Point groups

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§1. Basics of group theory

We skip elementary facts about groups, but remind terminology and formulas used in this work. Complete information on group theory can be found in Wikipedia and textbooks. For computations see FiniteGroups and related packages; commands from these packages are [`highlighted`].

Two elements $g_{1,2}$ in a group G are conjugate if there exists an element g such that $g_2 = g g_1 g^{-1}$. This equivalence relation partition the group G into conjugacy classes. A subgroup $F \subset G$ is normal if it is invariant under conjugation: $\forall g \in G, f \in F\ gfg^{-1} \in F$ (in fact $gFg^{-1} = F$). If H is a subgroup of G and F is a normal subgroup, then their elementwise product equals to G (with repetitions iff F and H overlap). In this case G is the inner semidirect product $G = F \rtimes H$. If H is also invariant then G is the direct product $G = F \times H$.

In what follows we consider group representations – finite-dimensional unitary representations in Hilbert space. Operators (matrices) of such representations satisfy the identities

$$T(g_1)T(g_2) = T(g_1 g_2), \quad T(g^{-1}) = T(g)^{-1} = T(g)^{+}, \quad T(g)\psi(\boldsymbol{r}) = \psi\left(g^{-1}\boldsymbol{r}\right),$$

where ψ are basis functions of the Hilbert space. Every such representation is the direct sum of irreducible representations (IR). IR operators are orthogonal:

$$\sum_{g\in G} \overline{T^{\Gamma}(g)_{\alpha\beta}}\, T^{\Gamma'}(g)_{\alpha'\beta'} = \frac{|G|}{|\Gamma|}\delta_{\Gamma\Gamma'}\delta_{\alpha\alpha'}\delta_{\beta\beta'}, \quad \alpha,\beta,\alpha'\beta' = 1,\ldots,|\Gamma|,$$

where Γ, Γ' are two IRs, $|\Gamma| = \dim\Gamma$, and $|G|$ is the number of elements in G. The character of a representation Λ is the function $\chi^{\Lambda}(g) = \operatorname{tr} T^{\Lambda}(g)$. IR characters form a complete orthogonal system in the space of functions constant on conjugacy classes.

A decomposition of a given representation Λ of a group G into IRs can be performed in two approaches. If only IR multiplicities ν are needed, it is enough to consider characters using the formula [`FGR_RepDecCh`]

$$\nu = \frac{1}{|G|}\sum_{g\in G}\overline{\chi^{\Gamma}(g)}\chi^{\Lambda}(g) \equiv \frac{1}{|G|}\sum_{g\in C} N_g^C\,\overline{\chi^{\Gamma}(g)}\chi^{\Lambda}(g),$$

where C denotes the representatives of the classes of conjugate elements of the group G, and N_g^C denotes the number of elements in the class represented by the element g. A complete decomposition requires determination of a unitary operator U such that the matrices $U^{+}T^{\Lambda}(g)U$ are block-diagonal for all $g \in G$, where each block corresponds to a single IR [`FGR_RepDec,FGR_RepU`]. It is convenient to write the matrices U in the corresponding block form $\begin{pmatrix} U^{\Gamma_1} & U^{\Gamma_2} & \ldots \end{pmatrix}$, where U^{Γ} are $|\Lambda| \times |\Gamma|$ unitary matrices such that $U^{\Gamma+}T^{\Lambda}(g)U^{\Gamma'} = \delta_{\Gamma\Gamma'}T^{\Gamma}(g)$, and $P^{\Gamma} = U^{\Gamma}U^{\Gamma+}$ is the Hermitian projector onto the IR space Γ. The matrices U^{Γ} are constructed according to the scheme given below.

For a fixed IR Γ, the $\Lambda \to \Gamma$ projection operators

$$P^{\Gamma}_{\alpha\beta} = \frac{|\Gamma|}{|G|}\sum_{g\in G}\overline{T^{\Gamma}(g)_{\beta\alpha}}\, T^{\Lambda}(g), \quad \alpha,\beta = 1,\ldots,|\Gamma| \tag{1.1}$$

have the following properties:[1]

$$1)\ P^{\Gamma+}_{\alpha\beta}=P^{\Gamma}_{\beta\alpha},\quad 2)\ P^{\Gamma+}_{\alpha\beta}P^{\Gamma'}_{\alpha'\beta'}=\delta_{\Gamma\Gamma'}\delta_{\beta\beta'}P^{\Gamma}_{\alpha'\alpha},\quad 3)\ T^{\Lambda}(g)P^{\Gamma}_{\alpha\beta}=\sum_{\gamma}P^{\Gamma}_{\alpha\gamma}T^{\Gamma}(g)_{\gamma\beta}.$$

From the second and third identities, it follows that for fixed index α and vector x, the set $\left\{P^{\Gamma}_{\alpha\beta}x,\ \beta=1,\ldots,|\Gamma|\right\}$ is an orthogonal system of vectors that transform under the IR Γ. From the first and second identities, it follows that $P^{\Gamma}_{\alpha\alpha}$ is a Hermitian projector onto the ν-dimensional subspace Γ^{ν} containing one vector from each Γ. Also note that $P^{\Gamma}=\sum_{\alpha}P^{\Gamma}_{\alpha\alpha}\equiv\frac{|\Gamma|}{|G|}\sum_{g\in G}\overline{\chi^{\Gamma}(g)}T^{\Lambda}(g)$ is also a Hermitian projector onto Γ^{ν}. Using these projectors, we construct the matrices U^{Γ} as follows. Let fix $\alpha=1$ and in the space obtained by the projector P^{Γ}_{11} introduce an orthonormal basis $\left\{e^{\Gamma}_{\mu},\ \mu=1,\ldots,\nu\right\}$ (i.e. orthonormalize column vectors of the matrix P^{Γ}_{11}). Then

$$\left(U^{\Gamma}_{\mu}\right)_{i\beta}=\frac{|\Gamma|}{|G|}\sum_{g\in G}\overline{T^{\Gamma}(g)_{\beta 1}}\ \left(T^{\Lambda}(g)e^{\Gamma}_{\mu}\right)_{i},\quad i=1,\ldots,|\Lambda|,\ \beta=1,\ldots,|\Gamma|. \tag{1.2}$$

Now let show that the resulting matrices perform a unitary transformation on Γ:

$$\left(U^{\Gamma+}_{\mu}T^{\Lambda}(g)U^{\Gamma'}_{\Lambda}\right)_{\alpha\beta}=\sum_{ij}\overline{\left(U^{\Gamma}_{\mu}\right)_{i\alpha}}\left(U^{\Gamma'}_{\Lambda}\right)_{j\beta}T^{\Lambda}(g)_{ij}=\frac{d^2}{N^2}\sum_{hf}T^{\Gamma}(h)_{\alpha1}\overline{T^{\Gamma'}(f)_{\beta1}}\sum_{ij}\overline{\left(T^{\Lambda}(h)e^{\Gamma}_{\mu}\right)_{i}}T^{\Lambda}(g)_{ij}\left(T^{\Lambda}(f)e^{\Gamma'}_{\nu}\right)_{j}$$

$$=\frac{d^2}{N^2}\sum_{hf}T^{\Gamma}(h)_{\alpha1}\overline{T^{\Gamma'}(f)_{\beta1}}\left\langle e^{\Gamma}_{\mu}\right|T^{\Lambda}(h^{-1}gf)\left|e^{\Gamma'}_{\nu}\right\rangle\overset{gf=hh'}{=}\frac{d^2}{N^2}\sum_{\gamma\delta h'f}T^{\Gamma}(g)_{\alpha\gamma}T^{\Gamma}(f)_{\gamma\delta}\overline{T^{\Gamma}(h')_{1\delta}T^{\Gamma'}(f)_{\beta1}}\left\langle e^{\Gamma}_{\mu}\right|T^{\Lambda}(h')\left|e^{\Gamma'}_{\nu}\right\rangle$$

$$=\frac{d}{N}\sum_{\gamma\delta h'}\delta_{\Gamma\Gamma'}\delta_{\gamma\beta}\delta_{\delta1}T^{\Gamma}(g)_{\alpha\gamma}\overline{T^{\Gamma}(h')_{1\delta}}\left\langle e^{\Gamma}_{\mu}\right|T^{\Lambda}(h')\left|e^{\Gamma'}_{\nu}\right\rangle=\delta_{\Gamma\Gamma'}T^{\Gamma}(g)_{\alpha\beta}\left\langle e^{\Gamma}_{\mu}\right|P^{\Gamma}_{11}\left|e^{\Gamma}_{\nu}\right\rangle=\delta_{\Gamma\Gamma'}\delta_{\mu\nu}T^{\Gamma}(g)_{\alpha\beta}.$$

A decomposition of tensor products of IRs can be performed using the formulas

$$\chi^{\Gamma_1\times\Gamma_2}(g)=\chi^{\Gamma_1}(g)\chi^{\Gamma_2}(g),\quad \chi^{[\Gamma^2]}(g)=\frac{1}{2}\chi^{\Gamma}(g)^2+\frac{1}{2}\chi^{\Gamma}(g^2),\quad \chi^{\{\Gamma^2\}}(g)=\frac{1}{2}\chi^{\Gamma}(g)^2-\frac{1}{2}\chi^{\Gamma}(g^2). \tag{1.3}$$

In terms of operators such decomposition expands products of IR basis functions into their linear combination:

$$|\Gamma_1\alpha_1\Gamma_2\alpha_2\rangle=\sum_{\Gamma\alpha}\langle\Gamma\alpha|\Gamma_1\alpha_1\Gamma_2\alpha_2\rangle\ |\Gamma\alpha\rangle\,, \tag{1.4}$$

where the coefficients are called Clebsch–Gordan coefficients. They can be obtained either from the decomposition or from the set of equations

$$\sum_{\beta}T^{\Gamma}(g)_{\beta\alpha}\langle\Gamma\beta|\Gamma_1\alpha_1\Gamma_2\alpha_2\rangle=\sum_{\beta_1\beta_2}T^{\Gamma_1}(g)_{\alpha_1\beta_1}T^{\Gamma_2}(g)_{\alpha_2\beta_2}\langle\Gamma\alpha|\Gamma_1\beta_1\Gamma_2\beta_2\rangle\,,\ \alpha_i=1,\ldots,|\Gamma_i|,\ g\in G \tag{1.5}$$

(it is enough to include here only generators of G).

