The Full Octahedral Group and the Cubic Lattice

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Description

In this Notebook we construct the Full Octahedral Group and we group its elements in conjugacy classes according to the nomenclature of Cristallography and Chemistry. Then all of the 10 irreducible Representations are constructed and the character table is also constructed. It follows the construction of the Self Dual Cubic lattice and the analysis of orbits of its vectors under O_h. In particular we study the spherical layers with quantized radii and their decompositions in orbits. Various routines are made available to the user.

Presentation of the NoteBook

The definitions of the Full and Proper Octahedral groups

▪ Presentation of the octahedral group in terms of generators

The proper octahedral group is abstractly defined by two generators

▪ The groups

The full octahedral group O_h has 48 group elements organized in 10 conjugacy classes whose names are standard in the chemical literature. A unique way to identify the group elements is by means of the action of the group element on the standard three vector {x,y,z} that is mapped into another triple,for instance {-z,x,-y}. In this way one creates for each group element $\gamma \in O_h$ a corresponding 3×3 matrix

$$\left(\begin{array}{llc}
\mathrm{EE} & 1 & \{\{x, y, z\}\} \\
\mathrm{C}_3 & 8 & \{\{-y, -z, x\}, \{-y, z, -x\}, \{-z, -x, y\}, \{-z, x, -y\}, \{z, -x, -y\}, \{z, x, \\
\mathrm{C}_4^2 & 3 & \{\{-x, -y, z\}, \{-x, y, -z\}, \{x, -y, -z\}\} \\
\mathrm{C}_2 & 6 & \{\{-x, -z, -y\}, \{-x, z, y\}, \{-y, -x, -z\}, \{-z, -y, -x\}, \{z, -y, \\
\mathrm{C}_4 & 6 & \{\{-y, x, z\}, \{-z, y, x\}, \{z, y, -x\}, \{y, -x, z\}, \{x, -z, y\}, \\
\mathrm{J} & 1 & \{\{-x, -y, -z\}\} \\
\mathrm{JC}_3 & 8 & \{\{-y, -z, -x\}, \{-y, z, x\}, \{-z, -x, -y\}, \{-z, x, y\}, \{z, -x, y\}, \{z, x, - \\
\mathrm{JC}_4^2 & 3 & \{\{-x, y, z\}, \{x, -y, z\}, \{x, y, -z\}\} \\
\mathrm{JC}_2 & 6 & \{\{-y, -x, z\}, \{-z, y, -x\}, \{z, y, x\}, \{y, x, z\}, \{x, -z, -y \\
\mathrm{JC}_4 & 6 & \{\{-x, -z, y\}, \{-x, z, -y\}, \{-y, x, -z\}, \{-z, -y, x\}, \{z, -y, -
\end{array}\right. \tag{1}$$

The proper octahedral group is made only of the first 5 conjugacy classes that close a subgroup $O_{24} \subset O_h$ with 24 elements.

$$\left(\begin{array}{llc}
\mathrm{EE} & 1 & \{\{x, y, z\}\} \\
\mathrm{C}_3 & 8 & \{\{-y, -z, x\}, \{-y, z, -x\}, \{-z, -x, y\}, \{-z, x, -y\}, \{z, -x, -y\}, \{z, x, y \\
\mathrm{C}_4^2 & 3 & \{\{-x, -y, z\}, \{-x, y, -z\}, \{x, -y, -z\}\} \\
\mathrm{C}_2 & 6 & \{\{-x, -z, -y\}, \{-x, z, y\}, \{-y, -x, -z\}, \{-z, -y, -x\}, \{z, -y, \\
\mathrm{C}_4 & 6 & \{\{-y, x, z\}, \{-z, y, x\}, \{z, y, -x\}, \{y, -x, z\}, \{x, -z, y\},
\end{array}\right. \tag{2}$$

The complete multiplication table of the proper octahedral group O_{24} is given in the following table:

