,-2 \ xyz \ 00$$

Axis 4

$$4,4 \ (x^4 - 6x^2y^2 + y^4) \ mc$$

$$4,-4 \ xy(x - y)(x + y) \ 0c$$

$$5,4 \ z(x^4 - 6x^2y^2 + y^4) \ m0$$

$$5,-4 \ xyz(x - y)(x + y) \ 000$$

Axis 1

$$1,1 \ x \ m0$$

$$1,-1 \ y \ 00$$

$$2,1 \ xz \ mc$$

$$2,-1 \ yz \ 0c$$

Axis 6

$$6,6 (x^6 - 15x^4y^2 + 15x^2y^4 - y^6) \quad mc$$

$$6,-6 xy(3x^4 - 10x^2y^2 + 3y^4) \quad 0c$$

$$7,6 z(\dots) \quad m0$$

$$7,-6 xyz(\dots) \quad 00$$

This can identify, and in fact identifies, harmonics having certain certain axes of rotation according to z. To be able to go ahead and combine these harmonics with certain crystal classes, however, it is necessary to examine the presence or absence of axes 2, perpendicular to the z axis.

Are there multiple axes?

I would say that for this it is necessary and enough to verify if the harmonic has an axis 2 of lateral symmetry according to x.

Naturally this axis 2 will then be repeated for the presence of the vertical axis ex. A3.

So: we need to examine whether or not there is symmetry with respect to the operation

$$\begin{array}{ccc} 1 & 0 & 0 \\ 2x\dots 0 & -1 & 0 \\ 0 & 0 & -1 \end{array} \quad x, y, z \gg x, -y, -z$$

Result: here it is. These are the harmonics with 2x symmetry

Spherical Harmonic	
2,-1 yz	X
3,-2 xyz	X
2,2 (x - y)(x + y)	X
3,3 x(x <sup>2</sup> - 3y <sup>2</sup> )	X
5,-4 xyz(x - y)(x + y)	X
4,4 (x <sup>4</sup> - 6x <sup>2</sup> y <sup>2</sup> + y <sup>4</sup> )	X

They are few. And it's difficult to see. With the graph of the harmonics you see badly. We can see it better if we consider the Spherical Harmonics that I had supposed 'redundant', that is discarded as duplicates.

In reality they represent the same symmetries already found, but they represent them in a better way. I'll clear up with examples.

Example n ° 1

Take the harmonic Y (3,3).

$$Y(3,3) = x(x^2 - 3y^2)$$

The examination of further harmonics always with the A3 rotation shows that Y (5.3) has the same symmetries.

$$Y(5,3) = x(x^2 - 3y^2)(x^2 + y^2 - 8z^2)$$

For this reason it has been discarded.

But is it really a duplicate?

And does it have the same symmetries?

It shows them better, the same symmetries but it shows very well that three axes of symmetry are added to the vertical axis.

Empirically we can show it by the following figure.

The figure shows a 3D image as well as a projection along the x, y and z direction.



The first image is a three-dimensional image of the Y harmonic (5.3)

The second image is a view along the x axis

Then the y axis. Then the last, according to the vertical axis, obviously shows the symmetry A3.

The view along the x axis clearly shows a symmetry 2. That is: we see that the figure remains the same if it is rotated 180°.



So the harmonic has an axis 2 of lateral symmetry.

Naturally this axis 2 is then tripled due to the presence of the vertical axis A3.

And just as naturally, there is also in Y (3.3) but it is difficult to see.

**Example n ° 2.**

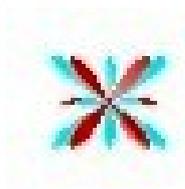
Very interesting the

$$Y(6,4) = (x^4 - 6x^2y^2 + y^4)(x^2 + y^2 - 10z^2)$$

**This, I had noticed, reposes the symmetries of Y (4.4) and as such discarded.**

$$Y(4,4) = (x^4 - 6x^2y^2 + y^4)$$

However, the view along the x axis suggests, it seems, a symmetry 4 also along this axis (see figure) and therefore as such it seems suitable to represent the class 432 as I had inserted it among the tetragonal classes, see my paper on '5 bits 32 crystal classes'.



Let's try it.

Symmetry 4x:

$$\begin{matrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{matrix}$$

Change x,y,z >> x,-z,y

Hmmm.....

It seems.

But there is not.

Only 2x.

