# Multipole Representation and Group Theory Learned through MultiPie and QtDraw

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## 1. Introduction

The editor asked me to write an article explaining how to use `MultiPie`. Therefore, I would like to introduce useful ways of using `MultiPie` from a user's perspective [*1].

`MultiPie` is a software package designed to generate complete bases of multipoles. Beyond its primary role as a computational tool, however, it also serves as an excellent educational platform for learning about multipoles. Since multipole bases in crystals are defined as irreducible representations of symmetry groups, understanding multipolar phenomena generally requires a solid background in group theory, including point groups and space groups. This often presents a significant barrier for beginners. With `MultiPie`, however, users can perform tasks such as irreducible decomposition without first mastering the underlying mathematical formalism. By examining concrete results and visualizing symmetry properties directly, users can develop an intuitive understanding of group theory and multipoles. Learning can then proceed from the interpretation of results rather than from abstract theoretical concepts, substantially lowering the barrier to entry for newcomers. With this philosophy in mind, this article introduces the fundamentals of multipoles through hands-on examples using `MultiPie`, while also explaining the basic operation and features of the software.

`MultiPie` and `QtDraw` are open-source software packages developed by Hiroaki Kusunose (Meiji University) and Rikuto Oiwa (Hokkaido University) [1–3]. They can generate complete bases of multipoles from crystal structure information. `QtDraw` is a drawing software package capable of rendering various three-dimensional objects, and its distinctive feature is that, in conjunction with `MultiPie`, it can visualize crystal structures as well as electronic orbitals and spins based on symmetry operations. Since `MultiPie` is a program that is executed from the command line using text-based input files, it may present a somewhat high barrier to entry for beginners. In contrast, `QtDraw` provides an intuitive graphical user interface (GUI) that allows users to operate it more easily. Therefore, in this article, we mainly introduce how to use `MultiPie` through `QtDraw`.

In this article, we provide an overview of the basic usage of `QtDraw` by presenting concrete procedures for carrying out the following tasks:

[*1] This short article was originally written in Japanese as an article in NewsLetter #6 for the Scientific Project, "Unveiling, Design, and Development of Asymmetric Quantum Matters", `https://asymmetry.hiroshima-u.ac.jp/en`.

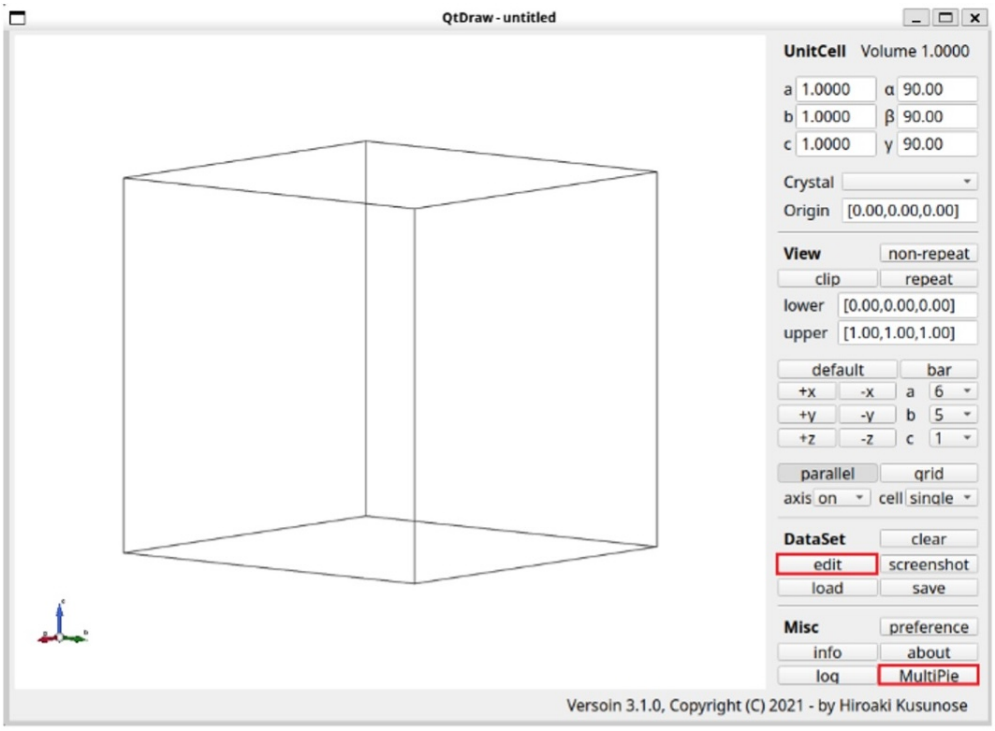



Fig. 1 `QtDraw` startup screen.

