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CLASSIFICATION OF SYMMETRIC COORDINATES FOR POINT CLUSTERS. II. EXAMPLES: A REGULAR TETRAHEDRON AND A CUBE

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A general group-theoretical method of classifying the symmetric coordinates of point clusters has been demonstrated for the nodes of a regular tetrahedron and a cube. This method is based on a factorisation of the mechanical representation into a positional and vector part. A procedure to determine an irreducible basis for the relevant mechanical representations has been explicitly demonstrated, showing that the proposed classification for these cases is complete. The classification schemes, associated with several chains of subgroups describing possible descents in symmetry, have been presented.

1. *Introduction*

In a previous paper of one of us [1], denoted hereafter by I, we proposed a general method for classifying and determining the symmetric coordinates for clusters of points, exhibiting in their equilibrium position the symmetry of a point group G. Classification schemes related to a descent in symmetry of a cluster have been discussed in that paper. In the present paper we are going to demonstrate this method for two nontrivial cases: clusters consisting of all nodes of a regular tetrahedron, and of a cube. We use throughout this paper the notation introduced in I.

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2. *Symmetric coordinates for a regular tetrahedron*

We consider a regular tetrahedron, spanned on nodes 1 2 3 4 (see Fig. 1), with the symmetry group T_d. Using Fig. 1, one can establish each permutation $\sigma(g)$ of Eq. (I.5), determining the positional representation P (I.6), e.g.

$$\sigma(C_{2x}) = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 1 & 4 & 3 \end{pmatrix}, \quad \sigma(C_{2y}) = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 3 & 4 & 1 & 2 \end{pmatrix}, \quad \sigma(C_{2z}) = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 \end{pmatrix},$$

$$\sigma(C_{31}) = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 1 & 3 & 4 & 2 \end{pmatrix}, \quad \sigma(C_{31}^{-1}) = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 1 & 4 & 2 & 3 \end{pmatrix}, \quad \sigma(S_{4z}) = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 3 & 1 & 4 & 2 \end{pmatrix}, \qquad (1)$$

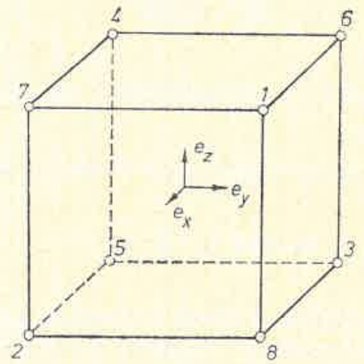

Fig. 1. The labeling of nodes of a cube and a tetrahedron

where C_{31} is the three-fold axis directed from the origin to the node 1. A stability group for each node G_i is isomorphic with C_{3v}, and the stability group for the cluster, $G(p)$, consists only of the unit element, so that the constituent set $\Sigma_p(T_d)$ is isomorphic with T_d.

Using Eq. (I. 12) and the standard character theory, one can obtain the decomposition (I. 10) of the positional representation P into irreducible representations Λ of the group T_d in a form

$$P = A_1 \oplus T_2, \qquad (2)$$

where T_2 is the vector representation V for the group T_d (we use the Mulliken notation: A_1, A_2, E, T_1, T_2 for irreducible representations of T_d).

The irreducible basis (I. 16) for P can be easily obtained from Eq. (I. 17) and the comment following that equation. Namely, the equilibrium position for the tetrahedron (Eq. (I.15)) is

$$r^0 = \frac{a}{2}(e_1^x+e_1^y+e_1^z+e_2^x-e_2^y-e_2^z-e_2^x+e_3^y-e_3^z-e_4^x-e_4^y+e_4^z)$$

$$= \frac{a}{2}[(|1\rangle+|2\rangle-|3\rangle-|4\rangle)e^x+(|1\rangle-|2\rangle+|3\rangle-|4\rangle)e^y+(|1\rangle-|2\rangle-|3\rangle+|4\rangle)e^z], \qquad (3)$$

where the first equality follows from Fig. 1 (a is the edge of the cube in Fig. 1), and the second is the consequence of the factorisation (I. 3) of the twelve-dimensional configuration space $\mathscr{M}$ of the cluster into the simple product of the four-dimensional positional space Π and a vector space $\mathscr{V}$, spanned on the basis $|1\rangle$, $|2\rangle$, $|3\rangle$, $|4\rangle$ and e^x, e^y, e^z, respectively. This notation has been defined by Eq. (I 2). An irreducible basis $|\Lambda\lambda\rangle$ for the positional representation P in Π is therefore given by

$$
\begin{aligned}
|A_1a_1\rangle &= \tfrac{1}{2}(|1\rangle+|2\rangle+|3\rangle+|4\rangle),\\
|T_2x\rangle &= \tfrac{1}{2}(|1\rangle+|2\rangle-|3\rangle-|4\rangle),\\
|T_2y\rangle &= \tfrac{1}{2}(|1\rangle-|2\rangle+|3\rangle-|4\rangle),\\
|T_2z\rangle &= \tfrac{1}{2}(|1\rangle-|2\rangle-|3\rangle+|4\rangle).
\end{aligned} \tag{4}
$$

The decomposition (2) includes only unit and vector representation, since the tetrahedron is a symplex in a three-dimensional space. Accordingly, the basis (4) can be determined immediately from Eq. (I. 17) and (3), which provide the basis $|A_1a_1\rangle$ and $|T_2\lambda\rangle$, respectively, without any tedious projection procedure.