Oh well, it's enough. That's what I wanted to show.

# Composed harmonics

There is another possibility available to represent a class that has one or more axes of rotational symmetry, and is to insert a sum.

Let me explain with an example.

For a class with A4 symmetry axis, consider the harmonics (Real Spherical Harmonics):

$$Y(4,4) = \frac{3}{16} \sqrt{\frac{35}{\pi}} (x^4 - 6x^2y^2 + y^4)$$

$$Y(4,0) = \frac{-72z^2(x^2+y^2) + 9(x^2+y^2)^2 + 24z^4}{16\sqrt{\pi}}$$

Then consider the sum, with appropriate weights, of Y (4.4) with Y (4.0).

$$\text{Sum} = a Y(4,4) + b Y(4,0)$$

This no longer has the eigenvalue  $m = 4$ , but nevertheless retains the property of possessing the A4 rotation symmetry. Consider, apart from proportionality coefficients, the following combination, with weights 1:15

$$1 (-72z^2(x^2+y^2) + 9(x^2+y^2)^2 + 24z^4) + 15 (x^4 - 6x^2y^2 + y^4)$$

The result that is obtained, always regardless of constant coefficients, is the harmonic

$$Y(4,4) \& Y(4,0) = (x^4 + y^4 + z^4) - 3((xy)^2 + (yz)^2 + (zx)^2)$$

This is completely symmetrical in x, y, z and enjoys all the symmetries of the holoedric class of the cubic system. For example, it is immediate to verify that it enjoys symmetry 4 according to the z axis

$$\begin{matrix} 0 & -1 & 0 \\ 1 & 0 & 0 \dots\dots\dots x,y,z \gg -y,x,z \\ 0 & 0 & 1 \end{matrix}$$

but also all the others that can be found in [5].

So this simple combination of two Spherical Harmonics represents the m3m class, holoedric class of the cubic system.

Note that it coincides with the Cubic Harmonic K (4, -4), see[6].

# Discussion

To sum up, at this point a certain number of classes are identified. I exclude the more uncertain ones. Compared to v2 version I have corrected some errors, I added new harmonics like Y (6, -3) etc, I hope I have not made mistakes of distraction or typing.

Her Maug	5 bit	Armoniche
1	00000	
1_	0000c	
m	000m0	1,1 x
2/m	000mc	2,1 xz
2	00200	1,-1 y
222	0020c	3,-2 xyz
mm2	002m0	3,2 z(x - y)(x + y)
mmm	002mc	2,2 (x - y)(x + y)
4	04000	
4_	0400c	
4mm	040m0	5,4 z(x <sup>4</sup> - 6x <sup>2</sup> y <sup>2</sup> + y <sup>4</sup> )
4/m	040mc	4,-4 xy(x - y)(x + y)
422	04200	
432	0420c	
4_2m	042m0	
4/mmm	042mc	4,4 (x <sup>4</sup> - 6x <sup>2</sup> y <sup>2</sup> + y <sup>4</sup> )
3	30000	3,-3 y(y <sup>2</sup> - 3x <sup>2</sup> )
3_	3000c	
3m	300m0	3,3 x(x <sup>2</sup> - 3y <sup>2</sup> )
3_2/m	300mc	6,-3 yz(y <sup>2</sup> - 3x <sup>2</sup> )(3(x <sup>2</sup> + y <sup>2</sup> ) - 8z <sup>2</sup> )
6	30200	
6_	3020c	
6mm	302m0	
6/m	302mc	6,-6 xy(3x <sup>4</sup> - 10x <sup>2</sup> y <sup>2</sup> + 3y <sup>4</sup> )
32	34000	
622	3400c	
6_m2	340mc	
6/mmm	340mc	6,6 (x <sup>6</sup> - 15x <sup>4</sup> y <sup>2</sup> + 15x <sup>2</sup> y <sup>4</sup> - y <sup>6</sup> )
23	34200	
m3	3420c	
4_3m	342m0	
m3m	342mc	K(-4) (x <sup>4</sup> - 3x <sup>2</sup> (y <sup>2</sup> + z <sup>2</sup> ) + y <sup>4</sup> - 3y <sup>2</sup> z <sup>2</sup> + z <sup>4</sup> )

Job evidently has to proceed with patience but what is the substance? The 32 crystal classes allowed and present in nature are, with patience, placed in correspondence with 32 Spherical Harmonics characterized by possessing exactly the same symmetries.