- Basic usage
- Perform irreducible decomposition: crystal-field splitting
- Investigate active multipoles
- Cluster multipoles: the case of URhSn

This article is based on `MultiPie` 2.0.7 and `QtDraw` 3.1.0, which were the latest versions available as of January 2026.

## 2. Basic Usage

First, let us set up the environment. To use `QtDraw`, Python 3.12 or later is required. Once Python is available on your system, `QtDraw` can be installed by following the instructions in the official documentation [3]. The documentation can easily be found by searching for keywords such as **qtdraw doc**.

From the command line, enter

```
$ pip install qtdraw
```

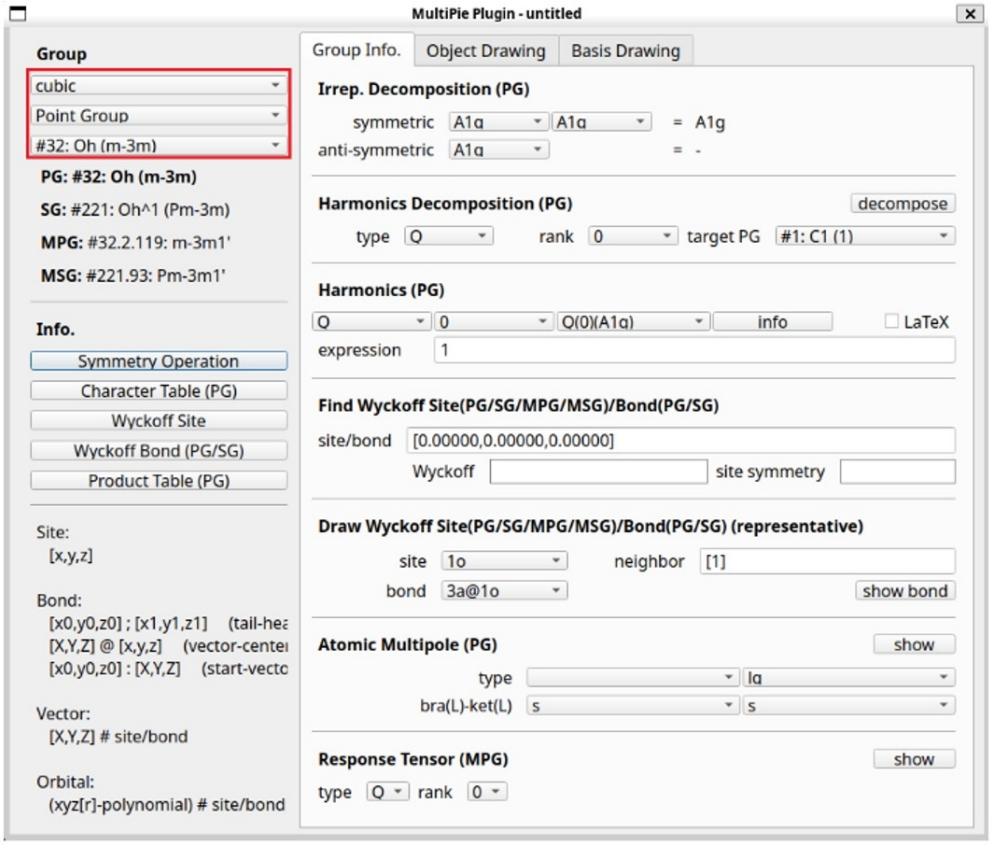



Fig. 2 Window for invoking `MultiPie` functions.

to install `QtDraw`. At this stage, `MultiPie` will also be installed automatically as a dependency. Next, configure the tool called `playwright` [3]. Once the setup is complete, enter

```
$ qtdraw
```

at the command line. If the window shown in Fig. 1 appears, the installation has been successful. At this point, only the unit-cell frame is displayed, but it can already be rotated interactively using the mouse.