§2. Rotation group

It is known that any proper orthogonal transformation of three-dimensional space $\boldsymbol{r}\to R\boldsymbol{r}$ is a rotation about some axis (Euler's rotation theorem). A rotation by an angle α about the axis $\boldsymbol{n}$ directed along (θ,ϕ) in spherical coordinates is given by the matrix [`RotationM`]:

$$R(\alpha,\boldsymbol{n})\equiv R(\alpha,[\theta,\phi])=R_z(\phi)R_y(\theta)R_z(\alpha)R_y(-\theta)R_z(-\phi), \tag{2.1}$$

where

$$R_z(\alpha)=R(\alpha,[001])=\begin{pmatrix}\cos\alpha & -\sin\alpha & 0\\ \sin\alpha & \cos\alpha & 0\\ 0 & 0 & 1\end{pmatrix},\qquad R_y(\theta)=R(\theta,[010])=\begin{pmatrix}\cos\theta & 0 & \sin\theta\\ 0 & 1 & 0\\ -\sin\theta & 0 & \cos\theta\end{pmatrix}.$$

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[1] See proof in the book of Petro Holod, Symmetry and group theory methods in physics (Kyiv, 2005), in Ukrainian.

Frequently used is the representation of rotations in terms of Euler angles, which in the so-called "y-convention" is defined as [`RotationMEulerY`]

$$R(\alpha,\beta,\gamma) = R_z(\gamma)R_y(\beta)R_z(\alpha). \tag{2.2}$$

We will distinguish these two representations by their arguments. Obviously,

$$R^{-1}(\alpha,\boldsymbol{n}) = R(-\alpha,\boldsymbol{n}) \equiv R(-\alpha,[\pi-\theta,\pi+\phi]), \qquad R^{-1}(\alpha,\beta,\gamma) = R(-\gamma,-\beta,-\alpha). \tag{2.3}$$

Since inversion commutes with rotations, any orthogonal transformation is generally given by a matrix of the form $\pm R(\alpha,\theta,\phi)$, where the plus corresponds to proper transformations and the minus to improper ones. Orthogonal transformations form the 3D rotation group denoted by $SO(3)$ in the case of proper rotations and $O(3) = SO(3)\times I$ in the general case. The infinitesimal operators of the rotation group are the "angular momentum" operators

$$L_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}, \quad L_y = \begin{pmatrix} 0 & 0 & \mathrm{i} \\ 0 & 0 & 0 \\ -\mathrm{i} & 0 & 0 \end{pmatrix}, \quad L_z = \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

which generate the rotation

$$R(\alpha,\boldsymbol{n}) = \exp\left[-\mathrm{i}\alpha\left(n_xL_x + n_yL_y + n_zL_z\right)\right],$$
$$R_x(\alpha_x)R_y(\alpha_y)R_z(\alpha_z) = \exp(-\mathrm{i}\alpha_xL_x)\exp(-\mathrm{i}\alpha_yL_y)\exp(-\mathrm{i}\alpha_zL_z)$$

and satisfy the commutation relations $[L_i,L_j] = \mathrm{i}\,e_{ijk}L_k$.

§3. Rotation group representations

Finite-dimensional irreducible representations of the proper group of rotations are numbered by the orbital (quantum) number $l\in\mathbb{Z}_+$ and denoted by D^l, $\dim D^l = 2l+1$. Representations of the rotation group are usually considered in the space of functions on the sphere using the basis spherical harmonics Y_{lm}, $m=-l,\dots,l$ [`Ylm`]. Infinitesimal operators are represented by the operators $L_i = -\mathrm{i}\sum_{jk} e_{ijk}x_j\partial_{x_k}$. The representation of symmetry elements is carried out by unitary Wigner D-matrix [`WignerD`]:

$$T[R(\alpha,\beta,\gamma)] = D^l(\alpha,\beta,\gamma), \quad D^l_{mm'}(\alpha,\beta,\gamma) = \mathrm{e}^{\mathrm{i}m\alpha+\mathrm{i}m'\gamma}d^l_{mm'}(\beta),$$

where $d^l_{mm'}$ is Wigner d-matrix. In particular,

$$D^l_{0m}(\alpha,\beta,\gamma) = (-1)^m\sqrt{\frac{4\pi}{2l+1}}Y_{lm}(\beta,\gamma),$$

$$d^0 = 1, \qquad d^1(\beta) = \begin{array}{|c|ccc|}\hline m\backslash m' & 1 & 0 & -1 \\ \hline 1 & c^2 & \sqrt{2}cs & s^2 \\ 0 & -\sqrt{2}cs & c^2-s^2 & \sqrt{2}cs \\ -1 & s^2 & -\sqrt{2}cs & c^2 \\ \hline \end{array}$$

$$d^2(\beta) = \begin{array}{|c|ccccc|}\hline m\backslash m' & 2 & 1 & 0 & -1 & -2 \\ \hline 2 & c^4 & 2c^3s & \sqrt{6}c^2s^2 & 2cs^3 & s^4 \\ 1 & -2c^3s & -c^2(4s^2-1) & \sqrt{6}cs(c^2-s^2) & s^2(4c^2-1) & 2cs^3 \\ 0 & \sqrt{6}c^2s^2 & -\sqrt{6}cs(c^2-s^2) & 1-6c^2s^2 & \sqrt{6}cs(c^2-s^2) & \sqrt{6}c^2s^2 \\ -1 & -2cs^3 & s^2(4c^2-1) & -\sqrt{6}cs(c^2-s^2) & -c^2(4s^2-1) & 2c^3s \\ -2 & s^4 & -2cs^3 & \sqrt{6}c^2s^2 & -2c^3s & c^4 \\ \hline \end{array},$$

where $c = \cos\frac{\beta}{2}$, $s = \sin\frac{\beta}{2}$. Spherical harmonics transforms as follows:

$$Y_{lm}(R\boldsymbol{r}) = \sum_{m'=-l}^{l} D^l_{mm'}(\alpha,\beta,\gamma)Y_{lm'}(\boldsymbol{r}) = \mathrm{e}^{\mathrm{i}m\alpha}\sum_{m'=-l}^{l} d^l_{mm'}(\beta)\left[\mathrm{e}^{\mathrm{i}m'\gamma}Y_{lm'}(\boldsymbol{r})\right].$$

The representations of the full group $O(3)$ are obtained as for the direct product. The inversion group has only two one-dimensional representations: the even g and the odd u. As a result, we obtain a doubling of the representations of the group $SO(3)$ into D^l_g and D^l_u, or briefly D^l_p, where $p = \pm 1$ is the parity.

It should be noted that in the space of functions on the sphere, the representations of the inversion group are realized by even and odd functions. However, the presence of $SO(3)$ symmetry exhausts the possible set of functions, since the system of eigenfunctions of this group is complete, and the symmetry of these functions with respect to inversion is fixed: the functions Y_{lm} have parity $(-1)^l$. Therefore, the function space is formally extended by introducing scalar and pseudoscalar functions: the former transform in the usual way under inversion, as functions of transformed coordinates ($\theta \to \pi - \theta$, $\phi \to \pi + \phi$), while pseudoscalars are additionally multiplied by -1. For example, the bases of D^0_g and D^0_u consist of the ordinary and pseudoscalar Y_{00} respectively. In contrast, for D^1_g and D^1_u one must take the pseudoscalar (axial vector) and ordinary Y_{1m}, respectively. The representations D^0_g, D^0_u, $V = D^1_u$, and $A = D^1_g$ are called scalar, pseudoscalar, vector, and axial, respectively.

The classes of conjugate elements of $SO(3)$ consist of all rotations by the same angle α. In the group $O(3)$, they are doubled by adding the inversion to each rotation yielding the improper rotation denoted by $\bar{\alpha}$. The characters are as follows:

$$\chi^l_p[\alpha] = \frac{\sin\left[\left(l + \frac{1}{2}\right)\alpha\right]}{\sin\left[\frac{1}{2}\alpha\right]}, \qquad \chi^l_p[\bar{\alpha}] = p\chi^l_p[\alpha].$$

The direct product of representations decomposes into IRs according to the formulas

$$D^{l_1}_{p_1} \times D^{l_2}_{p_2} = \sum_{l=|l_1-l_2|}^{l_1+l_2} D^l_{p_1p_2}, \qquad \left[D^l_p \times D^l_p\right] = \sum_{k=0}^{l} D^{2k}_g, \quad \left\{D^l_p \times D^l_p\right\} = \sum_{k=1}^{l} D^{2k-1}_g.$$

Clebsch–Gordan coefficients can be written in terms of 3j symbols [`MatrixElemYlm`]:

$$Y_{l_1m_1}Y_{l_2m_2} = \sum_{l=|l_1-l_2|}^{l_1+l_2} (-1)^{m_1+m_2} \sqrt{\frac{(2l_1+1)(2l_2+1)(2l+1)}{4\pi}} \begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix} Y_{l,m_1+m_2},$$

The representations of the two-dimensional group of proper rotations $SO(2)$ are all one-dimensional, since the group is abelian. They are numbered by the azimutal number $m \in \mathbb{Z}$, and the representation operators are the numbers $T[R(\alpha)] = \mathrm{e}^{-\mathrm{i}m\alpha}$.