The symmetric coordinates for the tetrahedron can be obtained from Eq. (I. 21) using standard Clebsch–Gordan coefficients for the group O, isomorphic with T_d. We take these coefficients from papers [2]. The symmetric coordinates can be written here as

$$|\Lambda\Gamma\gamma\rangle = \sum_{i,\alpha} B^{i\alpha}_{\Lambda\Gamma\gamma}|i\rangle e^{\alpha} \tag{5}$$

TABLE I

The symmetric coordinates for nodes of a regular tetrahedron. The coefficients $B^{i\alpha}_{\Lambda\Gamma\gamma}$ of Eq. (5) are in units of $\bar{B}_{\Lambda\Gamma\gamma}$; the latter are given under the headings of each column

$i\alpha$	Λ	A_1			T_2								
	Γ	T_2			A_1	E		T_1			T_2		
	γ	x	y	z	a_1	θ	ε	x	y	z	x	y	z
	$\bar{B}_{\Lambda\Gamma\gamma}$	1/2	1/2	1/2	$1/2\sqrt{3}$	$\frac{1}{2\sqrt{2\cdot 3}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$
1	x	1	0	0	1	−1	1	0	−1	1	0	−1	−1
	y	0	1	0	1	−1	−1	1	0	−1	−1	0	−1
	z	0	0	1	1	2	0	−1	1	0	−1	−1	0
2	x	1	0	0	1	−1	1	0	1	−1	0	1	1
	y	0	1	0	−1	1	1	−1	0	−1	1	0	−1
	z	0	0	1	−1	−2	0	1	1	0	1	−1	0
3	x	1	0	0	−1	1	−1	0	1	1	0	1	−1
	y	0	1	0	1	−1	−1	−1	0	1	1	0	1
	z	0	0	1	−1	−2	0	−1	−1	0	−1	1	0
4	x	1	0	0	−1	1	−1	0	−1	−1	0	−1	1
	y	0	1	0	−1	1	1	1	0	1	−1	0	1
	z	0	0	1	1	2	0	1	−1	0	1	1	0

(we omit all those indices of Eq. (I. 21), which are here irrelevant). The expansion coefficients B are listed in Table I.

According to a general interpretation given in Section 3 of I, the bases $|A_1T_2\gamma\rangle$ and $|T_2T_1\gamma\rangle$ ($\gamma = x, y, z$) describe respectively translations and rotations of the whole tetrahedron, $|T_2T_2A_1a_1\rangle$ is the "breathing mode", and $|T_2E\gamma\rangle$ ($\gamma = \theta, \varepsilon$) and $|T_2T_2\gamma\rangle$ are displacements violating the symmetry of the cluster. The bases $|T_2E\theta\rangle$ and $|T_2E\varepsilon\rangle$ can be related to a deformation of the cube in Fig. 1 to a parallelepiped with edges parallel with the axes x, y, z and lengths $(a-2b_\theta, a-2b_\theta, a+4b_\theta)$ and $(a+2b_\varepsilon, a-2b_\varepsilon, a)$, respectively, where $b_\theta = b/2\sqrt{2\cdot 3}$, $b_\varepsilon = b/2\sqrt{2}$, and b is a measure of the deformation. Similarly, $|T_2T_2\gamma\rangle$ can be related to a deformation of the cube to a regular truncate pyramid with square bases. E.g. for $|T_2T_2x\rangle$ the bases of the pyramid are parallel to the yz-plane, their edges are $a\pm 2b_x (b_x = b/2\sqrt{2})$, and the height is a.

3. *The symmetric coordinates for a cube*

The symmetry group for a cube (nodes 1, ..., 8 in Fig. 1) is O_h. Each stability group G_i is isomorphic with C_{3v}, and the stability group for the cluster is unity, and hence the constituent set $\Sigma_p(O_h)$ is isomorphic with O_h. The positional representation is now

$$P = A_{1g}\oplus A_{2u}\oplus T_{1u}\oplus T_{2g}, \tag{6}$$

where T_{1u} is the vector representation V. The corresponding bases $|\Lambda\lambda\rangle$ for $\Lambda = A_{1g}$ and T_{1u} can be found easily in a way demonstrated in the previous Section. The remaining bases have been determined by a projection procedure using a method proposed by Sakata [3] (we give an outline of this method in Appendix A). The irreducible basis

$$|\Lambda\lambda\rangle = \sum_i c^i_{\Lambda\lambda}|i\rangle \tag{7}$$

for the cube is given in Table II.

TABLE II

An irreducible basis $|\Lambda\lambda\rangle$ of the positional representation for the nodes of a cube. The coefficients $c^i_{\Lambda\lambda}$ are given in units of $1/2\sqrt{2}$

i \ Λ	A_{1g}	A_{2u}	T_{1u}			T_{2g}		
λ	a_{1g}	a_{2u}	x	y	z	x	y	z
1	1	1	1	1	1	1	1	1
2	1	1	1	−1	−1	1	−1	−1
3	1	1	−1	1	−1	−1	1	−1
4	1	1	−1	−1	1	−1	−1	1
5	1	−1	−1	−1	−1	1	1	1
6	1	−1	−1	1	1	1	−1	−1
7	1	−1	1	−1	1	−1	1	−1
8	1	−1	1	1	−1	−1	−1	1

TABLE III

Symmetric coordinates for nodes of a cube. The coefficients $B^{i\alpha}_{\Lambda\Gamma\gamma}$ of Eq. (5) are given in units of $\bar{B}_{\Lambda\Gamma\gamma}$; the latter are given under the headings of each column