I repeat, Spherical Harmonics or simple combinations of them.

The Spherical Harmonics in question are constructed with a logic like "complex signals", in which we have situations with

- single axes,
- multiple axes parallel to each other,
- multiple orthogonal axes, typically other frequency 2 axes that serve when, once the cyclic groups have been exhausted, the dihedral groups must be represented.

The thirty-two harmonics that solve the problem seem to be grouped together and be a variant of the set of orbitals  $p, d, f$  of the atom ( $l = 0, 1, 2, 3$ ). So a group of 16, and then, again, a second group of 16. Strange as it may seem, this is what guided me in writing the relationships involved, relationships whose complexity is such that it cannot be solved without a basic guiding idea .

So in summary further, the proposed job for me is solved but not methodically finished and completed as he requested. The rest of the work to be done is left for exercise. So to say "dirty work, but someone has to do it ...".

The set of harmonics involved can be considered an expression of what I call Spherical Harmonics Restriction Theorem in that it represents, in 3D, the analogue of the rule that isolates groups compatible with the creation of composite structures, equal and in scale with respect to an elementary cell (crystallographic restriction theorem excluding other symmetries not compatible with spatial periodicity). Such is the set of 32 harmonics, or combinations of, here identified, presumably a base in space for no better identified applications and a harbinger of who knows what other speculations.

Finally, I note that maybe what I seek can be found in 'Symmetry: An Introduction to Group Theory and Its Applications', McWeeny, or 'On the symmetries of spherical harmonics', Altmann, but I don't have them.

# Conclusions

I have shown, albeit in completely empirical ways, a series of properties involving the 32 crystal classes and the 16 Spherical Harmonics with  $l = 0, 1, 2, 3$  and so on.

In particular it is plausible that there is a one-to-one correspondence of the 32 classes and 32 very specific Spherical Harmonics or combinations of, such as to be able to talk about Spherical Harmonics Restriction Theorem, analogous to the Crystallographic Restriction Theorem. It would isolate the only harmonics or the only complex signals that allow a spatial periodicity, without holes. As if to say, coherent states of matter, association of bosons that as such can create structures with spatial periodicity, without overlaps and without holes. There is also the presence of a series of other properties and analogies, all of which include, for example properties analogous to the spin of quantum mechanics, the "5-bit" constitution of the 32 classes, and so on. In this regard, I believe that a treatment with the Clifford algebra or GA Geometric Algebra would be clarifying.

# Acknowledgments

I thank Giorgio Vassallo for the useful discussions but in particular for his persistent observation "It is not a question of coincidences".

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[5] Bilbao Server [http://www.cryst.ehu.es/cryst/get\\_point\\_genpos.html](http://www.cryst.ehu.es/cryst/get_point_genpos.html)

[6] Kubic Harmonics <http://www.quanty.eu/QuantyDocsu3.php>

# Appendix

## Asse4.

I try with the same symmetries, except that the possible existence of the improper axis 4 must be proven.

That is to say, I must also try the class 4\_ which has symmetry

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

which transforms x, y, z into y, -x, -z.

While instead the rotation 4 is

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

x, y, z become -y, x, z

The table this time is the following

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
$x,y,z \gg -y,x,z$	Asse di rotazione 4		
$x,y,z \gg y,-x,z$	Asse improprio 4_		
$x,y,z \gg x,-y,-z$	Piano xz di simmetria lungo l'asse x		
$x, y, z \gg -x, -y, -z$	inversione risp. centro		

And all the potentially involved Spherical Harmonics should be tried, ie those with m = 4

$$4,4 (x^4 - 6x^2y^2 + y^4)$$

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
$x,y,z \gg -y,x,z$	Asse di rotazione 4	X	
$x,y,z \gg y,-x,-z$	Asse improprio 4 <sub>-</sub>	X	
$x,y,z > x,-y,-z$	Piano xz di simmetria lungo l'asse x	X	
$x, y, z > -x, -y, -z$	inversione risp. centro	X	

$$4,-4 xy(x-y)(x+y)$$

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
$x,y,z \gg -y,x,z$	Asse di rotazione 4	X	
$x,y,z \gg y,-x,-z$	Asse improprio 4 <sub>-</sub>	X	
$x,y,z > x,-y,-z$	Piano xz di simmetria lungo l'asse x		X
$x, y, z > -x, -y, -z$	inversione risp. centro	X	