§4. Point group symmetry elements

The following symmetry elements of point groups are distinguished (alternative notations are given in curly brackets including Hermann–Mauguin (international) and Schoenflies notations):

- $\{1,\ e\}$ – identity transformation.
- $\{\bar{1}$, -1, $i\}$ – inversion.
- $\sigma(\theta,\phi) = -R(\pi,\theta,\phi)$ – reflection through the plane orthogonal to vector (θ,ϕ), $\sigma(\theta) \equiv \sigma(\theta, 0)$.
- $\{\cdot$/m, $\sigma_h\}$ – horizontal plane of symmetry $\sigma(0,0)$ (perpendicular to the principal axis).
- $\{\cdot$m, $\sigma_v\}$ – vertical plane of symmetry $\sigma(\pi/2,\phi)$, the default $\sigma_v = \sigma(\pi/2, 0)$ (yz-plane).
- $c(\alpha) = R(\alpha, [001]) = R_y(0, 0, \alpha)$ – rotation by angle α about z-axis (principal axis).
- $\{n,\ c_n = c(2\pi/n)\}$ – nth order rotation axis.
- $u_2(\theta,\phi) = R(\pi,\theta,\phi) = R_y(\pi - \phi, 2\theta, \phi)$ – 2nd order oblique axis;
- $\{\cdot/2,\ u_{2h}\}$ – horizontal 2nd order axis, the default $u_{2h} = R(\pi, [100])$ (x-axis).
- $\{\bar{n}$, -n, $c_{ni} = -c_n\}$ – rotoinversion (improper rotation) about the principal axis.

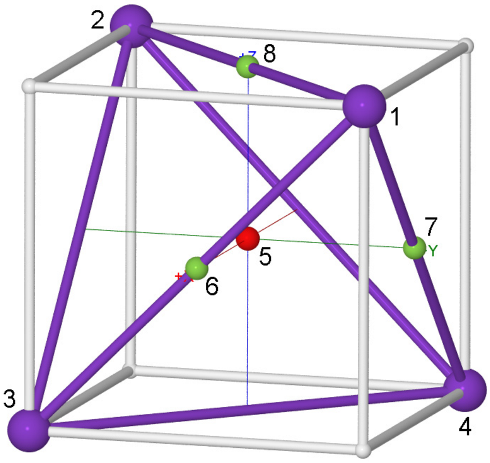

Figure 1: Tetrahedron in cube.

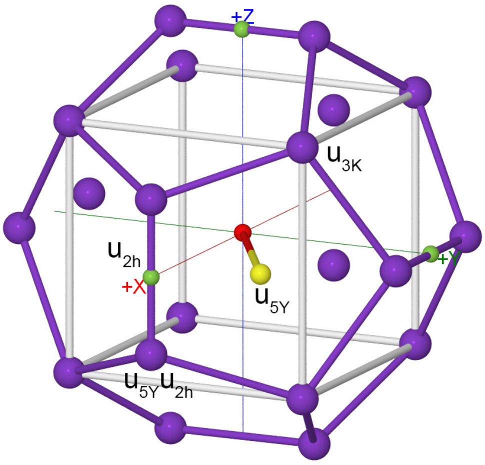

Figure 2: Dodecahedron in cube.

- $\{\tilde{n},\, s_n = c_n\sigma_h\}$ – rotoreflection, note that $s(\alpha) = c_i(\alpha - \pi)$ and $s_n = c_2 c_{ni}$.

Note that for polyhedral symmetry elements are conveniently considered in the "cubic" orientation where u_2 axes are aligned with the coordinates axes, see Figs. 1 and 2. This simplifies matrix form of all symmetry elements. We use special notations for non-horizontal and non-vertical axes: u_{2K} is the 2nd order generating axis of the cube and tetrahedron [101], $u_{3K} = R_y(\pi/2, \pi/2, 0)$ is the principal axis of the tetrahedron or through-vertex axis of the cube and dodecahedron [111], u_{5Y} is the principal axis of the dodecahedron $[\sqrt{5}+1, 2, 0]$.

Note that there are many relationships between these symmetry elements, in particular: $c_{1i} = s_2 = -1$, $c_{2i} = s_1 = \sigma_h$, $\sigma_v = -u_{2h}$.

All point groups can be constructed using the following principles. From Eq. (2.1) it follows that any rotation can be obtained by a combination of only two elements, $c(\alpha)$ and $u_2(\theta)$, namely:

$$R(\alpha, [\theta, \phi]) = c(\phi)u_2(\theta/2)c(\alpha)u_2(\theta/2)c(-\phi).$$

Consequently, any element of the group $O(3)$ can be obtained by a combination of only three elements, $c(\alpha)$, $u_2(\theta)$, and the inversion -1, in particular

$$\sigma(\theta, \phi) = -c(\phi)u_2(\theta/2)c_2u_2(\theta/2)c(-\phi).$$

The matrices of these basic symmetry elements have the following form:

$$c(\alpha) = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad u_2(\theta/2) = \begin{pmatrix} -\cos\theta & 0 & \sin\theta \\ 0 & -1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix}.$$

Point groups can be visualized using stereographic projection.

§5. Point groups

Point symmetry groups in three-dimensional space are finite (finiteness is equivalent to discreteness) subgroups of the group $O(3)$. They are divided into five classes corresponding to the five finite subgroups of the group $SO(3)$: C_n, D_n, T, O, Y. The generating elements of the point groups are cc_n, $u_2(\theta)$, and i, or their combinations. The construction of point groups proceeds in two stages. First, by adding a 2nd order oblique axis to the trivial cyclic group C_n, we obtain all proper point groups. Then by adding the inversion we obtain the rest of groups.

Let start with proper groups. Note that each proper point group is uniquely associated with a regular polyhedron or its dual, for which it is a symmetry group. In this case, the symmetry elements c_n pass through the vertices of the polyhedron, u_2 pass through the midpoints of the edges, and the elements $(c_n u_2)^{-1}$ pass through the centers of the faces. Let fix the orientation in such a way that the axes c_n, u_2, and $(c_n u_2)^{-1}$ form a right-handed triple of vectors of minimal volume, i.e. all of them are attached to a single face. To decide

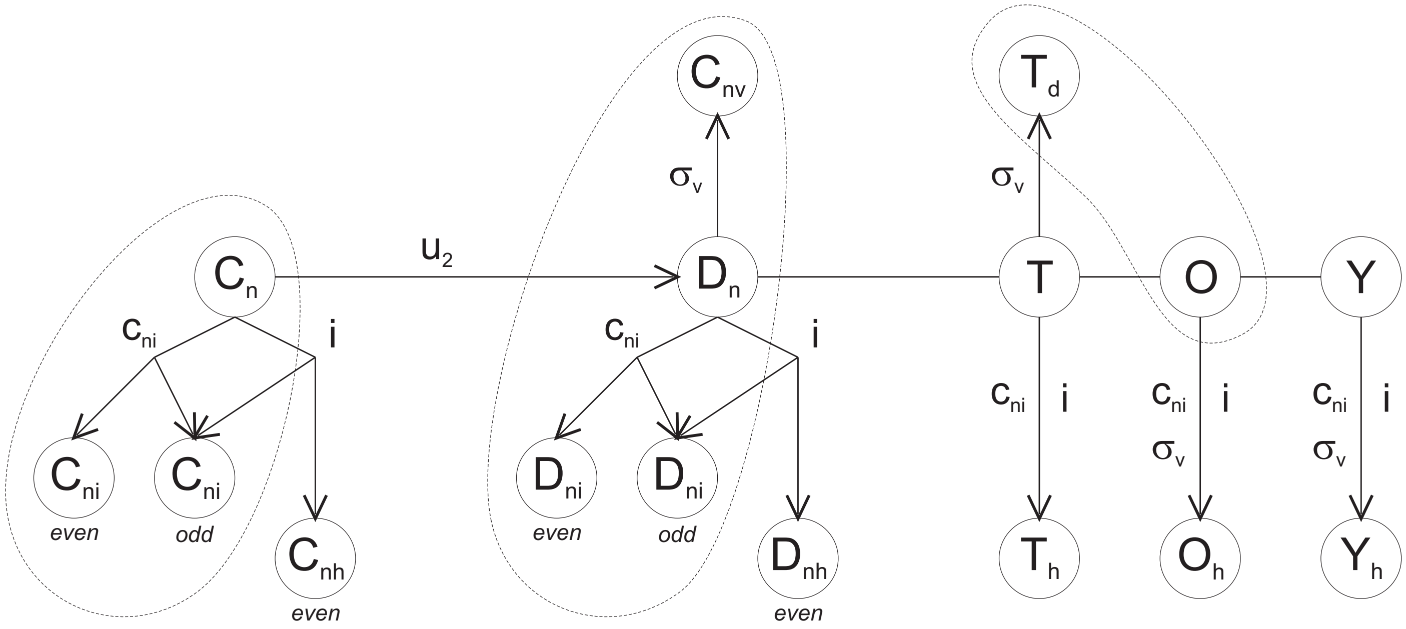

Figure 3: Hierarchy of point groups (isomorphic groups are combined).

between the polyhedron and its dual, we choose the simpler faces. Next,we note that combinations of only c_n and $u_2(\theta)$ do not yield new generating elements. Therefore, proper groups can have only two sets of generating elements: $\{c_n\}$ and $\{c_n, u_2(\theta)\}$. The first set generates C_n groups. For the second set, θ can take only a limited set of values (due to the finiteness of the generated group), which is summarized in the following table:

	n	θ	n'	polyhedron	dual
C_n	n			pyramid	pyramid
D_n	n	$\pi/2$	2	prism (dihedron)	bipyramid
T	3	$\cos 2\theta = -1/3$	3	tetrahedron	tetrahedron
O	4	$\pi/4$	3	octahedron	cube
Y	5	$\cos 2\theta = 1/\sqrt{5}$	3	icosahedron	dodecahedron

where n' is the order of the axis $(c_n u_2)^{-1}$, and for exceptional groups $\cos 2\theta = [1/\cos(2\pi/n) - 1]^{-1}$.