γ	XX	1_1	2_1	2_2	2_3	2_4	2_5	2_6	2_7	2_8	3_1	3_2	3_3	4_1	4_2	4_3	4_4	4_5	4_6	5_1	5_2	5_3
γ	XX	XX	XX	XX	XX	XX	XX	XX	XX	XX	XX	XX	XX	XX	XX	XX	XX	XX	XX	XX	XX	XX
1_1	XX	1_1	2_1	2_2	2_3	2_4	2_5	2_6	2_7	2_8	3_1	3_2	3_3	4_1	4_2	4_3	4_4	4_5	4_6	5_1	5_2	5_3
2_1	XX	2_1	2_5	2_4	3_3	3_2	1_1	3_1	2_6	2_3	2_7	2_2	2_8	5_3	4_4	5_6	4_6	5_4	4_2	4_1	4_3	5_1
2_2	XX	2_2	2_6	2_3	1_1	3_1	3_3	3_2	2_5	2_4	2_8	2_1	2_7	4_5	5_2	5_5	5_4	4_6	4_1	4_2	5_1	4_3
2_3	XX	2_3	3_2	1_1	2_2	2_8	2_7	2_1	3_3	3_1	2_4	2_6	2_5	4_6	5_1	5_3	5_6	4_1	4_5	5_2	4_2	5_5
2_4	XX	2_4	3_1	3_3	2_1	2_7	2_8	2_2	1_1	3_2	2_3	2_5	2_6	5_4	4_3	4_5	5_5	4_2	5_3	4_4	4_1	5_6
2_5	XX	2_5	1_1	3_2	2_8	2_2	2_1	2_7	3_1	3_3	2_6	2_4	2_3	5_1	4_6	5_2	4_2	5_5	4_4	5_3	5_6	4_1
2_6	XX	2_6	3_3	3_1	2_7	2_1	2_2	2_8	3_2	1_1	2_5	2_3	2_4	4_3	5_4	4_4	4_1	5_6	5_2	4_5	5_5	4_2
2_7	XX	2_7	2_3	2_6	3_1	1_1	3_2	3_3	2_4	2_5	2_1	2_8	2_2	5_2	4_5	4_2	5_1	4_3	5_6	5_5	5_4	4_6
2_8	XX	2_8	2_4	2_5	3_2	3_3	3_1	1_1	2_3	2_6	2_2	2_7	2_1	4_4	5_3	4_1	4_3	5_1	5_5	5_6	4_6	5_4
3_1	XX	3_1	2_8	2_7	2_6	2_5	2_4	2_3	2_2	2_1	1_1	3_3	3_2	5_6	5_5	4_6	5_3	5_2	4_3	5_4	4_5	4_4
3_2	XX	3_2	2_7	2_8	2_5	2_6	2_3	2_4	2_1	2_2	3_3	1_1	3_1	5_5	5_6	5_4	4_5	4_4	5_1	4_6	5_3	5_2
3_3	XX	3_3	2_2	2_1	2_4	2_3	2_6	2_5	2_8	2_7	3_2	3_1	1_1	4_2	4_1	5_1	5_2	5_3	5_4	4_3	4_4	4_5
4_1	XX	4_1	5_4	4_6	4_5	5_3	5_2	4_4	5_1	4_3	5_5	5_6	4_2	1_1	3_3	2_8	2_6	2_3	2_2	2_7	2_5	2_4
4_2	XX	4_2	4_6	5_4	5_3	4_5	4_4	5_2	4_3	5_1	5_6	5_5	4_1	3_3	1_1	2_7	2_5	2_4	2_1	2_8	2_6	2_3
4_3	XX	4_3	5_3	5_2	5_6	4_2	5_5	4_1	4_5	4_4	4_6	5_1	5_4	2_6	2_4	1_1	2_8	2_7	3_1	3_2	2_2	2_1
4_4	XX	4_4	4_2	5_5	5_1	5_4	4_6	4_3	5_6	4_1	5_2	4_5	5_3	2_8	2_1	2_6	1_1	3_2	2_5	2_3	3_1	3_3
4_5	XX	4_5	5_6	4_1	4_6	4_3	5_1	5_4	4_2	5_5	5_3	4_4	5_2	2_2	2_7	2_4	3_2	1_1	2_3	2_5	3_3	3_1
4_6	XX	4_6	4_4	4_5	4_1	5_5	4_2	5_6	5_2	5_3	4_3	5_4	5_1	2_3	2_5	3_1	2_1	2_2	1_1	3_3	2_7	2_8
5_1	XX	5_1	4_5	4_4	5_5	4_1	5_6	4_2	5_3	5_2	5_4	4_3	4_6	2_5	2_3	3_3	2_7	2_8	3_2	3_1	2_1	2_2
5_2	XX	5_2	4_1	5_6	4_3	4_6	5_4	5_1	5_5	4_2	4_4	5_3	4_5	2_7	2_2	2_5	3_3	3_1	2_6	2_4	3_2	1_1
5_3	XX	5_3	5_5	4_2	5_4	5_1	4_3	4_6	4_1	5_6	4_5	5_2	4_4	2_1	2_8	2_3	3_1	3_3	2_4	2_6	1_1	3_2
5_4	XX	5_4	5_2	5_3	4_2	5_6	4_1	5_5	4_4	4_5	5_1	4_6	4_3	2_4	2_6	3_2	2_2	2_1	3_3	1_1	2_8	2_7
5_5	XX	5_5	4_3	5_1	4_4	5_2	5_3	4_5	4_6	5_4	4_1	4_2	5_6	3_2	3_1	2_2	2_4	2_5	2_8	2_1	2_3	2_6
5_6	XX	5_6	5_1	4_3	5_2	4_4	4_5	5_3	5_4	4_6	4_2	4_1	5_5	3_1	3_2	2_1	2_3	2_6	2_7	2_2	2_4	2_5