Various operations can be performed using the buttons located in the panel on the right side of Fig. 1. Among these, we briefly explain the two functions highlighted by the red boxes. Pressing the **edit** button displays a list of the objects currently being drawn. From this list, each object can be shown or hidden, and objects can also be deleted. The properties of each object can be edited as well by double-clicking it. Pressing the **MultiPie** button opens the window shown in Fig. 2. From this window, the functions of `MultiPie` can be accessed. On the left side is a panel for selecting point groups and space groups, where basic group-theoretical information can be referenced, such as character tables of point groups and Wyckoff positions of space groups.

On the right side are three tabs. The **Group Info.** tab provides basic information on multipoles. The **Object Drawing** tab can be used to draw objects generated by applying symmetry operations. The **Basis Drawing** tab can be used to draw objects classified according to irreducible representations.

## 3. Irreducible Decomposition: Crystal-Field Splitting

Let us begin by examining crystal-field splitting of atomic orbitals. As an example, we will confirm that the threefold degeneracy of the $p$ orbitals is split into the $(p_x, p_y)$ orbitals and the $p_z$ orbital in a tetragonal crystal field.

First, select the symmetry of the system in the red-boxed area of Fig. 2. Both point groups and space groups can be selected; here, we choose the point group $O_{\rm h}$.

To investigate crystal-field splitting, use the **Harmonics Decomposition (PG)** function located in the **Group Info.** tab on the right-hand side. To examine crystal-field states of electrons, select **type=Q**, which corresponds to charge distributions, and choose **rank 1** for $p$ orbitals. Specify the point group $D_{4\rm h}$ as the target PG, and then press the **decompose** button.

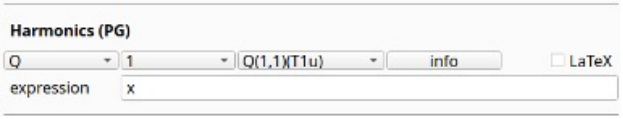

As a result, the table shown on the right will appear in a new window. The first and second columns display the irreducible representations of the $p$ orbitals under the point groups $O_{\rm h}$ and $D_{4\rm h}$, respectively.

| | Oh | D4h |
|---|---|---|
| 1 | $\mathbb{Q}_{1,1}(T_{1u})$ | $\mathbb{Q}_{1,1}(E_u)$ |
| 2 | $\mathbb{Q}_{1,2}(T_{1u})$ | $\mathbb{Q}_{1,2}(E_u)$ |
| 3 | $\mathbb{Q}_{1,3}(T_{1u})$ | $\mathbb{Q}_{1}(A_{2u})$ |

Here, for example, the symbol $\mathbb{Q}_{1,2}(T_{1u})$ represents a rank-1 electric multipole belonging to the irreducible representation $T_{1u}$. The second subscript is a label used to distinguish basis functions within a degenerate representation; it is omitted for one-dimensional representations. From this table, we find that the $p$ orbitals are classified into the threefold-degenerate irreducible representation $T_{1u}$ in the point group $O_{\rm h}$, whereas under tetragonal symmetry they split into $E_u$ and $A_{2u}$. This compatibility relation can be written as

$$T_{1u}(O_{\rm h}) \downarrow D_{4\rm h} = A_{2u} \oplus E_u.$$

The form (anisotropy) of each basis function can be examined using **Harmonics (PG)** (see the figure). Select **Q** and **1**, and then press the **info** button located to the right. A new window will open displaying the table shown.



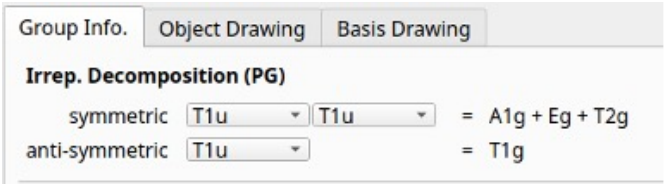

From this table, we find that the three basis functions are represented by $x$, $y$, and $z$, respectively. Combining this information with the previous result, we conclude that the irreducible representation $E_u$ is represented by $(x, y)$, while $A_{2u}$ is represented by $z$. This result means that, in a tetragonal crystal field, the $p$ orbitals split into the $p_z$ orbital and the $(p_x, p_y)$ orbitals. In the same manner, the reader is encouraged as an exercise to verify how the fivefold degeneracy of the $d$ orbitals is split by crystal fields of cubic and tetragonal symmetry.