Now we need to include the inversion. For the generating set $\{c_n\}$, there are only two new sets of generators: $\{-c_n\}$ and $\{c_{2k}, -1\}$, because $G\{c_{2k+1}, -1\} = G\{-c_{2k+1}\}$. The corresponding groups are

$$G\{-c_n\} = C_{ni}, \quad G\{c_{2k}, -1\} = C_{2k,h}.$$

For the generating set $\{c_n, u_2(\theta)\}$, three new sets of generators are possible: $\{-c_n, u_2(\theta)\}$, $\{c_n, -u_2(\theta)\}$, and $\{c_n, u_2(\theta), -1\}$. This expand the dihedral class with the following groups:

$$G\{-c_n, u_{2h}\} = D_{ni}, \quad G\{c_n, -u_{2h}\} = C_{nv}, \quad G\{c_{2k}, u_{2h}, -1\} = D_{2k,h},$$

where $G\{c_{2k+1}, u_{2h}, -1\} = G\{-c_{2k+1}, u_{2h}\}$. For the exceptional classes, we obtain:

$$\begin{gathered} G\{-c_3, u_{2T}\} = G\{c_3, u_{2T}, -1\} = T_h,\ G\{c_3, -u_{2T}\} = T_d, \\ G\{-c_4, u_{2K}\} = G\{c_4, -u_{2K}\} = G\{c_4, u_{2K}, -1\} = O_h, \\ G\{-c_5, u_{2Y}\} = G\{c_5, u_{2Y}, -1\} = Y_h \sim G\{c_5, -u_{2Y}\}. \end{gathered}$$

This exhausts all possible point groups; see Fig. 3 and Table 1.

From the perspective of abstract group theory, some point groups are isomorphic, as can be seen by the generators in Table 1. Up to isomorphism, the set of point groups include only C_n, D_n, T, O, Y, and their direct products with C_2 for even n. The latter condition follows from the isomorphisms $C_2 \times C_{2k+1} \sim C_{4k+2}$ and $C_2 \times D_{2k+1} \sim D_{4k+2}$. Reduction of other point groups to this set is given in Table 1.

In practical applications, alternative notations for some point groups are used, based on replacing the inversion as the generating element with σ_h. In this case the rotoinversion axes are replaced by rotoreflection

group		ord	a	b	c	$(ab)^{-1}$	generators	isomorphisms
C_n		n	c_n				$1= a^n =$	
C_{ni}	$2k$	n	c_{ni}				$1= a^n =$	$\sim C_{2k}$
	$2k{+}1$	$2n$	c_{ni}				$1= a^{2n}=$	$\sim C_{4k+2}$
C_{nh}	$2k$	$2n$	c_n		i		$1= a^n =$	$= c^2, ac = ca$
D_n		$2n$	c_n	u_{2h}		u'_{2h}	$1= a^n = b^2 = (ab)^2$	
D_{ni}	$2k$	$2n$	c_{ni}	u_{2h}		σ'_v	$1= a^n = b^2 = (ab)^2$	$\sim D_{2k}$
	$2k{+}1$	$4n$	c_{ni}	u_{2h}		σ'_v	$1= a^{2n}= b^2 = (ab)^2$	$\sim D_{4k+2}$
D_{nh}	$2k$	$4n$	c_n	u_{2h}	i	u'_{2h}	$1= a^n = b^2 = (ab)^2$	$= c^2, ac = ca, bc = cb$
C_{nv}		$2n$	c_n	σ_v		σ'_v	$1= a^n = b^2 = (ab)^2$	$\sim D_n$
T		12	c_3	u_{2T}		c'_3	$1= a^3 = b^2 = (ab)^3$	$\sim A_4$
T_h		24	c_{3i}	u_{2T}		c'_{3i}	$1= a^6 = b^2 = (ab)^6$	
T_d		24	c_3	σ_{vT}		c'_{4i}	$1= a^3 = b^2 = (ab)^4$	$\sim O$
O		24	c_4	u_{2K}		u_{3K}	$1= a^4 = b^2 = (ab)^3$	$\sim S_4$
O_h		48	c_{4i}	u_{2K}		u_{3iK}	$1= a^4 = b^2 = (ab)^6$	
Y		60	c_5	u_{2Y}		u_{3Y}	$1= a^5 = b^2 = (ab)^3$	$\sim A_5$
Y_h		120	c_{5i}	u_{2Y}		u_{3iY}	$1= a^{10}= b^2 = (ab)^6$	

Table 1: Point groups classified by generators. For exceptional groups, the relations between generating elements do not determine the group uniquely except for T and Y.

G	ord	a	b	c	$(ab)^{-1}$	polyhedron
C_n	n	c_n				proper pyramid
C_{nd}	$2n$	s_{2n}				pseudoantiprism
C_{nh}	$2n$	c_n		σ_h		pseudoprism
C_{nv}	$2n$	c_n	σ_v		σ'_v	pyramid
D_n	$2n$	c_n	u_{2h}		u'_{2h}	proper prism
D_{nd}	$4n$	s_{2n}	u_{2h}		σ'_v	antiprism
D_{nh}	$4n$	c_n	u_{2h}	σ_h	u'_{2h}	prism
T	12	c_3	u_{2T}		c'_3	proper tetrahedron
T_h	24	s_6	u_{2T}		s'_6	pseudocube
T_d	24	c_3	σ_{vT}		s'_4	tetrahedron
O	24	c_4	u_{2K}		u_{3K}	proper cube
O_h	48	s_4	u_{2K}		s'_6	cube
Y	60	c_5	u_{2Y}		u_{3Y}	proper icosahedron
Y_h	120	s_{10}	u_{2Y}		s'_6	icosahedron

Table 2: Alternative choice of point groups.

Scho	C_n	C_{ni}	C_{nh}	D_n	D_{nd}	D_{nh}	C_{nv}	E_n	E_{nh}	E_{nv}	
H-M odd	n	-n		n2	-nm	-(2n)m2	nm				
H-M even	n	-n	n/m	n22	-(2n)2m	n/mmm	$n$mm				
1	1	-1	m	(2)	(2/m)	(2/m)	(m)				
2	2	(m)	2/m	222	-42m	mmm	mm2				
3	3	-3	-6	32	-3m	-62m	3m	23	m-3	-43m	T
4	4	-4	4/m	422	-82m	4/mmm	4mm	432	m-3m		O
5	5	-5	-10	52	-5m	-102m	5m	25	m-5		Y
6	6	(-6)	6/m	622	-122m	6/mmm	6mm				
...	...	...	...	...	...	...	...				
∞	∞	∞/m	∞/m	∞2	∞/mm	∞/mm	∞mm	∞∞	∞∞m	∞∞m	

Table 3: Correspondence between Schoenflies and Hermann–Mauguin notations (duplicates are in parentheses).

axes. This allows to associate each point group with the symmetry of a decorated regular polyhedron. The decoration assigns “signs” to the vertices which flips under improper transformations. In particular, all vertices of proper polyhedra have the same sign; a pseudoprism and a pseudoantiprism have positive and negative vertices on their upper and lower faces, respectively; a pseudocube consists of a cube formed by joining a positive and negative tetrahedrons. Thus introduced groups are listed in Table 2 together with their generators and polyhedra. The relation between the alternatively defined groups are as follows:

$$\begin{pmatrix}C\\D\end{pmatrix}_{2k+1,h}=\begin{pmatrix}C\\D\end{pmatrix}_{4k+2,i},\quad \begin{pmatrix}C\\D\end{pmatrix}_{2k+1,d}=\begin{pmatrix}C\\D\end{pmatrix}_{2k+1,i},\quad \begin{pmatrix}C\\D\end{pmatrix}_{2k,d}=\begin{pmatrix}C\\D\end{pmatrix}_{4k,i}.$$

Sometimes groups $S_n = G\{s_n\}$ are introduced. They relate to “canonical” point groups by the identities $S_{2k+1} = C_{4k+2,i}$, $S_{4k} = C_{4k,i}$, $S_{4k+2} = C_{2k+1,i}$.

International notations for point groups are given in Table 3.