$i\alpha$	Λ	A_{1g}			A_{2u}			T_{1u}											T_{2g}										
	Γ	T_{1u}			T_{2g}			A_{1g}	E_g		T_{1g}			T_{2g}			A_{2u}	E_u		T_{1u}			T_{2u}		
	γ	x	y	z	x	y	z	a_{1g}	θ	ε	x	y	z	x	y	z	a_{2u}	θ	ε	x	y	z	x	y	z
	$\bar{B}_{\Lambda\Gamma\gamma}$	$1/2\sqrt{2}$			$1/2\sqrt{2}$			$1/2\sqrt{2\cdot 3}$	$1/2^2\sqrt{3}$	$1/2^2$	$1/2^2$			$1/2^2$			$1/2\sqrt{2\cdot 3}$	$1/2^2\sqrt{3}$	$1/2^2$	$1/2^2$			$1/2^2$		
1	x	1	0	0	1	0	0	1	−1	1	0	−1	1	0	−1	−1	−1	−1	−1	0	−1	−1	0	−1	1
	y	0	1	0	0	1	0	1	−1	−1	1	0	−1	−1	0	−1	−1	1	−1	−1	0	−1	1	0	−1
	z	0	0	1	0	0	1	1	2	0	−1	1	0	−1	1	0	−1	0	2	−1	−1	0	−1	1	0
2	x	1	0	0	1	0	0	1	−1	1	0	1	−1	0	1	1	−1	−1	−1	0	1	1	0	1	−1
	y	0	1	0	0	1	0	−1	1	1	−1	0	−1	1	0	−1	1	−1	1	1	0	−1	−1	0	−1
	z	0	0	1	0	0	1	−1	−2	0	1	1	0	1	−1	0	1	0	−2	1	−1	0	1	1	0
3	x	1	0	0	1	0	0	−1	1	−1	0	1	1	0	1	−1	1	1	1	0	1	−1	0	1	1
	y	0	1	0	0	1	0	1	−1	−1	−1	0	1	1	0	1	−1	1	−1	1	0	1	−1	0	1
	z	0	0	1	0	0	1	−1	−2	0	−1	−1	0	−1	1	0	1	0	−2	−1	1	0	−1	−1	0
4	x	1	0	0	1	0	0	−1	1	−1	0	−1	−1	0	−1	1	1	1	1	0	−1	1	0	−1	−1
	y	0	1	0	0	1	0	−1	1	1	1	0	1	−1	0	1	1	−1	1	−1	0	1	1	0	1
	z	0	0	1	0	0	1	1	2	0	1	−1	0	1	1	0	−1	0	2	1	1	0	1	−1	0
5	x	1	0	0	−1	0	0	−1	1	−1	0	1	−1	0	1	1	−1	−1	−1	0	−1	−1	0	−1	1
	y	0	1	0	0	−1	0	−1	1	1	−1	0	1	1	0	1	−1	1	−1	−1	0	−1	1	0	−1
	z	0	0	1	0	0	−1	−1	−2	0	1	−1	0	1	1	0	−1	0	2	−1	−1	0	−1	1	0
6	x	1	0	0	−1	0	0	−1	1	−1	0	−1	1	0	−1	−1	−1	−1	−1	0	1	1	0	1	−1
	y	0	1	0	0	−1	0	1	−1	−1	1	0	1	−1	0	1	1	−1	1	1	0	−1	−1	0	−1
	z	0	0	1	0	0	−1	1	2	0	−1	−1	0	−1	1	0	1	0	−2	1	−1	0	1	1	0
7	x	1	0	0	−1	0	0	1	−1	1	0	−1	−1	0	−1	1	1	1	1	0	1	−1	0	1	1
	y	0	1	0	0	−1	0	−1	1	1	1	0	−1	−1	0	−1	−1	1	−1	1	0	1	−1	0	1
	z	0	0	1	0	0	−1	1	2	0	1	1	0	1	−1	0	1	0	−2	−1	1	0	−1	−1	0
8	x	1	0	0	−1	0	0	1	−1	1	0	1	1	0	1	−1	1	1	1	0	−1	1	0	−1	−1
	y	0	1	0	0	−1	0	1	−1	−1	−1	0	−1	1	0	−1	1	−1	1	−1	0	1	1	0	1
	z	0	0	1	0	0	−1	−1	−2	0	−1	1	0	−1	−1	0	−1	0	2	1	1	0	1	−1	0

The symmetric coordinates for the cube can be labelled by means of Eq. (5), without any additional repetition indices. The numerical values of the coefficients B are listed in Table III (we have assumed that the Clebsch–Gordan coefficients for the group O_h are equal to those of O after suppression of parity indices g and u).

In an interpretation of the symmetric coordinates $|\Lambda\Gamma\gamma\rangle$ it is convenient to consider the cube as two mutually interplaced regular tetrahedrons

$$t_1 = (1\ 2\ 3\ 4), \quad t_2 = (5\ 6\ 7\ 8), \tag{8}$$

each transforming into the other under inversion. It is easy to check that the part $A_{1g} \oplus T_{1u}$ of the positional representation (6) of the cube corresponds to positional representations (2), i.e. $A_1 \otimes T_2$, of tetrahedrons t_1 and t_2. Indeed, the coefficients $c^i_{\Lambda\lambda}$ from Table II for $i = 1\ldots, 4$ are equal, apart from a constant factor, to the corresponding coefficients determined by Eq. (4) for the tetrahedron t_1, and the coefficients for $i = 5, \ldots, 8$ determine evidently the positional representation for t_2. Moreover, the positional representation (6) for the cube can be written in a form

$$P = (A_{1g} \oplus T_{1u}) \oplus A_{2u} \otimes (A_{1g} \oplus T_{1u}), \tag{9}$$

allowing the introduction of the associated bases $|\check{\Lambda}\check{\lambda}\rangle$ by means of the relation

$$|\hat{\Lambda}\hat{\lambda}\rangle = \begin{bmatrix} \Lambda & A_2 & \check{\Lambda} \\ \lambda & a_2 & \check{\lambda} \end{bmatrix} |\Lambda\lambda\rangle \tag{10}$$

(cf. paper [4] for details related to the associated bases). Accordingly, the part $(A_{1g} \oplus T_{1u})$ of the positional representation (9) can be related to the same displacements for both tetrahedrons (e.g. translations or rotations in the same direction), and the remaining part $A_{2u} \otimes (A_{1g} \oplus T_{1u})$ corresponds to mutually opposite displacements of nodes of each tetrahedron.