| | symbol | expression |
|---|---|---|
| 1 | $\mathbb{Q}_{1,1}(T_{1u})$ | $x$ |
| 2 | $\mathbb{Q}_{1,2}(T_{1u})$ | $y$ |
| 3 | $\mathbb{Q}_{1,3}(T_{1u})$ | $z$ |

# 4. Investigating Active Multipoles

Next, let us investigate the active multipolar degrees of freedom within a specific degenerate irreducible representation. Continuing with the example from the previous section, we consider the $p$ orbitals. Since the $p$ orbitals have three basis functions, the number of multipolar degrees of freedom is $3^2 = 9$. This example is also discussed in Part 3 of the review article series by Hayami *et al.* [4]. Readers may find it helpful to consult that article alongside the present discussion.

(a) Irreducible decomposition




First, let us classify the multipolar degrees of freedom according to irreducible representations by using irreducible decomposition. For this purpose, use **Irrep. Decomposition (PG)** in the **Group Info.** tab. From the field to the right of symmetric, select $T_{1u}$, the irreducible representation to which the $p$ orbitals belong. The result of the irreducible decomposition of the symmetric product will then be displayed on the right. This result is expressed as

$$[T_{1u} \otimes T_{1u}] = A_{1g} \oplus E_g \oplus T_{2g}.$$

Next, select $T_{1u}$ in the anti-symmetric field as well. The irreducible decomposition of the antisymmetric product is obtained as

$$\{T_{1u} \otimes T_{1u}\} = T_{1g}.$$

When dealing with a single shell, as in the present example, it is known that the symmetric product corresponds to multipoles that are even under time reversal, whereas the antisymmetric product corresponds to multipoles that are odd under time reversal. Denoting the time-reversal parity by the superscripts $+$ and $-$, the above results can be summarized as

$$T_{1u} \otimes T_{1u} = A_{1g}^{+} \oplus E_g^{+} \oplus T_{2g}^{+} \oplus T_{1g}^{-}.$$

From this, we find that electrons in the $p$ orbitals possess $1+2+3=6$ electric degrees of freedom and 3 magnetic degrees of freedom, all of which have even spatial parity.

(b) Matrix element


Although irreducible decomposition allows us to classify multipoles according to irreducible representations, it does not reveal their ranks (monopole, dipole, quadrupole, etc.). To determine this, it is necessary to examine the matrix elements of the multipole operators[*2]. This can be done using **Atomic Multipole (PG)** in the **Group Info.** tab. Select **type=Q**, and then **lg** from the field on the right. This

[*2] Strictly speaking, the rank is not a good quantum number in a point group, and linear combinations between basis functions belonging to the same irreducible representation are allowed. In many cases, the lowest rank appearing in such a linear combination is used as the nomenclature of the multipole.

specifies the basis in which the matrix elements are displayed. In the **bra(L)-ket(L)** field below, select the $p$ orbitals. Press **show**, and the table shown below will appear (it has been reformatted to fit within the frame). The symbols in the second column indicate the type of multipole. Here, the superscript (a) stands for atomic multipole. From the results, we find that there is one rank-0 multipole and five rank-2 multipoles. The matrices in the third column represent the matrix elements of the multipoles in the basis $(p_x, p_y, p_z)$.

| No | multipole | matrix |
|---|---|---|
| | bra | $\langle p_x \vert, \langle p_y \vert, \langle p_z \vert$ |
| | ket | $\vert p_x \rangle, \vert p_y \rangle, \vert p_z \rangle$ |
| | | |
| 1 | $\mathbb{Q}_0^{(a)}(A_{1g})$ | $\begin{bmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$ |
| 2 | $\mathbb{Q}_{2,1}^{(a)}(E_g)$ | $\begin{bmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{bmatrix}$ |
| 3 | $\mathbb{Q}_{2,2}^{(a)}(E_g)$ | $\begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$ |
| 4 | $\mathbb{Q}_{2,1}^{(a)}(T_{2g})$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$ |
| 5 | $\mathbb{Q}_{2,2}^{(a)}(T_{2g})$ | $\begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \end{bmatrix}$ |
| 6 | $\mathbb{Q}_{2,3}^{(a)}(T_{2g})$ | $\begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ |

These matrices agree with Eq. (6) of Ref. [3], apart from the normalization factor. In `MultiPie`, the matrices are normalized such that, for a matrix $\hat{O}$,

$$\mathrm{Tr}\,\hat{O}\hat{O}^\dagger = \sum_{ij} O_{ij} O_{ij}^* = 1.$$

In the same way, the matrix elements of the magnetic multipoles $M$ can also be obtained, although the results are omitted here. Note that nothing is displayed when the toroidal multipoles $T$ and $G$ are selected. This is because electrons within a single shell do not possess toroidal degrees of freedom. In contrast, $T$ and $G$ multipoles do exist between different shells, such as $p$-$d$ and $p$-$f$, and the reader is encouraged to verify this.

From the above results, we conclude that the multipolar degrees of freedom within the $p$ orbitals are classified under the point group $O_\mathrm{h}$ into one electric monopole $\mathbb{Q}_0(A_{1g})$, two and three electric quadrupoles $\mathbb{Q}_2(E_g)$ and $\mathbb{Q}_2(T_{2g})$, respectively, and three magnetic dipoles $\mathbb{M}_1(T_{1g})$.

## 5. Cluster Multipoles: The Example of URhSn

Finally, let us examine the classification of cluster multipoles. As an example, we consider URhSn, which has a distorted kagome structure. URhSn exhibits phase transitions originating from the U $5f$ electrons at temperatures $T_c = 16$ K and $T_o = 54$ K [5]. The intermediate phase, $T_c < T < T_o$, is most likely characterized by ordering of the electric quadrupole $O_{zx}$ or $O_{yz}$ [6]. The former corresponds to a polar structure, whereas the latter corresponds to a chiral (Sohncke) structure. NMR measurements strongly support the chiral-order scenario [7]. Since chirality is generated spontaneously by electronic ordering in a crystal structure that is not itself chiral, this material has attracted attention in this

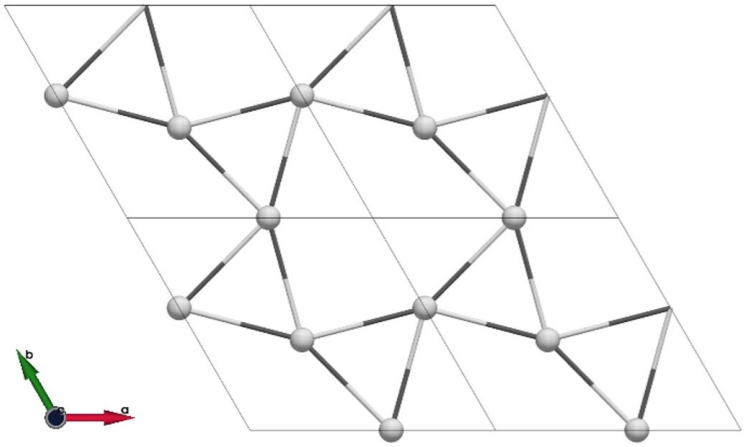
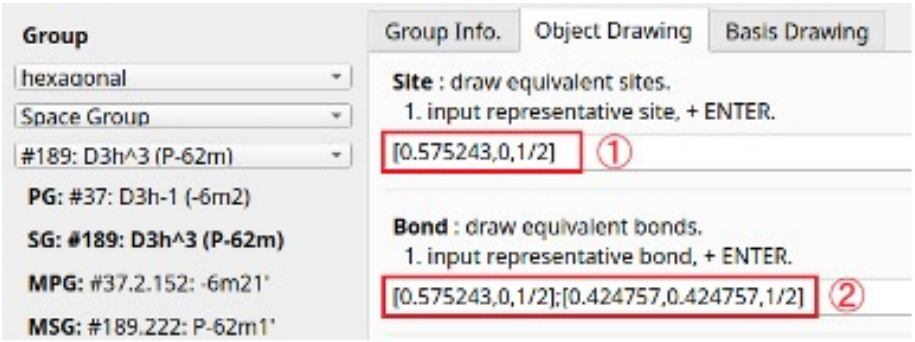



Fig. 3 Crystal structure of URhSn (U atoms only).