The full octahedral group O_h has 10 irreducible representations and the corresponding character table is diplayed below

Class	{EE, 1}	{C_3, 8}	{C_4^2, 3}	{C_2, 6}	{C_4, 6}	{J, 1}	{JC_3, 8}	{JC_4^2, 3}
Irrep	{x, y, z}	{-y, -z, x}	{-x, -y, z}	{-x, -z, -y}	{-y, x, z}	{-x, -y, -z}	{-y, -z, -x}	{-x, y, z}
D_1	1	1	1	1	1	1	1	1
D_2	1	1	1	1	1	-1	-1	-1
D_3	1	1	1	-1	-1	1	1	1
D_4	1	1	1	-1	-1	-1	-1	-1
D_5	2	-1	2	0	0	2	-1	2
D_6	2	-1	2	0	0	-2	1	-2
D_7	3	0	-1	-1	1	3	0	-1
D_8	3	0	-1	-1	1	-3	0	1
D_9	3	0	-1	1	-1	3	0	-1
D_{10}	3	0	-1	1	-1	-3	0	1

(4)

As we see O_h has four 1-dimensional representations, two 2-dimensional representations and four 3-dimensional representations.
The proper octahedral group O_{24} has 5 irreducible representations and the corresponding character table is diplayed below:

Class	{EE, 1}	{C_3, 8}	{C_4^2, 3}	{C_2, 6}	{C_4, 6}
Irrep	{x, y, z}	{-y, -z, x}	{-x, -y, z}	{-x, -z, -y}	{-y, x, z}
D_1	1	1	1	1	1
D_2	1	1	1	-1	-1
D_3	2	-1	2	0	0
D_4	3	0	-1	-1	1
D_5	3	0	-1	1	-1

(5)

As we see O_{24}, which is isomorphic to S_4, has two 1-dimensional representations, one 2-dimensional representaion and two 3-dimensional representations.