4. The reduction in symmetry

Now we consider a classification of symmetric coordinates for a cube and a tetrahedron, adapted to a chain of subgroups $G_c \to G$. We restrict the discussion to a few non--trivial cases, when the cluster decomposes into simple subclusters.

We begin with the chain $T_d \to C_{3v}$. Let

$$\boldsymbol{i}^x = (1/\sqrt{2\cdot 3})\,(e^x+e^y+e^z), \quad \boldsymbol{i}^y = (1/\sqrt{2})\,(-e^x+e^y), \quad \boldsymbol{i}^z = (1/\sqrt{3})\,(e^x+e^y+e^z), \tag{11}$$

then $\boldsymbol{i}^z$ can be chosen as the trigonal axis, and $\boldsymbol{i}^x$ lies in a mirror plane. The tetrahedron (1234) (Fig. 1) decomposes in the subgroup C_{3v} into two simple clusters: (1) and (234). For the cluster (1) the stability group $G_1 \equiv G(1) = C_{3v}$ so the constituent set $\Sigma(1)$ is isomorphic with the quotient C_{3v}/C_{3v} and hence is the trivial group, whereas for the cluster (234) each G_i, $i = 2, 3, 4$, is isomorphic with C_s, and G (234) $= C_1$ so the constituent set is isomorphic with C_{3v}. The equilibrium positions $\boldsymbol{r}^0(p)$ for both clusters are

$$\boldsymbol{r}^0(1) = a\sqrt{3}\,\boldsymbol{i}^z, \tag{12}$$

$$\boldsymbol{r}^0(234) = [(1/\sqrt{2\cdot 3})(|2\rangle+|3\rangle-2|4\rangle)\boldsymbol{i}^x+(1/\sqrt{2})(-|2\rangle+|3\rangle)\boldsymbol{i}^y$$
$$+(1/\sqrt{3})(|2\rangle+|3\rangle+|4\rangle)i^z] \tag{13}$$

(we assume for simplicity, that the equilibrium positions of the nodes of the cube in Fig. 1 are not changed under the reduction in symmetry; an eventual change can be accounted for by replacing a by a' for the coefficients related to $\boldsymbol{i}^z$). Using these formulas, we can easily obtain the irreducible bases $|pA\lambda\rangle$ for the positional representations for each cluster as

$$|(1)A_1a_1\rangle = |1\rangle, \tag{14}$$

$$|(234)A_1a_1\rangle = (1/\sqrt{3})(|2\rangle+|3\rangle+|4\rangle),$$
$$|(234)Ex\rangle = (1/\sqrt{2\cdot 3})(|2\rangle+|3\rangle-2|4\rangle),$$
$$|(234)Ey\rangle = (1/\sqrt{2})(-|2\rangle+|3\rangle). \tag{15}$$

Eqs (14) and (15) are an example of the geometric reduction (the case (*iii*) of Secton 4 of I). In order to determine the bases of the positional representation in the formal reduction scheme (the case (*ii*)) one has to establish the decomposition coefficients $a_{A\lambda}^{A_c\lambda_c}$ (cf. Eq. (I. 25)). Assuming that

$$a_{A_1a_1}^{A_{1c}a_{1c}} = 1 \tag{16}$$

and that appropriate coefficients for $A_c = T_2$ are determined by Eq. (11) (note that T_2 is here the vector representation V, and (11) is its basis), one gets

$$|A_{1c}A_1a_1\rangle = (1/2)(|1\rangle+|2\rangle+|3\rangle+|4\rangle),$$
$$|T_2A_1a_1\rangle = (1/2\sqrt{3})(3|1\rangle-|2\rangle-|3\rangle-|4\rangle),$$
$$|T_2Ex\rangle = (1/\sqrt{2\cdot 3}(|2\rangle+|3\rangle-2|4\rangle),$$
$$|T_2Ey\rangle = (1/\sqrt{2})(-|2\rangle+|3\rangle). \tag{17}$$

Now it is easy to evaluate the coefficients $A_p^{A_c}(A)$ for the transformation (I. 26) between the geometric and formal basis (Eqs. (14)–(15), and Eq. (17), respectively). This transformation is

$$|(1)A_1a_1\rangle = (1/2)\,|A_{1c}A_1a_1\rangle+(\sqrt{3}/2)\,|T_2A_1a_1\rangle,$$
$$|(234)A_1a_1\rangle = (\sqrt{3}/2)\,|A_{1c}A_1a_1\rangle-(1/2)\,|T_2A_1a_1\rangle,$$
$$|(234)Ex\rangle = |T_2Ex\rangle, \quad |(234)Ey\rangle = |T_2Ey\rangle. \tag{18}$$

Eqs. (18) can be interpreted in terms of an "interference" of "waves". E.g., a result of an "interference" of basis functions $|A_{1c}A_1a_1\rangle$ and $|T_2A_1a_1\rangle$ of the positional representation for a tetrahedron, with "amplitudes" and "phases" defined by the first of Eqs. (18), is an "annihilation" of nodes 2, 3, 4, so that there remains only the node 1. In the other three cases the node 1 is annihilated, and three independent "superpositions" of the nodes 2, 3, 4 are realized.