Project [8].

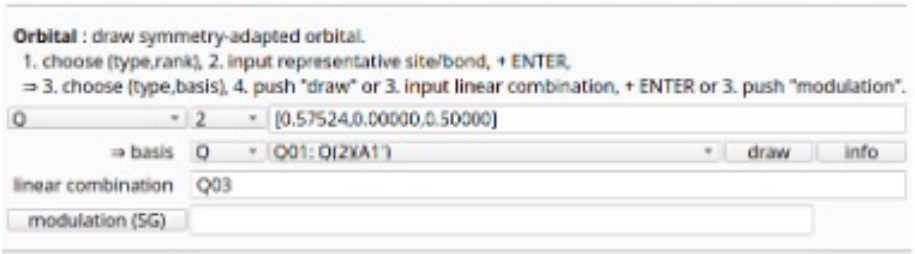
Let us first prepare the crystal structure. For this purpose, use the **Object Drawing** tab. First, select the space group $P\bar{6}2m$ (No. 189) from the **Group** panel on the left. Then, in the **Site** field of the **Object Drawing** tab, enter the coordinates of one U site. The U atoms occupy the $3g$ Wyckoff positions,




$$(x, 0, 1/2), \quad (0, x, 1/2), \quad (-x, -x, 1/2),$$

with $x = 0.5752$. Enter one of these coordinates into field 1 in the figure and press Enter. Spheres will then be drawn at all symmetry-equivalent positions generated by the space-group operations. Next, let us also draw the bonds connecting the U atoms. In field 2 of the **Bond** field in the figure, enter the coordinates of two U sites separated by a semicolon (;). After pressing Enter, all symmetry-equivalent bonds generated by the symmetry operations will be drawn. The resulting structure is shown in Fig. 3. It should be noted that there are also methods for importing CIF files or VESTA files, as well as methods for providing crystal and other structural information input file to `MultiPie` and generating `QtDraw` format files via `MultiPie` (with the extension `.qtdw`).

Let us now investigate how an ordered state of electric quadrupoles carried by the $5f$ electrons on the U sites is classified



in terms of cluster multipoles. For this purpose, use the **Basis Drawing** tab. In the **Orbital** field, enter the multipole type, rank, and coordinates. Since we wish to place electric quadrupoles on the U sites, select the multipole type **Q**, rank **2**, and the coordinates of a U site as shown in the figure above, and then press Enter. Next, select the type of cluster multipole from the field next to basis. Since the charge distribution associated with an electric quadrupole is even under time reversal, the cluster multipoles constructed from it must be either $Q$ or $G$, namely electric or electric-toroidal multipoles.

Let us first select **Q**. After selecting $Q$ and pressing the **info** button, a list of 14 $Q$ multipoles appears, as shown in the right figure. The first and second columns give the symbols of the cluster multipoles. The third column shows their symmetry (anisotropy), while the fourth column shows the anisotropy of the constituent atomic multipoles at a representative site. Among these multipoles, the three entries whose third column contains one of the first-order functions $x$, $y$, or $z$ correspond to polar electric quadrupole ordered states. Among them, `Q04`, which belongs to the irreducible representation $A_2''$, corresponds to a polar ordered state with the $z$-axis as its principal axis. The polar nature of $A_2''$ can also be understood from the character table shown in Fig. 4. The mirror symmetry $\sigma_h$ with respect to the horizontal ($xy$) plane is broken, as indicated by the character $-1$ (odd), whereas the mirror symmetries $\sigma_v$ with respect to the vertical ($zx$ and $yz$) planes are preserved, as indicated by the character $+1$ (even). Selecting `Q04` and pressing the **draw** button produces the structure shown in Fig. 5. This is the cluster-multipole ordered state corresponding to the electric quadrupole $O_{zx}$.