▪ Orbits of lattice vectors under the group O_{24}

The vectors in the cubic lattice arrange under the action of the two octahedral groups into the following type of orbits

1. Vectors of type {n,0,0} with n $\in \mathbb{Z}$ generate orbits of length 6 under both groups
2. Vectors of type {n,n,n} with n $\in \mathbb{Z}$ generate orbits of length 8 under both groups
3. Vectors of type {n,0,n} with n $\in \mathbb{Z}$ generate orbits of length 12 under both groups
4. Vectors of type {n,n,r} with n,r $\in \mathbb{Z}$ generate orbits of length 24 under both groups
5. Vectors of type {n,r,s} with n,r,s $\in \mathbb{Z}$ generate orbits of length 48 under O_h and 24 under O_{24}

Objects and Commands available to the user

The names of the created objects available to the user are the following ones:

1. The set of all group elements of O_h given as 3×3 orthogonal matrices and organized according into conjugacy classes accordin with the nomenclature of eq. (1) is encoded in the object **chemclassa**
2. The action on the three coordinates {x,y,z} of each element of the full octahedral group organized in conjugacy classes as displayed in eq. (1) is encoded in the object **repchemclassa.**
3. The array containing all the 48 group elements of O_h given as 3×3 orthogonal matrices but not ordered in conjugacy classes is encoded in the object **octahedroD**
4. The array containing all the 24 group elements of O_{24} given as 3×3 orthogonal matrices but not ordered in conjugacy classes is encoded in the object **octahedroP**
5. The array containing all the 24 group elements of O_{24} given as 3×3 orthogonal matrices and labeled by their name n_r where n=1,2,3,4,5 enumerates the conjugacy classes C_n and r=1,..,$|C_n|$ is encoded in the object **GroupO**
6. The multiplication table of the O_{24} group is encoded in the objects **tabloid** or **multab** (with or without column and row heads).
7. The 10 irreducible representations of the full octahedral group O_h are encoded in the object **DHclassa** whose elements have the following structure **DHclassa[[irrep,conj class]]**
   `={name of conj class, # of elelemnts in the class ,`
   `{D[element 1], D[element 2], ..., D[last element in the class]}}`
8. The characters of the 10 irreducible representations of the full octahedral group O_h are encoded in the object **chi .** The characters are organized into a table encoded in the object named **Tabella**.
9. The 5 irreducible representations of the proper octahedral group O_{24} are encoded in the object **PDclassa** whose elements have the following structure whose elelments have the same structure as those of DHclassa.
10. The characters of the 5 irreducible representations of the proper octahedral group O_{24} are encoded in the object **Pchi .** The characters are organized into a table encoded in the object named **PTabella**.

Auxiliary group theoretical routines used by the package but available also to the user

Besides the basic commands described in the previous section this package contains also some general group-theoretical routines that are internally utilized but available to the user. These are

1. **generone**. Given a set of matrices named **Allgroup** the routine generone generates the set of all their products. Repeated use of generone arrives at a set that closes under multiplication if the original matrices were elements of a finite group.
2. **generoneName**. Given a set of matrices named **AllgroupN** , associated, each of them with a name, the routine generone generates the set of all their products keeping track of the non--commutative product of names. Repeated use of generoneName arrives at a set that closes under multiplication if the original matrices were elements of a finite group
3. **coniugatoL**. If you give a set of matrices forming a finite group and you name it **gruppone**, **coniugatoL** produces the set of conjugacy classes into which the finite group is organized. The output of this calculation is named **orgclas**.
4. **verifiosub**. Given a set of matrices that form a finite group, named **gruppone** and a subset named **settino**, verifiosub verifies whether settino is a subgroup and moreover it verifies whether it is a normal subgroup.
5. **quozientus**. Given a set of matrices forming a finite group, named gruppone and a normal subgroup named gruppino, quozientus constructs the equivalence classes G/H namely the quotient group. The output of this calculation is named **equaclass.**
6. The routines **genorb** and **genorbP**. Given any three vector $\{v_1,v_2,v_3\}$ named **vec** the routines create its orbit under the action of the full octahedral group (genorb) or under the action of the proper octahedral group (genorbP).
7. **latticePS**. This is a routine that generates finite portions of the space lattice and of the momentum lattice.
   In order to activate this routine you have to give two data:
   spaz = ? is the lattice spacing a that you want;
   nplan = ? is the number of lattice points that you want to place on the cubic rays.
   Then you type **latticePS**.
   Running the routine one obtains a lattice with a certain finite number **N** of points that depends on the initial user chosen number of points **nplan**. The computer calculates N and also calculates how many point of the lattice intersect the sherical surface centered at the origin {0,0,0} and of radius n a where n∈ℕ. We name such collection of points *spherical arrays* and they are encoded into an