TABLE IV

Classification schemes of formal and geometric reduction for a few chains $O_h \to G$. Each of the four columns related to the formal reduction presents the decomposition of an appropriate representation A_c occurring in Eq. (6) into irreducible representations of the group G. The column p contains labels of nodes belonging to a given simple cluster, G_i is the stability group of an i-th node of the cluster, and P_p — the corresponding positional representation. The representations constituting the vector part V of the positional representation P_p are underlined. For a geometric identification of a particular group cf. Appendix B

G	The formal reduction				The geometric reduction		
	A_{1g}	A_{2u}	T_{1u}	T_{2g}	p	G_i	P_p
T_d	A_1	A_1	T_2	T_2	1234 5678	C_{3v}	$A_1\oplus\underline{T_2}$
C_{4v}	A_1	B_2	$A_1\oplus E$	$B_2\oplus E$	1647 8352	C_s	$\underline{A_1}\oplus B_2\oplus\underline{E}$
$D_2(a)$	A_1	A_1	$A_2\oplus B_1\oplus B_2$	$A_2\oplus B_1\oplus B_2$	1234 5678	C_1	$A_1\oplus\underline{A_2}\oplus\underline{B_1}\oplus\underline{B_2}$
$D_2(b)$	A_1	A_2	$A_2\oplus B_1\oplus B_2$	$A_1\oplus B_1\oplus B_2$	1458 6732	C_1	$A_1\oplus\underline{A_2}\oplus\underline{B_1}\oplus B_2$ $A_1\oplus\underline{A_2}\oplus B_1\oplus\underline{B_2}$
D_{3d}	A_{1g}	A_{2u}	$A_{2u}\oplus E_u$	$A_{1g}\oplus E_g$	15 234678	C_{3v} C_s	$A_{1g}\oplus\underline{A_{2u}}$ $A_{1g}\oplus\underline{A_{2u}}\oplus\underline{E_u}\oplus E_g$

All cases of reduction $O_h \to G$ analyzed in this work are listed in Table IV. This Table provides a detailed classification of irreducible bases for the positional space for nodes of a cube in both formal and geometric reduction schemes. It follows from an inspection of Table IV that

$$G(p) = \begin{cases} C_{3v} & \text{for } G = D_{3d},\ p = (15) \\ C_1 & \text{for other cases} \end{cases} \tag{19}$$

(cf. Eq. (I. 9)), so that the constituent sets $\Sigma_p(G)$ are isomorphic with the corresponding groups G, with the exception of the linear cluster $p = (15)$, for which

$$\Sigma_{(15)}(D_{3d}) \sim D_{3d}/C_{3v} \sim \Sigma_2, \tag{20}$$

that is, the constituent set $\Sigma_{(15)}$ is isomorphic with the group Σ_2 of permutations of two elements.

A determination of bases for the formal reduction scheme is reduced to a careful determination of the decomposition coefficients $a_{A\lambda}^{A_c\lambda_c}$ for each of the subgroups G. The coefficients related to cases listed in Table IV are compiled in Appendix B.

TABLE V

Irreducible bases for clusters from Table IV. The bases for $\Lambda = A_1$ are omitted — they are determined by Eq. (I.16). The exchange of indices is determined by the sequence of nodes in a cluster (e.g. "8352 as 1647 after the exchange of indices" means that 1 should be substituted by 8, 6 by 3, etc). Symbols $|Vx\rangle$, $|Vy\rangle$, and $|Vz\rangle$ denote appropriate vector components of the positional representation, associated with the Cartesian system for the corresponding group G according to definitions given in Appendix B

G	p	Λ λ	$\lvert p\Lambda\lambda\rangle$
T_d	1234	T_2 x	$(1/2)(\lvert 1\rangle+\lvert 2\rangle-\lvert 3\rangle-4\rangle) = \lvert Vx\rangle$
		y	$(1/2)(\lvert 1\rangle-\lvert 2\rangle+\lvert 3\rangle-\lvert 4\rangle) = \lvert Vy\rangle$
		z	$(1/2)(\lvert 1\rangle-\lvert 2\rangle-\lvert 3\rangle+\lvert 4\rangle) = \lvert Vz\rangle$
	5678		as 1234 after the exchange of indices
C_{4v}	1647	E x	$(1/2)(\lvert 1\rangle-\lvert 6\rangle-\lvert 4\rangle+\lvert 7\rangle) = \lvert Vx\rangle$
		y	$(1/2)(\lvert 1\rangle+\lvert 6\rangle-\lvert 4\rangle-\lvert 7\rangle) = \lvert Vy\rangle$
		B_2 b_2	$(1/2)(\lvert 1\rangle-\lvert 6\rangle+\lvert 4\rangle-\lvert 7\rangle)$
	8352		as 1467 after the exchange of indices
$D_2(a)$	1234	A_2 a_2	as $\lvert T_2z\rangle$ for this cluster in T_d
		B_1 b_1	as $\lvert T_2x\rangle$ for this cluster in T_d
		B_2 b_2	as $\lvert T_2y\rangle$ for this cluster in T_d
	5678		as 1234 after the exchange of indices
$D_2(b)$	1458	A_2 a_2	$(1/2)(\lvert 1\rangle+\lvert 4\rangle-\lvert 5\rangle-\lvert 8\rangle) = \lvert Vz\rangle$
		B_1 b_1	$(1/2)(\lvert 1\rangle-\lvert 4\rangle-\lvert 5\rangle+\lvert 8\rangle) = \lvert Vx\rangle$
		B_2 b_2	$(1/2)(\lvert 1\rangle-\lvert 4\rangle+\lvert 5\rangle-\lvert 8\rangle)$
	6732	A_2 a_2	$(1/2)(\lvert 6\rangle+\lvert 7\rangle-\lvert 3\rangle-\lvert 2\rangle) = \lvert Vz\rangle$
		B_1 b_1	$(1/2)(\lvert 6\rangle-\lvert 7\rangle-\lvert 3\rangle+\lvert 2\rangle)$
		B_2 b_2	$(1/2)(\lvert 6\rangle-\lvert 7\rangle+\lvert 3\rangle-\lvert 2\rangle) = \lvert Vy\rangle$
D_{3d}	15	A_{2u} a_{2u}	$(1/\sqrt{2})(\lvert 1\rangle-\lvert 5\rangle) = \lvert Vz\rangle$
	234678	A_{u2} a_{2u}	$(1/\sqrt{2\cdot 3})(-\lvert 2\rangle-\lvert 3\rangle-\lvert 4\rangle+\lvert 6\rangle+\lvert 7\rangle+\lvert 8\rangle) = \lvert Vz\rangle$
		E_u x	$(1/2)(\lvert 2\rangle-\lvert 3\rangle-\lvert 6\rangle+\lvert 7\rangle) = \lvert Vx\rangle$
		y	$(1/2\sqrt{3})(\lvert 2\rangle+\lvert 3\rangle-2\lvert 4\rangle-\lvert 6\rangle-\lvert 7\rangle+2\lvert 8\rangle) = \lvert Vy\rangle$
		E_g x	$(1/2\sqrt{3})(\lvert 2\rangle+\lvert 3\rangle-2\lvert 4\rangle+\lvert 6\rangle+\lvert 7\rangle-2\lvert 8\rangle)$
		y	$(1/2)(-\lvert 2\rangle+\lvert 3\rangle-\lvert 6\rangle+\lvert 7\rangle)$