There are many group relations between point groups. Any group $G_h = G \times I$, where I is the inversion group and G can be $C_{2k,h}$, $D_{2k,h}$, T, O, or Y. Other direct products:

$$\begin{pmatrix}C\\D\end{pmatrix}_{nh}=\begin{pmatrix}C\\D\end{pmatrix}_{n}\times\Sigma_h,\quad \begin{pmatrix}C\\D\end{pmatrix}_{2k+1,i}=\begin{pmatrix}C\\D\end{pmatrix}_{2k+1}\times I,\quad O_h=T_d\times I.$$

Semidirect products:

$$D_n = C_n \rtimes U_{2h},\quad C_{nv} = C_n \rtimes \Sigma_v,\quad D_{nd} = D_n \rtimes \Sigma_v\left(\frac{\pi}{2}+\frac{\pi}{2n}\right),$$
$$T = D_2 \rtimes U_{3K},\quad T_d = D_2 \rtimes U_{3vK},\quad O = T \rtimes U_{2K},$$

where U_2, U_3, and U_{3v} are rotated groups C_2, C_3, and C_{3v}. Regarding C_{nd}, we can only say that C_n is its invariant subgroup. A series of relations can be obtained by taking into account the arbitrariness of the position of the group I in direct and semidirect products. The maximal subgroups of Y_h are T_h, D_{5d}, and D_{2h}.

There are also 7 limiting symmetry groups (see also Table 3):

C_∞	∞	proper cone
$C_{\infty i} = C_{\infty h}$	∞/m	pseudocylinder
D_∞	∞2	proper cylinder
$D_{\infty i} = D_{\infty h}$	∞/mm	cylinder
$C_{\infty v}$	∞mm	cone
E_∞	$\infty\infty$	proper sphere
$E_{\infty h} = E_{\infty v}$	$\infty\infty$m	sphere

In two-dimensional space, there are only two types of point groups: C_n and D_n, which belong to the same class C_n.

§6. Point group representations

There are standard notations for IRs: letters A and B denote one-dimensional IRs that are symmetric and antisymmetric with respect to the principal rotation c_n; single or double prime denote symmetry or antisymmetry with respect to the reflection σ_h; multidimensional IRs are denoted by letters E, F (or T), G, H; indices g and u denote even and odd IRs with respect to the inversion; indices 1 and 2 denote symmetric and antisymmetric IRs with respect to the rotation u_2 or the reflection σ_v (or simply enumerate representations for high-order axes).

Since the representations of isomorphic groups are identical, it is enough to consider only non-isomorphic groups. Furthermore, IRs of the direct product $G \times I$ are obtained by doubling the representations of the group G into symmetric and antisymmetric ones, using the formula $T(ig) = \pm T(g)$. If we denote by R the column of irreducible representations of the group G and by M its characters table, then the characters of the IRs of the direct product can be written as

	G	$i \cdot G$
R_g	M	M
R_u	M	$-M$

C_1				e	
	C_i			e	$\boldsymbol{i}$
		C_s		e	$\boldsymbol{\sigma_h}$
			C_2	e	$\boldsymbol{c_2}$
A	A_g	A'	A	1	1
	A_u	A''	B	1	−1
			C_{2h}	$\boldsymbol{i}$	σ_h

C^{2d}_{4i}	e	c_2	$\boldsymbol{c_{4i}}$	c^{-1}_{4i}
C_4	e	c_2	$\boldsymbol{c_4}$	c^{-1}_4
A	1	1	1	1
B	1	1	−1	−1
E	1	−1	i	−i
	1	−1	−i	i
C_{4h}	$\boldsymbol{i}$	σ_h	c_{4i}	c^{-1}_{4i}

C_3				e	$\boldsymbol{c_3}$	c^{-1}_3			
	C^{3d}_{3i}			e	c_3	c^{-1}_3	i	$\boldsymbol{c_{3i}}$	c^{-1}_{3i}
		C^{3h}_{6i}		e	c_3	c^{-1}_3	σ_h	$\boldsymbol{c_{6i}}$	c^{-1}_{6i}
			C_6	e	c^{-1}_3	c_3	c_2	$\boldsymbol{c_6}$	c^{-1}_6
A	A_g	A'	A	1	1	1	1	1	1
E	E_g	E'	E_2	1	q	q^2	1	q	q^2
				1	q^2	q	1	q^2	q
	A_u	A''	B	1	1	1	−1	−1	−1
	E_u	E''	E_1	1	q	q^2	−1	$-q$	$-q^2$
				1	q^2	q	−1	$-q^2$	$-q$
			C_{6h}	$\boldsymbol{i}$	c^{-1}_{3i}	c_{3i}	σ_h	c_{6i}	c^{-1}_{6i}

C_2				e	$\boldsymbol{c_2}$		
	C_{2h}			e	$\boldsymbol{c_2}$	$\boldsymbol{i}$	σ_h
		C_{2v}		e	$\boldsymbol{c_2}$	$\boldsymbol{\sigma_v}$	σ'_v
			D_2	e	$\boldsymbol{c_2}$	$\boldsymbol{u_2}$	u'_2
A	A_g	A_1	A	1	1	1	1
B	B_g	B_1	B_2	1	−1	1	−1
	A_u	A_2	B_3	1	1	−1	−1
	B_u	B_2	B_1	1	−1	−1	1
			D_{2h}	$\boldsymbol{i}$	σ_h	σ_v	σ'_v

C_{4v}	e	c_2	$2\boldsymbol{c_4}$	$2\boldsymbol{\sigma_v}$	$2\sigma'_v$
D^{2d}_{4i}	e	c_2	$2\boldsymbol{c_{4i}}$	$2\boldsymbol{u_2}$	$2\sigma'_v$
D_4	e	c_2	$2\boldsymbol{c_4}$	$2\boldsymbol{u_2}$	$2u'_2$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
B_1	1	1	−1	1	−1
B_2	1	1	−1	−1	1
E	2	−2	0	0	0
D_{4h}	$\boldsymbol{i}$	σ_h	$2c_{4i}$	$2\sigma_v$	$2\sigma'_v$

C_{3v}				e	$2\boldsymbol{c_3}$	$3\boldsymbol{\sigma_v}$			
D_3				e	$2\boldsymbol{c_3}$	$3\boldsymbol{u_2}$			
	D^{3d}_{3i}			e	$2c_3$	$3\boldsymbol{u_2}$	i	$2\boldsymbol{c_{3i}}$	$3\sigma_v$
		D^{3h}_{6i}		e	$2c_3$	$3\boldsymbol{u_2}$	σ_h	$2\boldsymbol{c_{6i}}$	$3\sigma'_v$
			C_{6v}	e	$2c_3$	$3\boldsymbol{\sigma_v}$	c_2	$2\boldsymbol{c_6}$	$3\sigma'_v$
			D_6	e	$2c_3$	$3\boldsymbol{u_2}$	c_2	$2\boldsymbol{c_6}$	$3u'_2$
A_1	A_{1g}	A'_1	A_1	1	1	1	1	1	1
A_2	A_{2g}	A'_2	A_2	1	1	−1	1	1	−1
E	E_g	E'	E_2	2	−1	0	2	−1	0
	A_{1u}	A''_1	B_1	1	1	1	−1	−1	−1
	A_{2u}	A''_2	B_2	1	1	−1	−1	−1	1
	E_u	E''	E_1	2	−1	0	−2	1	0
			D_{6h}	$\boldsymbol{i}$	$2c_{3i}$	$3\sigma_v$	σ_h	$2c_{6i}$	$3\sigma'_v$

T	e	$4\boldsymbol{c_3}$	$4c^{-1}_3$	$3\boldsymbol{u_2}$
A	1	1	1	1
E	1	q	q^2	1
	1	q^2	q	1
F	3	0	0	−1
T_h	i	$4\boldsymbol{c_{3i}}$	$4c^{-1}_{3i}$	$3\sigma_v$

T_d	e	$8c_3$	$3u_2$	$6\boldsymbol{c_{4i}}$	$6\boldsymbol{\sigma_v}$
O	e	$8u_3$	$3c_2$	$6\boldsymbol{c_4}$	$6\boldsymbol{u_2}$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
F_1	3	0	−1	1	−1
F_2	3	0	−1	−1	1
O_h	i	$8u_{3i}$	$3\sigma_h$	$6\boldsymbol{c_{4i}}$	$6\sigma_v$

Y	e	$12\boldsymbol{c_5}$	$12c^2_5$	$15\boldsymbol{u_2}$	$20u_3$
A	1	1	1	1	1
F_1	3	$\frac{1+\sqrt{5}}{2}$	$\frac{1-\sqrt{5}}{2}$	−1	0
F_2	3	$\frac{1-\sqrt{5}}{2}$	$\frac{1+\sqrt{5}}{2}$	−1	0
G	4	−1	−1	0	1
H	5	0	0	1	−1
Y_h	i	$12\boldsymbol{c_{5i}}$	$12c^3_{5i}$	$15\sigma_v$	$20u_{3i}$

Table 4: Irreducible representation of point groups classified by generators (in bold), $q = \mathrm{e}^{2\pi\mathrm{i}/3}$. For direct products with the inversion group, only the list of additional classes is given, the representations themselves can be obtained using examples of C_i, C_{3i}, C_{2h}, D_{3i}. The groups C_2 and C_{2h} are duplicated for convenience. Upper indexes denote alternative group names, in this case the rotoinversion should be replaced by the corresponding rotoreflection as follows: $c_{3i} = s^{-1}_6$, $c_{4i} = s^{-1}_4$, $c_{6i} = s^{-1}_3$. Self-representations: $C_{3,4,6}$ and $D_{3,4,6}$ – E, $T_{,h}$ – F, T_d – F_2, $O_{,h}$ and $Y_{,h}$ – F_1.