object named **strata.** The various radii and the number of lattice points intersected by the sphere of the corresponding radius are contained in a file named **multip.**

8. When you run **latticePS** you generate graphical objects that can be displayed by typing **Show[....]** . The generated graphical objects are **skeletonPS** and **vertexPS**, namely the links between points in the cubic lattice (skeletonPS) and the points of the cubic lattice (vertexPS). These objects can be combined with other graphical objects ar polyedra, spheres and special points in the lattice.
9. **orbitandus.** The routine orbitandus organizes the lattice points contained in a spherical layer into orbits of the proper ocathedral group. In order to utilize this routine you have first to generate a lattice by means of the routine **latticePS**. Next if you type **orbitandus** you obtain a file named **filtro** that is an array of arrays. Each entry of the array has three entries and it looks like it follows

$$\left\{ 25 \ , 30 \ , \ \left\{\left\{O_1^{25}, 6\right\}, \left\{O_2^{25}, 24\right\}\right\} \right\}$$

The first entry 25 is the radius squared of the spherical orbit, the second entry 30 is the number of lattice points that intersect this sphere, the third entry tells you that in this case the 30 points organize into an orbit of 6 points under the proper octahedral group ⊕ an orbit of 24 points under the action of the same group.
10. Routines for the analysis of group representations. Suppose that you have constructed a group representation. The matrices have to be organized in an array of 5 entries corresponding to the 5 conjugacy classes each of which as the form **Repra[[r]]={p,{$D[g_1]$,$D[g_2]$,....,$D[g_p]$}}** where p is the population of the r class and **{$D[g_1]$,$D[g_2]$,....,$D[g_p]$}** are the matrices representing the p elements in that class. Then you can utilize the following routines
   (a) **homverifioinvers** verifies that the representation is indeed a homomorphism where the product is from right to left D[A]D[B] == D[BA]. Next it utilizes the routine ortogverifio that verifies if it is an ortogonal representation. Finally it utilizes the routine brutcaratter to decompose the given representation into irreducible ones.
   (b) **homverifiodirec** verifies that the representation is indeed a homomorphism where the product is from left to right D[A]D[B] == D[AB]. Next it utilizes the routine ortogverifio that verifies if it is an ortogonal representation. Finally it utilizes the routine brutcaratter to decompose the given representation into irreducible ones.
   (c) **brutcaratter**. It can be called directly to decompose the given representation into irreducible ones.

The MATHEMATICA NoteBook

General routines

Construction of the Full Octahedral Group O_h and of the proper Octahedral Group O_{24}.

Irreducible Representations of O_h and O.