| tag | symbol | symmetry | 1st cluster (c.c.) |
|---|---|---|---|
| Q01: Q(2)(A1') | $\mathbb{Q}_2(A_1')$ | $-\frac{x^2}{2}-\frac{y^2}{2}+z^2$ | $\frac{\sqrt{3}\left(-\frac{x^2}{2}-\frac{y^2}{2}+z^2\right)}{3}$ |
| Q02: Q(3)(A1') | $\mathbb{Q}_3(A_1')$ | $\frac{\sqrt{10}x\left(x^2-3y^2\right)}{4}$ | $\frac{(x-y)(x+y)}{2}$ |
| Q03: Q(3)(A2') | $\mathbb{Q}_3(A_2')$ | $\frac{\sqrt{10}y\left(3x^2-y^2\right)}{4}$ | $xy$ |
| Q04: Q(1)(A2") | $\mathbb{Q}_1(A_2'')$ | $z$ | $xz$ |
| Q05: Q(1,1)(E') | $\mathbb{Q}_{1,1}(E')$ | $x$ | $\frac{\sqrt{21}(x-y)(x+y)}{14}-\frac{\sqrt{21}\left(-\frac{x^2}{2}-\frac{y^2}{2}+z^2\right)}{21}$ |
| Q06: Q(1,2)(E') | $\mathbb{Q}_{1,2}(E')$ | $y$ | $\frac{\sqrt{21}xy}{7}$ |
| Q07: Q(2,1)(E') | $\mathbb{Q}_{2,1}(E')$ | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ | $\frac{\sqrt{2}(x-y)(x+y)}{4}$ |
| Q08: Q(2,2)(E') | $\mathbb{Q}_{2,2}(E')$ | $-\sqrt{3}xy$ | $-\frac{\sqrt{2}xy}{2}$ |
| Q09: Q(3,1)(E') | $\mathbb{Q}_{3,1}(E')$ | $-\frac{\sqrt{6}x\left(x^2+y^2-4z^2\right)}{4}$ | $\frac{\sqrt{14}(x-y)(x+y)}{28}+\frac{\sqrt{14}\left(-\frac{x^2}{2}-\frac{y^2}{2}+z^2\right)}{7}$ |
| Q10: Q(3,2)(E') | $\mathbb{Q}_{3,2}(E')$ | $-\frac{\sqrt{6}y\left(x^2+y^2-4z^2\right)}{4}$ | $\frac{\sqrt{14}xy}{14}$ |
| Q11: Q(2,1)(E") | $\mathbb{Q}_{2,1}(E'')$ | $\sqrt{3}yz$ | $\frac{\sqrt{2}yz}{2}$ |
| Q12: Q(2,2)(E") | $\mathbb{Q}_{2,2}(E'')$ | $-\sqrt{3}xz$ | $-\frac{\sqrt{2}xz}{2}$ |
| Q13: Q(3,1)(E") | $\mathbb{Q}_{3,1}(E'')$ | $\sqrt{15}xyz$ | $\frac{\sqrt{2}yz}{2}$ |
| Q14: Q(3,2)(E") | $\mathbb{Q}_{3,2}(E'')$ | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ | $\frac{\sqrt{2}xz}{2}$ |

| | $E$ | $3C_2'$ | $2C_3$ | $\sigma_h$ | $3\sigma_v$ | $2S_3$ |
|---|---|---|---|---|---|---|
| irrep. | 1(1) | $2_{100}(3)$ | $3^{+}_{001}(2)$ | $m_{001}(1)$ | $m_{120}(3)$ | $-6^{+}_{001}(2)$ |
| $A_1'$ | 1 | 1 | 1 | 1 | 1 | 1 |
| $A_2'$ | 1 | −1 | 1 | 1 | −1 | 1 |
| $A_1''$ | 1 | 1 | 1 | −1 | −1 | −1 |
| $A_2''$ | 1 | −1 | 1 | −1 | 1 | −1 |
| $E'$ | 2 | 0 | −1 | 2 | 0 | −1 |
| $E''$ | 2 | 0 | −1 | −2 | 0 | 1 |

Fig. 4 Character table of the $D_{3h}$ point group. Schönflies symbols (e.g., $C_3$) have been added to the table generated by `QtDraw`.