Therefore, for direct products with the inversion, only the correct order of the new classes should be specified.

Let start with the class C_n. The IRs of cyclic groups are one-dimensional with the IR operators given by

$$T^{A_m}(c_n^l) = q^{ml}, \quad q = \mathrm{e}^{2\pi \mathrm{i}/n}, \quad m, l = 0, \dots, n-1, \tag{6.1}$$

where m enumerates IRs and l enumerates conjugacy classes. In physics, complex-conjugate one-dimensional representations are combined into real two-dimensional. Therefore, we have the following characters table for $n = 2k+1$:

C_n	e	c_n	c_n^{-1}	$\dots$	c_n^l	c_n^{-l}	$\dots c_n^{-k}$
A	1	1	1	$\dots$	1	1	$\dots$
E_1	1	q	q^{-1}	$\dots$	q^l	q^{-l}	$\dots$
	1	q^{-1}	q	$\dots$	q^{-l}	q^l	$\dots$
$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$
E_m	1	q^m	q^{-m}	$\dots$	q^{ml}	q^{-ml}	$\dots$
	1	q^{-m}	q^m	$\dots$	q^{-ml}	q^{ml}	$\dots$
$\dots E_k$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$
C_{ni}	i	c_{ni}	c_{ni}^{-1}	$\dots$	ic_n^l	ic_n^{-l}	$\dots ic_n^{-k}$

and for $n = 2k$:

C_{ni}	e	$(-1)^k c_2$	c_{ni}	c_{ni}^{-1}	$\dots$	c_{ni}^l	c_{ni}^{-l}	$\dots c_{ni}^{-k+1}$
C_n	e	c_2	c_n	c_n^{-1}	$\dots$	c_n^l	c_n^{-l}	$\dots c_n^{-k+1}$
A	1	1	1	1	$\dots$	1	1	$\dots$
B	1	1	-1	-1	$\dots$	$(-1)^l$	$(-1)^l$	$\dots$
E_1	1	-1	q	q^{-1}	$\dots$	q^l	q^{-l}	$\dots$
	1	-1	q^{-1}	q	$\dots$	q^{-l}	q^l	$\dots$
$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$
E_m	1	$(-1)^m$	q^m	q^{-m}	$\dots$	q^{ml}	q^{-ml}	$\dots$
	1	$(-1)^m$	q^{-m}	q^m	$\dots$	q^{-ml}	q^{ml}	$\dots$
$\dots E_{k-1}$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$
C_{nh}	i	σ_h	c_{ni}	c_{ni}^{-1}	$\dots$	ic_n^l	ic_n^{-l}	$\dots ic_n^{-k}$

Moreover, for odd k, the group $C_{2k,i}$ has an element σ_h, and in this case the IRs are denoted differently: $A', A'', E_1', E_1'', E_2', \dots$

The elements of the groups of class D_n are generally represented by two-dimensional matrices, whose values on the generators are as follows:

$$T^{E_m}(c_n) = \begin{pmatrix} q^m & 0 \\ 0 & q^{-m} \end{pmatrix}, \quad T(\sigma) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{6.2}$$

where σ is u_{2h} for D_n or D_{ni} and σ_v for C_{nv}. For some m such representations are reducible thus creating $A_{1,2}$ and $B_{1,2}$ pairs. The resulting IRs for $n = 2k+1$

C_{nv}	e	$n\sigma_v$	$2c_n$	$\dots$	$2c_n^l$	$\dots 2c_n^k$
D_n	e	nu_{2h}	$2c_n$	$\dots$	$2c_n^l$	$\dots 2c_n^k$
A_1	1	1	1	$\dots$	1	$\dots$
A_2	1	-1	1	$\dots$	1	$\dots$
E_1	2	0	$2\cos\frac{2\pi}{n}$	$\dots$	$2\cos\frac{2\pi l}{n}$	$\dots$
$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$
E_m	2	0	$2\cos\frac{2\pi m}{n}$	$\dots$	$2\cos\frac{2\pi ml}{n}$	$\dots$
$\dots E_k$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$
D_{ni}	i	$n\sigma_v$	$2c_{ni}$	$\dots$	$2ic_n^l$	$\dots 2ic_n^k$

and for $n = 2k$

D_{ni}	e	$(-1)^k c_2$	ku_{2h}	$k\sigma'_v$	$2c_{ni}$	$\dots$	$2c^l_{ni}$	$\dots 2c^{k-1}_{ni}$
C_{nv}	e	c_2	$k\sigma_v$	$k\sigma'_v$	$2c_n$	$\dots$	$2c^l_n$	$\dots 2c^{k-1}_n$
D_n	e	c_2	ku_{2h}	ku'_{2h}	$2c_n$	$\dots$	$2c^l_n$	$\dots 2c^{k-1}_n$
A_1	1	1	1	1	1	$\dots$	1	$\dots$
A_2	1	1	-1	-1	1	$\dots$	1	$\dots$
B_1	1	$(-1)^k$	1	-1	-1	$\dots$	$(-1)^l$	$\dots$
B_2	1	$(-1)^k$	-1	1	-1	$\dots$	$(-1)^l$	$\dots$
E_1	2	-2	0	0	$2\cos\frac{2\pi}{n}$	$\dots$	$2\cos\frac{2\pi l}{n}$	$\dots$
$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$
E_m	2	$2(-1)^m$	0	0	$2\cos\frac{2\pi m}{n}$	$\dots$	$2\cos\frac{2\pi ml}{n}$	$\dots$
$\dots E_{k-1}$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$
D_{nh}	i	σ_h	$k\sigma_v$	$k\sigma'_v$	$2c_{ni}$	$\dots$	$2ic^l_n$	$\dots 2ic^{k-1}_n$

Again, for odd k, the group $D_{2k,i}$ contains the element σ_h, and the IRs are denoted as $A'_1, A'_2, A''_1, A''_2, E'_1, E''_1, E'_2, \dots$ Real-valued two-dimensional representations can be obtained by rotating the basis with a unitary matrix

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ \mathrm{i} & -\mathrm{i}\end{pmatrix},\ \text{yielding } \tilde{T}(c_n) \equiv UT(c_n)U^{-1} = \begin{pmatrix}\cos\frac{2\pi m}{n} & \sin\frac{2\pi m}{n}\\ -\sin\frac{2\pi m}{n} & \cos\frac{2\pi m}{n}\end{pmatrix},\ \tilde{T}(\sigma) = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{6.3}$$

Irreducible representations of exclusive groups are constructed using special methods not discussed here. The resulting characters tables are given in Table 4. Three-dimensional IRs are self-representations: for the octahedron, F_1 and F_2 are self-representations by the groups O and T_d, respectively; for the icosahedron, F_1 is a self-representation, and F_2 is a self-representation with an alternative choice of the oblique second-order axis. The three one-dimensional IRs of the tetrahedron correspond to IRs of the group $C_3 \sim T/D_2$. The two one-dimensional and one two-dimensional IRs of the octahedron correspond to IRs of the group $C_{3v} \sim T_d/D_2$. The four-dimensional IR G of the icosahedron together with the one-dimensional A is a self-representation of the group $A_5 \sim Y$. The five-dimensional IR H together with A is one of the IRs of the group S_6, acting on six pairs of opposite vertices of the icosahedron.

To decompose the representations of the rotation group into IRs of point groups, the following characters table is used:

		e	c_2	c_n	i	σ	c_{ni}
S	χ^0_g	1	1	1	1	1	1
A	χ^1_g	3	-1	$1+2\cos(2\pi/n)$	3	-1	$1+2\cos(2\pi/n)$
	χ^0_u	1	1	1	-1	-1	-1
V	χ^1_u	3	-1	$1+2\cos(2\pi/n)$	-3	1	$-1-2\cos(2\pi/n)$
	χ^l_p	$2l+1$	$(-1)^l$	$\frac{\sin[(2l+1)\pi/n]}{\sin[\pi/n]}$	$p(2l+1)$	$p(-1)^l$	$p\frac{\sin[(2l+1)\pi/n]}{\sin[\pi/n]}$

§7. Cubic symmetry m-3m

In this and subsequent sections, we will follow the notations of the Bilbao Crystallographic Server.

The group O_h=m-3m and its subgroups are special: they are frequently found in nature and possess all symmetry elements up to 4th order axis. Its proper subgroup O=432 consists of $3c_4$ axes aligned with the coordinate axes, $4c_3$ axes along the main diagonals of the cube, and $6c_2$ axes along the minor diagonals of the cube. Their representatives are

$$c_4 = R(\pi/2,[001]) = \begin{pmatrix}0 & -1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 1\end{pmatrix},\ u_{3K} = R(2\pi/3,[111]) = \begin{pmatrix}0 & 0 & 1\\ 1 & 0 & 0\\ 0 & 1 & 0\end{pmatrix},\ u_{2K} = R(\pi,[101]) = \begin{pmatrix}0 & 0 & 1\\ 0 & -1 & 0\\ 1 & 0 & 0\end{pmatrix}.$$

Any two elements from this triple are generators because $c_4u_{2K}u_{3K} = 1$. Multiplying by the inverse yields the elements c_{4i}, u_{3iK}, σ_{vK}. The generating elements of the group O_h will be the same as those for the group O, but one of them is replaced by an improper rotation.