Generating the Cubic Self Dual Lattice and introducing routines for orbits

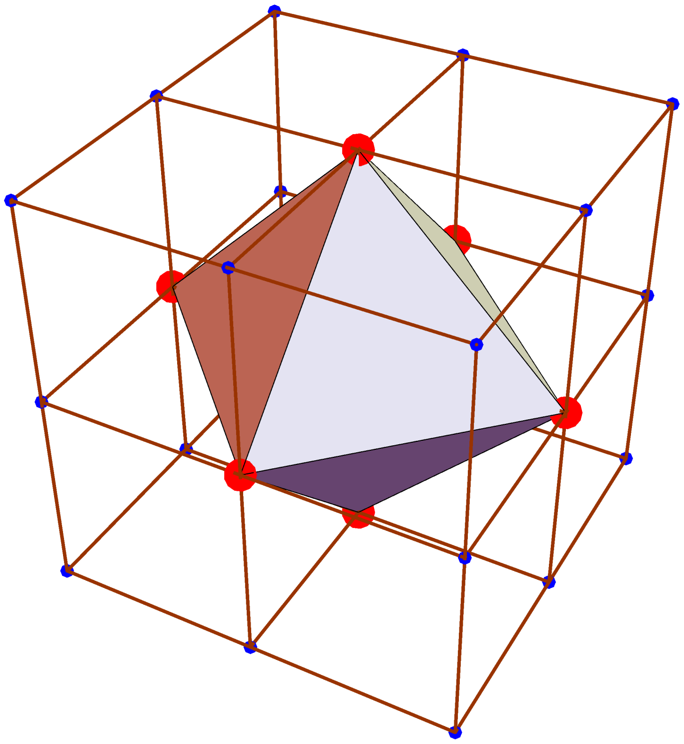
Study of Orbits of the Proper Octahedral Group in the Momentum Lattice

Lattice orbits of the Octahedral Group and the regular polyehdra

Inscription of the Octahedron and the 6 dimensional orbit

- **Calculations**
- **Visualization of this orbit**

```
Show[vertexPS, skeletonPS, punte6, ottone, Boxed → False]
```

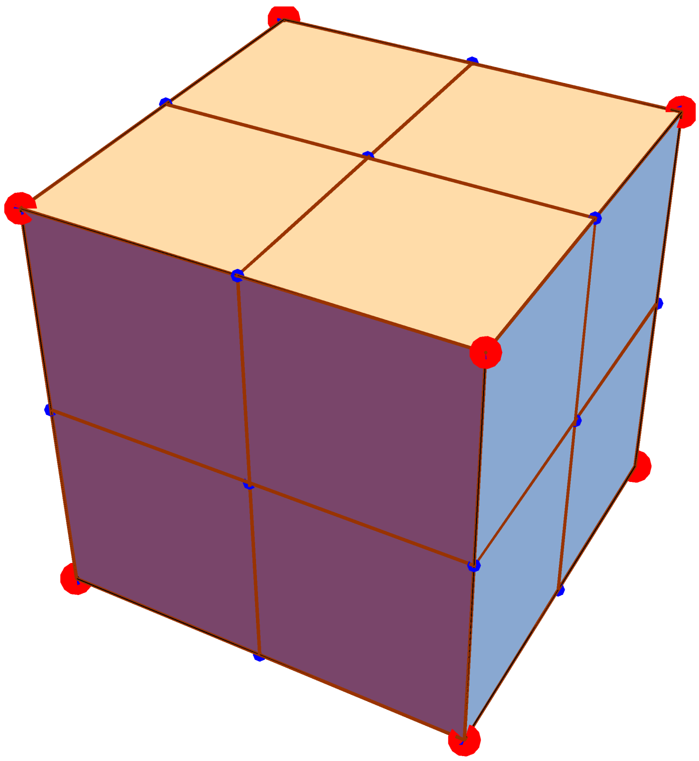


Inscription of the Cube and the 8 dimensional orbit

- **Calculations**

- **Visualization of this orbit**

```
Show[vertexPS, skeletonPS, cubone, punte8, Boxed → False]
```



Orbit of Length 12

- **calculations**

■ Visualization of this orbit

```
Show[vertexPS, skeletonPS, cubone, punte12, Boxed → False]
```