Bases in the geometric reduction scheme, i.e. irreducible bases for subclusters p, associated with a group G, are listed in Table V. The equilibrium positions of clusters listed in Table IV are given by

$$r^0(p) = \begin{cases} \pm a(|Vx\rangle e^x+|Vy\rangle e^y+|Vz\rangle e^z) & \text{for} \quad G = T_d, C_{4v}, D_2(a), \\ a(\sqrt{2}\,|Vx\rangle e^x+|Vz\rangle e^z) & \text{for} \quad G = D_2(b),\ p = 1458, \\ a(\sqrt{2}\,|Vy\rangle e^y+|Vz\rangle e^z) & \text{for} \quad G = D_2(b),\ p = 6732, \\ a\sqrt{3}\,|Vz\rangle e^z & \text{for} \quad G = D_{3d},\ p = 15, \\ a\sqrt{2}\,(|Vx\rangle e^x+|Vy\rangle e^y+|Vz\rangle e^z) & \text{for} \quad G = D_{3d},\ p = 234678, \end{cases} \tag{21}$$

where the sign "—" in the first line corresponds to $p = 5678$ and 8352, and $|Vx\rangle$, $|Vy\rangle$, $|Vz\rangle$ are the vector components of an appropriate positional representation, defined by Tables IV and V, where the Cartesian axes x, y, z are associated with the symmetry group G of the cluster according to the definitions of Appendix B. Note that for $G = C_{4v}$ both 1647 and 8352 are plane clusters perpendicular to the z-axis. Nevertheless, the positional representation contains the vector component $|Vz\rangle = |A_1 a_1\rangle$, associated with a translation of the plane of a cluster along the z-axis (cf. comments following Eq. (I. 15)).

TABLE VI

Matrix elements $A_p^{A_c}(A)$ of transformations between the geometric and formal reduction schemes for the cases listed in Table IV. The matrices, their rows, and columns are labelled by A, A_c, and p, respectively

$O_h \to T_d$:

A_1	1234	5678
A_{1g}	$1/\sqrt{2}$	$1/\sqrt{2}$
A_{2u}	$1/\sqrt{2}$	$-1/\sqrt{2}$

T_2	1234	5678
T_{1u}	$1/\sqrt{2}$	$-1/\sqrt{2}$
T_{2g}	$1/\sqrt{2}$	$1/\sqrt{2}$

$O_h \to C_{4v}$:

A_1	1647	8352
A_{1g}	$1/\sqrt{2}$	$1/\sqrt{2}$
T_{1u}	$1/\sqrt{2}$	$-1/\sqrt{2}$

B_2	1647	8352
A_{2u}	$1/\sqrt{2}$	$-1/\sqrt{2}$
T_{2g}	$1/\sqrt{2}$	$1/\sqrt{2}$

E	1647	8352
T_{1u}	$1/\sqrt{2}$	$1/\sqrt{2}$
T_{2g}	$1/\sqrt{2}$	$-1/\sqrt{2}$

$O_h \to D_2(a)$: The matrix $A(A_1)$, and each of the three matrices $A(A_2)$, $A(B_1)$, $A(B_2)$ coincides with $A(A_1)$, and $A(T_2)$, respectively, for the case $O_h \to T$.

$O_h \to D_2(b)$:

A_1	1458	6732
A_{1g}	$1/\sqrt{2}$	$1/\sqrt{2}$
T_{2g}	$1/\sqrt{2}$	$-1/\sqrt{2}$

A_2	1458	6732
A_{2u}	$1/\sqrt{2}$	$-1/\sqrt{2}$
T_{1u}	$1/\sqrt{2}$	$1/\sqrt{2}$

B_1	1458	6732
T_{1u}	1	0
T_{2g}	0	1

B_2	1458	6732
T_{1u}	0	1
T_{2g}	1	0

$O_h \to D_{3d}$:

A_{1g}	15	234678
A_{1g}	$1/2$	$\sqrt{3}/2$
T_{2g}	$\sqrt{3}/2$	$-1/2$

A_{2u}	15	234678
A_{2u}	$1/2$	$-\sqrt{3}/2$
T_{1u}	$\sqrt{3}/2$	$1/2$

E_g	234678
T_{2g}	1

E_u	234678
T_{2u}	1

The transformation matrices between bases in the geometric and formal reduction schemes (cf. Eq. (I. 26)) are given in Table VI. This Table demonstrates also the general structure of the transformation matrices $A(A)$.