It is convenient to denote elements of cubic groups by the transformation of the three functions $\{x, y, z\}$, where a bar above a function denotes a minus sign in front of it. For example, $c_4 = \bar{y}xz$, $u_{3K} = zxy$, $u_{2K} = z\bar{y}x$, $i = \bar{x}\bar{y}\bar{z}$. Using these notations, the equality $c_4 u_{2K} u_{3K} = 1$ is proven as follows:

$$\begin{array}{ccccccc}
 & & xyz & \xrightarrow{u_{2K}} & z\bar{y}x & & \\
\hline
\multicolumn{1}{|c}{xyz} & \xrightarrow[u_{3K}]{} & zxy & \to & y\bar{x}z & \to & \multicolumn{1}{c|}{xyz} \\
\hline
 & & & & xyz & \xrightarrow[c_4]{} & \bar{y}xz
\end{array}$$

The functionally simplest IR basis functions of the group O_h are listed in Table 5. These functions often conveniently replace spherical harmonics. Sometimes the monomial basis $x^k y^m z^n$ is used but it permutes IRs of the rotation group. Interestingly, the functions of all F_2 IRs from Table 5 can be obtained by rotating a single function of another representation: $x'y'$, xyz, $x'y'(7z^2 - r^2)$, but this rotation is not an element of cubic symmetry.

The decomposition of the IRs the rotation group into IRs of the group O_h is as follows (see the basis functions in Table 5)

	1	3	2	4	$2'$	-1	-3	m	-4	m'	S	P	D	F	G	H				
	1	8	3	6	6	1	8	3	6	6	0	1	2	3	4	5	6	7	8	9
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	.	.	.	1	.	1	.	1	.
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1	.	.	.	.	.	.	.	.	.	1
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1	.	.	.	.	.	.	1	.	.	.
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1	.	.	.	1	.	.	.	1	.	1
E_g	2	-1	2	0	0	2	-1	2	0	0	.	.	1	.	1	.	1	.	2	.
E_u	2	-1	2	0	0	-2	1	-2	0	0	.	.	.	.	.	1	.	1	.	1
F_{1g}	3	0	-1	1	-1	3	0	-1	1	-1	.	.	.	.	1	.	1	.	2	.
F_{1u}	3	0	-1	1	-1	-3	0	1	-1	1	.	1	.	1	.	2	.	2	.	3
F_{2g}	3	0	-1	-1	1	3	0	-1	-1	1	.	.	1	.	1	.	2	.	2	.
F_{2u}	3	0	-1	-1	1	-3	0	1	1	-1	.	.	.	1	.	1	.	2	.	2

The IR multiplication table for the group O is as follows

	A_2	E	F_1	F_2
A_2	A_1	E	F_2	F_1
E		$A_1 + A_2 + E$	$F_1 + F_2$	$F_1 + F_2$
F_1			$A_1 + E + F_1 + F_2$	$A_2 + E + F_1 + F_2$
F_2				$A_1 + E + F_1 + F_2$

§8. Tetrahedral symmetry -43m

The decomposition of the IRs the rotation group into IRs of the group T_d=-43m is as follows

	e	$8c_3$	$3c_2$	$6c_{4i}$	$6\sigma_v$	0	1	2	3	4	5	6
A_1	1	1	1	1	1	1	.	.	1	1	.	1
A_2	1	1	1	-1	-1	.	.	.	.	.	.	1
E	2	-1	2	0	0	.	.	1	.	1	1	1
F_1	3	0	-1	1	-1	.	.	.	1	1	1	1
F_2	3	0	-1	-1	1	.	1	1	1	1	2	2

Orbits (see Fig. 4), decomposition of regular representation, stabilizer:

	e	$8c_3$	$3c_2$	$6c_{4i}$	$6\sigma_v$		
Λ, Λ'	4	1	0	0	2	$A_1 + F_2$	C_{3v}
Δ	6	0	2	0	2	$A_1 + E + F_2$	C_{2v}
$\Lambda\Lambda', \Lambda\Delta, \Lambda'\Delta$	12	0	0	0	2	$A_1 + E + F_1 + 2F_2$	C_{1v}

L	IR	label	harmonic polynomials	real spherical harmonics
0	A_{1g}	S	1	$\tilde{Y}_{00}$
1	F_{1u}	X	x	$\tilde{Y}_{11}$
		Y	y	$\tilde{Y}_{1-1}$
		Z	z	$\tilde{Y}_{10}$
2	E_g	$X2$	$x'y'$	$\tilde{Y}_{22}$
		$Z2$	$3z^2 - r^2$	$\tilde{Y}_{20}$
	F_{2g}	YZ	yz	$\tilde{Y}_{2-1}$
		ZX	zx	$\tilde{Y}_{21}$
		XY	xy	$\tilde{Y}_{2-2}$
3	A_{2u}	XYZ	xyz	$\tilde{Y}_{3-2}$
	F_{1u}	$X3$	$x(5x^2 - 3r^2)$	$-\sqrt{\frac{3}{8}}\ \tilde{Y}_{31}\ +\sqrt{\frac{5}{8}}\ \tilde{Y}_{33}$
		$Y3$	$y(5y^2 - 3r^2)$	$-\sqrt{\frac{3}{8}}\ \tilde{Y}_{3-1}\ -\sqrt{\frac{5}{8}}\ \tilde{Y}_{3-3}$
		$Z3$	$z(5z^2 - 3r^2)$	$\tilde{Y}_{30}$
	F_{2u}	$XY2$	$xy'z'$	$-\sqrt{\frac{5}{8}}\ \tilde{Y}_{31}\ -\sqrt{\frac{3}{8}}\ \tilde{Y}_{33}$
		$YZ2$	$yz'x'$	$\sqrt{\frac{5}{8}}\ \tilde{Y}_{3-1}\ -\sqrt{\frac{3}{8}}\ \tilde{Y}_{3-3}$
		$ZX2$	$zx'y'$	$\tilde{Y}_{32}$
4	A_{1g}	$S4$	$5(x^4 + y^4 + z^4) - 3r^4$	$\sqrt{\frac{7}{12}}\ \tilde{Y}_{40}\ +\sqrt{\frac{5}{12}}\ \tilde{Y}_{44}$
	E_g	$X2Z2$	$x'y'(7z^2 - r^2)$	$\tilde{Y}_{42}$
		$Z4$	$r^4 + 4z^2r^2 - 7z^4 - 14x^2y^2$	$-\sqrt{\frac{5}{12}}\ \tilde{Y}_{40}\ +\sqrt{\frac{7}{12}}\ \tilde{Y}_{44}$
	F_{1g}	$YZY2$	$yzy'z'$	$-\sqrt{\frac{7}{8}}\ \tilde{Y}_{4-1}\ -\sqrt{\frac{1}{8}}\ \tilde{Y}_{4-3}$
		$ZXZ2$	$zxz'x'$	$\sqrt{\frac{7}{8}}\ \tilde{Y}_{41}\ -\sqrt{\frac{1}{8}}\ \tilde{Y}_{43}$
		$XYX2$	$xyx'y'$	$\tilde{Y}_{4-4}$
	F_{2g}	$YZX2$	$yz(7x^2 - r^2)$	$-\sqrt{\frac{1}{8}}\ \tilde{Y}_{4-1}\ +\sqrt{\frac{7}{8}}\ \tilde{Y}_{4-3}$
		$ZXY2$	$zx(7y^2 - r^2)$	$-\sqrt{\frac{1}{8}}\ \tilde{Y}_{41}\ -\sqrt{\frac{7}{8}}\ \tilde{Y}_{43}$
		$XYZ2$	$xy(7z^2 - r^2)$	$\tilde{Y}_{4-2}$
5	E_u	$XYZX2$	$xyzx'y'$	$\tilde{Y}_{5-4}$
		$XYZZ2$	$xyz(3z^2 - r^2)$	$\tilde{Y}_{5-2}$
6	A_{2g}	$X2Y2Z2$	$(x'y')(y'z')(z'x')$	$-\sqrt{\frac{11}{16}}\ \tilde{Y}_{62}\ +\sqrt{\frac{5}{16}}\ \tilde{Y}_{66}$
9	A_{1u}		$xyz(x'y')(y'z')(z'x')$	$-\sqrt{\frac{17}{24}}\ \tilde{Y}_{9-4}\ +\sqrt{\frac{7}{24}}\ \tilde{Y}_{9-8}$

Table 5: Cubic harmonics. Here $r^2 = x^2 + y^2 + z^2$. Primes denote pairs of coordinates rotated by $\pi/4$: $x', y' = (x \pm y)/\sqrt{2}$ such that $x'y' \equiv x^2 - y^2$; note that $x'y'$ is not a product but a shorthand notation for the expression $x^2 - y^2$. Different pairs are distinguished by parentheses: $(x'y')(y'z') \equiv (x^2 - y^2)(y^2 - z^2)$. For $L > 4$, the functions are listed selectively to include the function with the smallest L for all IRs. The function $S4$ can also be written in another form $r^4 - 5(x^2y^2 + y^2z^2 + z^2x^2)$.

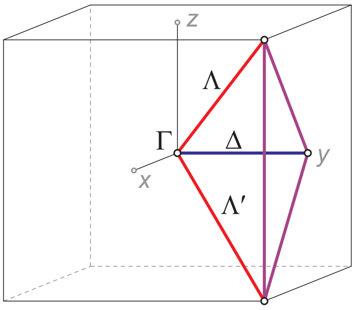

Figure 4: Orbits of the group -43m.