$$5,4 z(x^4 - 6x^2y^2 + y^4)$$

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
$x,y,z \gg -y,x,z$	Asse di rotazione 4	X	
$x,y,z \gg y,-x,-z$	Asse improprio 4 <sub>-</sub>		X
$x,y,z > x,-y,-z$	Piano xz di simmetria lungo l'asse x	X	
$x, y, z > -x, -y, -z$	inversione risp. centro		X

$$5,-4 xyz(x-y)(x+y)$$

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
$x,y,z \gg -y,x,z$	Asse di rotazione 4	X	
$x,y,z \gg y,-x,-z$	Asse improprio 4 <sub>-</sub>		X
$x,y,z > x,-y,-z$	Piano xz di simmetria lungo l'asse x		X
$x, y, z > -x, -y, -z$	inversione risp. centro		X

Again the motif 00 0c m0 mc.

But there are some strange things that will have to be discussed.

Now I examine what, according to my ideas, is the first group of 4 classes.

Hermann Mauguin	5 bit symbols	Generators	Generators modificati
1	00000		
1 <sub>c</sub>	0000c	c	c
m	000m0	my	my
2/m	000mc	2y,c	my,c

I have 4 Spherical Harmonics available.

1,1<sub>x</sub>

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
Asse/assi di rotazione	Rotazione A1	X	
$x,y,z > x,-y,z$	Piano xz di simmetria lungo l'asse x	X	
$x, y, z > -x, -y, -z$	inversione risp. centro		X

1,-1<sub>y</sub>

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
Asse/assi di rotazione	Rotazione A2	X	
$x,y,z > x,-y,z$	Piano xz di simmetria lungo l'asse x		X
$x, y, z > -x, -y, -z$	inversione risp. centro		X

2,1<sub>xz</sub>

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
Asse/assi di rotazione	Rotazione A2	X	
$x,y,z > x,-y,z$	Piano xz di simmetria lungo l'asse x	X	
$x, y, z > -x, -y, -z$	inversione risp. centro	X	

2,-1<sub>yz</sub>

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
Asse/assi di rotazione	Rotazione A2	X	
$x,y,z > x,-y,z$	Piano xz di simmetria lungo l'asse x		X
$x, y, z > -x, -y, -z$	inversione risp. centro	X	

Again the motif 00 0c m0 mc.

Go on.

Axis 6.

$$6,6 (x^6 - 15x^4y^2 + 15x^2y^4 - y^6)$$

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
Asse/assi di rotazione	Rotazioni A2, A3	X	
$x, y, z > x, -y, z$	Piano xz di simmetria lungo l'asse x	X	
$x, y, z > -x, -y, -z$	inversione risp. centro	X	

$$6,-6 xy(3x^4 - 10x^2y^2 + 3y^4)$$

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
Asse/assi di rotazione	Rotazioni A2, A3	X	
$x, y, z > x, -y, z$	Piano xz di simmetria lungo l'asse x		X
$x, y, z > -x, -y, -z$	inversione risp. centro	X	

7,6 z(...)

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
Asse/assi di rotazione	Rotazioni A2, A3	X	
$x, y, z > x, -y, z$	Piano xz di simmetria lungo l'asse x	X	
$x, y, z > -x, -y, -z$	inversione risp. centro		X

7,-6 xyz(...)

Cambio di coordinate	Significato	Simmetria rispettata	Simmetria non rispettata
Asse/assi di rotazione	Rotazioni A2, A3	X	
$x, y, z > x, -y, z$	Piano xz di simmetria lungo l'asse x		X
$x, y, z > -x, -y, -z$	inversione risp. centro		X

Still the motif 00 0c m0 mc? I believe that the classes to be interpreted are these, also considering that I made hypotheses.

Hermann Mauguin	5 bit symbols	Generators	Generators modificati
<b>6</b>	<b>30200</b>	<b>3z, 2z</b>	<b>3z, 2z</b>
<b>6<sub>-</sub></b>	<b>3020c</b>	<b>mz, 3z</b>	<b>((3z, 2z) &amp;c)</b>
<b>6mm</b>	<b>302m0</b>	<b>3z, 2z, m110</b>	<b>3z, 2z, m110</b>
<b>6/m</b>	<b>302mc</b>	<b>3, 2z, c</b>	<b>3z, 2z, m001, c</b>