The bases related to a reduction in symmetry strongly depend on an orientation of elements of a subgroup G of O_h. E.g. two isomorphic subgroups $D_2(a)$ and $D_2(b)$ lead to essentially different bases: the basis in the case of $D_2(a)$ is determined by three-dimensional clusters $p = 1234$ and 5678, related to the intermediate subgroup T_d in the chain $O_h \to T_d$

$\to D_2(a)$ where the chain $T_d \to D_2(a)$ is associated only with the formal reduction, whereas the basis in the case of $D_2(b)$ is associated with two plane clusters $p = 1458$ and 6732, situated on the plane xz, and yz, respectively (in the system of coordinates for the group $D_2(b)$).

5. *Final remarks and conclusions*

We have presented in this paper an application of a general method for the determination of the symmetric coordinates for point clusters invariant under a point group to the non-trivial cases of nodes of a regular tetrahedron and of a cube. We have shown how the factorisation of the corresponding mechanical representation into the positional and vector part allows one to simplify the projection procedure by using standard Clebsch–Gordan coefficients. The determination of an irreducible basis for the positional representation can be further simplified by exploiting the information about the equilibrium position of the cluster. It allows us to obtain immediately, without any tedious projection, the bases related to the vectorial part of the positional representation. Consequently, bases for the positional representation for the regular tetrahedron, as well as for all subclusters listed in Table IV, with an exception of the last one, can be obtained in a very simple way (when only one component is unknown, e.g. $|B_2b_2\rangle$ for the case $G = D_2(b)$, $p = 1458$ of Table IV, we can determine it from the orthogonality conditions: $\langle B_2\, b_2|A_1a_1\rangle$ $\langle B_2b_2|A_2a_2\rangle = \langle B_2b_2|B_1b_1\rangle = 0$ – cf. Table V).

We note that the mechanical representation M for a cube decomposes into irreducible representations Γ as

$$M = A_{1g}\oplus A_{2u}\oplus E_g\oplus E_u\oplus T_{1g}\oplus 2T_{1u}\oplus 2T_{2g}\oplus T_{2u}, \tag{22}$$

hence a simple classification based only on Γ and γ is not complete for the cases $\Gamma = T_{1u}$ and T_{2g}. Whereas the two representations $\Gamma = T_{1u}$ can be easily distinguished by relating one of them to translations of the whole cube, the resolution of two identical representations T_{2g} is not so obvious. The scheme proposed in this paper provides a natural label distinguishing these representations, namely the representation Λ, which is related to the equilibrium position of the cluster. Consequently, the proposed scheme is complete for the cases considered here.

APPENDIX A

A brief outline of the projection method of Sakata [3]

Let P be a representation of a compact group G, with the decomposition

$$P = \sum_{\Lambda} n(P, \Lambda)\Lambda \tag{A1}$$

into irreducible representations Λ of this group. According to a method proposed by Sakata [3], an irreducible basis $|P\Lambda t\lambda\rangle$, $t = 1, 2, \ldots, n(P, \Lambda)$ is given, with an accuracy to a λ-independent normalisation, by columns of the matrix

$$\check{F}(G) = \sum_{g \in G} \check{P}(g)\check{A}\check{P}^{(q)}(g)^{\dagger}, \tag{A2}$$

where $\check{P}(g)$ is the matrix of the representation P for an element $g \in G$, $\check{A}$ is an arbitrary square matrix of the order $[P]$, and $\check{P}^{(q)}(g)$ is a quasidiagonal matrix composed from standard irreducible matrices $\check{D}^{\Lambda}(g)$ according to the decomposition (A1), with a fixed sequence of Λ's.

The method of Sakata accounts for all conditions imposed by the symmetry of the group G as well as by the assumed conventions for matrix elements $D^{\Lambda}_{\lambda\lambda'}(g)$, and the whole remaining arbitrariness (a choice of phases, normalisation, a choice of a system of repetition indices t) can be removed only way of some extra physical or mathematical conditions. In particular, this method automatically assures the coherence of any two states $|\Lambda\lambda\rangle$ and $|\Lambda\lambda'\rangle$ belonging to the same representation Λ, whereas traditional methods of projection (see e.g. Lyubarskii [5], § 26) require not only the operators which project on $|\Lambda\lambda\rangle$ but also step operators which transform $|\Lambda\lambda\rangle$ into $|\Lambda\lambda'\rangle$.

For cases when the group manifold G can be decomposed into left cosets with respect to a subgroup H as

$$G = \bigcup_{x=1}^{|G|/|H|} g_x H, \tag{A3}$$

the matrix $\check{F}(G)$ is given, with an accuracy to an unimportant multiplicative constant, by

$$\check{F}(G) = \sum_{x=1}^{|G|/|H|} \check{P}(g_x)\check{F}(H)\check{P}^{(q)}(g_x)^{\dagger}, \tag{A4}$$

where $\check{F}(H)$ should be evaluated using Eq. (A2) with the summation limited to the subgroup H. The formula (A4) provides a considerable simplification of calculations, e.g. using the chain

$$O_h \to O \to T \to D_2 \to C_1 \tag{A5}$$

one can restrict the summation in (A2) from 48 to 8 elements, namely to E, C_{2x}, C_{2y} and C_{2z} (the elements of D_2), C_{31} and C_{31}^{-1} (left coset representatives for D_2 in T), C_{4x} (that for T in O), and I (that for O in O_h). The method can be easily demonstrated for the case of positional representation of the regular tetrahedron (2). It involves only the summation over elements quoted in Eq. (1), and leads also to the irreducible basis (4).