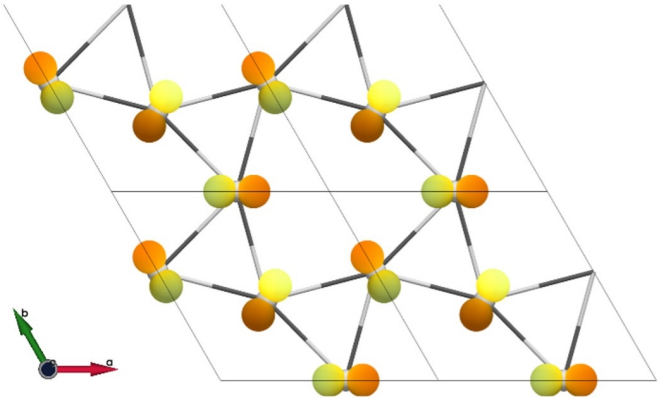



Fig. 5 Polar cluster order $Q_1$ ($A_2''$) consisting of electric quadrupoles,$O_{zx}$.

| tag | symbol | symmetry | 1st cluster (c.c.) |
|---|---|---|---|
| G01: G(2)(A1") | $\mathbb{G}_2(A_1'')$ | $-\frac{x^2}{2}-\frac{y^2}{2}+z^2$ | $-yz$ |

Next, select **G** as the basis. A table consisting of a single multipole is then obtained, as shown in the right figure. This irreducible representation, $A_1''$, is chiral because, as can be seen from the character table in Fig. 4, it breaks both types of mirror symmetries, $\sigma_h$ and $\sigma_v$. Pressing the **draw** button displays the corresponding quadrupole arrangement. The result is shown in Fig. 6. There are a total of $5\times3 = 15$ ways to place electric quadrupoles, corresponding to the product of the number of electric quadrupole types (5) and the number of U sites (3) within the unit cell. This number corresponds to the total number of basis functions for the cluster electric multipoles. From the above results, we find that 14 of these basis functions are classified as $Q$, while 1 is classified as $G$. As demonstrated by this example, `MultiPie` enables one to identify the irreducible representations of cluster multipoles with great ease, even for complicated arrangements such as electric-quadrupole ordering on a distorted kagome lattice.

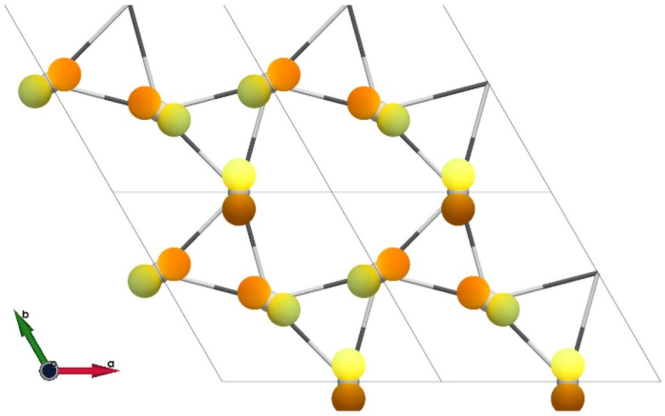



Fig. 6 Chiral cluster order $G_2$ ($A_1''$) consisting of electric quadrupoles,$O_{yz}$.

## 6. Concluding Remarks

In this article, we introduced methods for obtaining the irreducible representations of electronic crystal-field states and multipolar ordered states using `MultiPie`. Classification of complex ordered structures in terms of irreducible representations has traditionally required considerable expertise and experience, but `MultiPie` makes this task accessible to anyone. Although we focused on electric quadrupole ordered states in this article, magnetic ordered states can of course also be treated. Furthermore, the drawing functions based on symmetry operations are compatible with magnetic point groups and magnetic space groups as well (via the **Object Drawing** tab). More advanced usage than that presented here is introduced in the official documentation [3]. For example, it is possible to specify arrangements of atoms and multipoles directly in Python code which creates `.qtdw` file as a background job. This functionality can also be used via iPython interactive interface. This makes repetitive tasks, such as generating figures for all multipoles, straightforward to perform.

In recent years, a wide variety of open-source software packages have been developed. One of the advantages of open-source software is the close relationship between developers and users. By communicating feedback to the developers, users themselves can contribute to the development of the software. We encourage readers to actively share their opinions and requests.

In preparing this article, Hiroaki Kusunose kindly provided extensive guidance on the use of `MultiPie` and `QtDraw`. The author would like to express sincere gratitude for his assistance.

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