Decomposition over irreducible representations of stabilizers:

		e	c_3	c_2	σ_v	σ'_v		A_1	A_2	E	F_1	F_2
C_{3v}	A_1	1	1		1		$S; P_z$	1	.	.	.	1
	A_2	1	1		-1		D_{xy}	.	1	.	1	.
	E	2	-1		0		P_x, P_y	.	.	1	1	1
C_{2v}	A_1	1		1	1	1	$S; P_z$	1	.	1	.	1
	A_2	1		1	-1	-1	D_{xy}	.	1	1	1	.
	B_1	1		-1	1	-1	P_y	.	.	.	1	1
	B_2	1		-1	-1	1	P_x	.	.	.	1	1
C_{1v}	A'	1			1		$S; P_y, P_z$	1	.	1	1	2
	A''	1			-1		P_x	.	1	1	2	1

Multiplication table

	A_2	E	F_1	F_2
A_2	A_1	E	F_2	F_1
E		$A_1 + A_2 + E$	$F_1 + F_2$	$F_1 + F_2$
F_1			$A_1 + E + F_1 + F_2$	$A_2 + E + F_1 + F_2$
F_2				$A_1 + E + F_1 + F_2$

§9. Hexagonal symmetry 6/mmm

The decomposition of the IRs the rotation group into IRs of the group D_{6h}=6/mmm is as follows

	1	6	3	2_z	2_y	2_x	-1	-6	-3	m_z	m_y	m_x	0	1	2	3	4	5	6	7
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1	1	.	1	.	1	.	2	.
A_{1u}	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	.	.	.	.	.	.	.	1
A_{2g}	1	1	1	1	-1	-1	1	1	1	1	-1	-1	.	.	.	.	.	.	1	.
A_{2u}	1	1	1	1	-1	-1	-1	-1	-1	-1	1	1	.	1	.	1	.	1	.	2
B_{1g}	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	.	.	.	.	1	.	1	.
B_{1u}	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1	.	.	.	1	.	1	.	1
B_{2g}	1	-1	1	-1	-1	1	1	-1	1	-1	-1	1	.	.	.	.	1	.	1	.
B_{2u}	1	-1	1	-1	-1	1	-1	1	-1	1	1	-1	.	.	.	1	.	1	.	1
E_{1g}	2	1	-1	-2	0	0	2	1	-1	-2	0	0	.	.	1	.	1	.	2	.
E_{1u}	2	1	-1	-2	0	0	-2	-1	1	2	0	0	.	1	.	1	.	2	.	3
E_{2g}	2	-1	-1	2	0	0	2	-1	-1	2	0	0	.	.	1	.	2	.	2	.
E_{2u}	2	-1	-1	2	0	0	-2	1	1	-2	0	0	.	.	.	1	.	2	.	2

§10. Ellipsoid symmetry mmm

The D_{2h}=mmm group has 16 subgroups, which can be conveniently parametrized using four bits, as shown in Table 6.

subG	x	y	z	i
1	0	0	0	0
m$_x$	1	0	0	0
m$_y$	0	1	0	0
m$_z$	0	0	1	0
2$_x$	0	1	1	0
2$_y$	1	0	1	0
2$_z$	1	1	0	0
222	1	1	1	0
-1	0	0	0	1
2/m$_x$	1	0	0	1
2/m$_y$	0	1	0	1
2/m$_z$	0	0	1	1
mm2$_x$	0	1	1	1
mm2$_y$	1	0	1	1
mm2$_z$	1	1	0	1
mmm	1	1	1	1

Table 6: Parametrization of subgroups of the group mmm.

The decomposition of the IRs the rotation group into IRs of the group mmm is as follows

	1	2_z	2_y	2_x	-1	m_z	m_y	m_x	0	1	2	3	4	5
A_g	1	1	1	1	1	1	1	1	1	.	2	.	3	.
A_u	1	1	1	1	-1	-1	-1	-1	.	.	.	1	.	2
B_{1g}	1	1	-1	-1	1	1	-1	-1	.	.	1	.	2	.
B_{1u}	1	1	-1	-1	-1	-1	1	1	.	1	.	2	.	3
B_{2g}	1	-1	1	-1	1	-1	1	-1	.	.	1	.	2	.
B_{2u}	1	-1	1	-1	-1	1	-1	1	.	1	.	2	.	3
B_{3g}	1	-1	-1	1	1	-1	-1	1	.	.	1	.	2	.
B_{3u}	1	-1	-1	1	-1	1	1	-1	.	1	.	2	.	3

The decomposition of the IRs of the group m-3m s into IRs of the group mmm is as follows (see Table 5 for the notation of the basis functions)

$$
\begin{array}{lll}
A_{1g} & = A_g\ S & \text{or } S4 \\
A_{1u} & = A_u\ XYZX2Y2Z2 & \\
A_{2g} & = A_g\ X2Y2Z2 & \\
A_{2u} & = A_u\ XYZ & \\
E_g & = A_g/A_g\ Z2 \oplus A_g/B_{1g}\ X2 & \text{or } X2Z2 \oplus Z4 \\
E_u & = A_u/A_u\ -XYZX2 \oplus A_u/B_{1u}\ XYZZ2 & \\
F_{1g} & = B_{3g}\ YZY2 \oplus B_{2g}\ ZXZ2 \oplus B_{1g}\ XYX2 & \\
F_{1u} & = B_{3u}\ X \oplus B_{2u}\ Y \oplus B_{1u}\ Z & \text{or } X3 \oplus Y3 \oplus Z3 \\
F_{2g} & = B_{3g}\ YZ \oplus B_{2g}\ ZX \oplus B_{1g}\ XY & \text{or } YZX2 \oplus ZXY2 \oplus XYZ2 \\
F_{2u} & = B_{3u}\ XY2 \oplus B_{2u}\ YZ2 \oplus B_{1u}\ ZX2 &
\end{array}
$$

where the axes of the group mmm are aligned with the 4th order axes of the cube. However, the IRs E_g and E_u do not decompose into distinct IRs in this orientation. For a complete decomposition, the two axes of the group mmm should be aligned with the 2nd order axes of the cube, and the resulting IRs are shown after a slash. However, using such an orientation for three-dimensional IRs is inconvenient due to the increased complexity of the basis functions. Here and in what follows, the basis functions are chosen such that they transform by the matrices (6.3). The decomposition of the IRs of the group 6/mmm into IRs of the mmm group is as follows

$$\begin{aligned}
A_{1g} &= A_g\ 1 \text{ or } 3z^2 - r^2\\
A_{1u} &= A_u\ zs_3c_3\\
A_{2g} &= B_{1g}\ s_3c_3\\
A_{2u} &= B_{1u}\ z\\
B_{1g} &= B_{2g}\ zx(x^2-3y^2) = zc_3\\
B_{2g} &= B_{3g}\ zy(y^2-3x^2) = zs_3\\
B_{1u} &= B_{2u}\ \ y(y^2-3x^2) = \ \ s_3\\
B_{2u} &= B_{3u}\ \ x(x^2-3y^2) = \ \ c_3\\
E_{1g} &= B_{3g}\ zy \oplus B_{2g}\ \ -zx\\
E_{1u} &= B_{3u}\ \ x \oplus B_{2u}\ \ \ y\\
E_{2g} &= A_g\ x'y' \oplus B_{1g}\ \ \ xy\\
E_{2u} &= A_u\ zxy \oplus B_{1u}\ \ -zx'y'
\end{aligned}$$

where $c/s_m = \sin^m\theta\cos/\sin m\phi \sim \tilde{Y}_{m\pm m}$.

§11. Icosahedral symmetry m-5m

Similar to the tetrahedron, it is convenient to choose a "cubic" coordinate system (Fig. 2) such that the 8 vertices of the dodecahedron with coordinates $|x| = |y| = |z| = 1/\sqrt{3}$ form a cube, and the remaining 12 vertices form 3 mutually perpendicular rectangles, one of which has coordinates $x = 0$, $y = \pm\frac{\sqrt{5}-1}{2\sqrt{3}}$, $z = \pm\frac{\sqrt{5}+1}{2\sqrt{3}}$, and the rest are formed by third-order rotations around the main axes of the cube.

For the group Y=m-5, the generating elements are the rotation about the principal axis $a = u_{5Y}$ and the rotation about the nearest second order axis $b = u_{2h}$. Then we have the following non-trivial classes

$12c_5$ & $12c_5^2$	$a^q,\ a^pba^qba^{-p}$	$p = 0,\dots,4,\ q = (1,4)$ & $(2,3)$
$15u_2$	$a^pba^qba^{-q}ba^{-p},\ p = \overline{0,4}$	$q = 0,\dots,2$
$20u_3$	$a^{p\pm1}ba^{-p},\ a^{p\pm1}ba^{\pm3}ba^{-p}$	$p = 0,\dots,4$

The second-order axis perpendicular to the principal axis is given by the expression $b' = c_2 = a^2ba^{-2}ba^2b$ and, together with u_{5Y}, generates the subgroup $D_5 = C_5\cdot\{1,b'\}$, where $C_5 = \{1,a,a^2,a^3,a^4\}$. Then $Y = \{1, C_5b\}\cdot D_5 \equiv \{a^i, a^iba^j, a^ib', a^iba^jb'\}$. Note that $c = ab$ is the 3rd order axis closest to the axes u_{2h} and u_{5Y} such that $\{a,b,c\}$ is a right-handed triple.