APPENDIX B

The formal reduction for selected chains $O_h \to G$

We give here the irreducible bases

$$|\Gamma_c\Gamma\gamma\rangle = \sum_{\gamma_c} a^{\Gamma_c\gamma_c}_{\Gamma\gamma}|\Gamma_c\gamma_c\rangle \tag{B1}$$

assumed in this paper for subgroups G of the group O_h, listed in Table IV, and for representations Γ_c appearing in Eq. (6). Γ_c and Γ denote the irreducible representations of O_h and G, respectively, and γ_c and γ – the corresponding standard basis functions.

For the subgroup T_d, we choose the cartesian system e^x, e^y, e^z (Fig. 1). Then

$$|A_{1g}A_1a_1\rangle = |A_{1g}a_{1g}\rangle, \quad |A_{2u}A_1a_1\rangle = |A_{2u}a_{2u}\rangle,$$

$$|T_{1u}T_2\gamma\rangle = |T_{1u}\gamma\rangle, \quad |T_{2g}T_2\gamma\rangle = |T_{2g}\gamma\rangle, \quad \gamma = x, y, z. \tag{B2}$$

We choose the four-fold axis of the subgroup C_{4v} to be parallel *to* e^z. Then we have (in the same system e^x, e^y, e^z)

$$|A_{1g}A_1a_1\rangle = |A_{1g}a_{1g}\rangle, \quad |A_{2u}B_2b_2\rangle = |A_{2u}a_{2u}\rangle,$$

$$|T_{1u}A_1a_1\rangle = |T_{1u}z\rangle, \quad |T_{2g}B_2b_2\rangle = |T_{2g}z\rangle,$$

$$|T_{1u}Ex\rangle = |T_{1u}x\rangle, \quad |T_{2g}Ex\rangle = |T_{2g}y\rangle,$$

$$|T_{1u}Ey\rangle = |T_{1u}y\rangle, \quad |T_{2g}Ey\rangle = |T_{2g}x\rangle. \tag{B3}$$

The group O_h has two kinds of geometrically unequivalent subgroups D_2. The subgroup $D_2(a)$ is a normal subgroup of O_h, and its two-fold axes are parallel to e^x, e^y, and e^z. We have

$$|A_{1g}A_1a_1\rangle = |A_{1g}a_{1g}\rangle, \quad |A_{2u}A_1a_1\rangle = |A_{2u}a_{2u}\rangle,$$

$$|T_{1u}B_1b_1\rangle = |T_{1u}x\rangle, \quad |T_{2g}B_1b_1\rangle = |T_{2g}y\rangle,$$

$$|T_{1u}B_2b_2\rangle = |T_{1u}y\rangle, \quad |T_{2g}B_2b_2\rangle = |T_{2g}x\rangle,$$

$$|T_{1u}A_2a_2\rangle = |T_{1u}z\rangle, \quad |T_{2g}A_2a_2\rangle = |T_{2g}z\rangle. \tag{B4}$$

As the subgroup $D_2(b)$, we choose the one having horizontal two-fold axes rotated with respect to $D_2(a)$ through the angle $\pi/4$ around e^z. It is therefore convenient to choose in this case the cartesian system

$$j^x = (1/\sqrt{2})\,(e^x+e^y), \quad j^y = (1/\sqrt{2})\,(-e^x+e^y), \quad j^z = e^z. \tag{B5}$$

Then

$$|A_{1g}A_1a_1\rangle = |A_{1g}a_{1g}\rangle, \quad |A_{2u}A_2a_2\rangle = |A_{2u}a_{2u}\rangle,$$

$$|T_{1u}A_2a_2\rangle = |T_{1u}z\rangle, \quad |T_{2g}A_1a_1\rangle = |T_{2g}z\rangle,$$

$$|T_{1u}B_1b_1\rangle = (1/\sqrt{2})\,(|T_1x\rangle+|T_1y\rangle),$$

$$|T_{1u}B_2b_2\rangle = (1/\sqrt{2})\,(|T_1x\rangle-|T_1y\rangle),$$

$$|T_{2g}B_1b_1\rangle = (1/\sqrt{2})\,(|T_{2g}x\rangle-|T_{2g}y\rangle),$$

$$|T_{2g}B_2b_2\rangle = (1/\sqrt{2})\,(|T_{2g}x\rangle+|T_{2g}y\rangle). \tag{B6}$$

Note that the subgroups $D_2(a)$ and $D_2(b)$, despite their isomorphism, have different decompositions of the same octahedral representation T_{2g}, as a consequence of their geometric unequivalence.

We relate the subgroup D_{3d} to the cartesian system

$$\boldsymbol{k}^x = (1/\sqrt{2})(\boldsymbol{e}^x-\boldsymbol{e}^y), \quad \boldsymbol{k}^y = (1/\sqrt{2\cdot 3})(\boldsymbol{e}^x+\boldsymbol{e}^y-2\boldsymbol{e}^z), \quad \boldsymbol{k}^z = (1/\sqrt{3})(\boldsymbol{e}^x+\boldsymbol{e}^y+\boldsymbol{e}^z), \tag{B7}$$

so that the trigonal axis coincides with $\boldsymbol{k}^z$, and $\boldsymbol{k}^x$ is a two-fold axis. Then the decomposition coefficients $a_{\Gamma\gamma}^{\Gamma_c\gamma_c}$ are given by Table A 17 of Griffith [6] for the chain $O \rightarrow D_3$.

A comparison of the system (B7) with that for the subgroup C_{3v} (cf. Eq. (11)) is given by

$$\boldsymbol{k}^x = -\boldsymbol{i}^y, \quad \boldsymbol{k}^y = \boldsymbol{i}^x, \quad \boldsymbol{k}^z = \boldsymbol{i}^z. \tag{B8}$$

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