SAMB for "`MoS2`"

- Group: No. 187 D_{3h}^1 $P-6m2$ [hexagonal]
- Associated point group: No. 26 D_{3h} $-6m2$ (-6m2 setting)   [hexagonal]

- Generation condition
    - model type: `tight_binding`
    - time-reversal type: `electric`
    - irrep: `[A1']`
    - `spinless`

- Unit cell:
    $a = 3.1661,\ b = 3.1661,\ c = 20.0,\ \alpha = 90.0,\ \beta = 90.0,\ \gamma = 120.0$
- Lattice vectors:
    $\boldsymbol{a}_1 = \begin{pmatrix} 3.1661 & 0 & 0 \end{pmatrix}$
    $\boldsymbol{a}_2 = \begin{pmatrix} -1.58305 & 2.74192303092191 & 0 \end{pmatrix}$
    $\boldsymbol{a}_3 = \begin{pmatrix} 0 & 0 & 20.0 \end{pmatrix}$

Table 1: High-symmetry line: Γ-M-K-Γ-K'.

symbol	position	symbol	position	symbol	position
Γ	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	M	$\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	K	$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & 0 \end{pmatrix}$
K'	$\begin{pmatrix} -\frac{1}{3} & -\frac{1}{3} & 0 \end{pmatrix}$				

- Kets: dimension = 11

Table 2: Hilbert space for full matrix.

No.	ket	No.	ket	No.	ket	No.	ket	No.	ket
1	d_u@Mo$_1$	2	d_v@Mo$_1$	3	d_{yz}@Mo$_1$	4	d_{zx}@Mo$_1$	5	d_{xy}@Mo$_1$
6	p_x@S$_1$	7	p_y@S$_1$	8	p_z@S$_1$	9	p_x@S$_2$	10	p_y@S$_2$
11	p_z@S$_2$								

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S$_1$ [1a: -6m2]	Mo$_1$	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,2,3,4,5,6,7,8,9,10,11,12]
S$_2$ [2i: 3m.]	S$_1$	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0.12425 \end{pmatrix}$	[1,5,6,7,8,9]
	S$_2$	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0.87575 \end{pmatrix}$	[2,3,4,10,11,12]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	$\boldsymbol{b}$@$\boldsymbol{c}$	mapping
B$_1$ [3j: mm2]	b$_1$	Mo$_1$	Mo$_1$	1	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix}$ @ $\begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[1,-3,-8,10]
	b$_2$	Mo$_1$	Mo$_1$	1	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[2,-5,7,-12]
	b$_3$	Mo$_1$	Mo$_1$	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[-4,6,-9,11]
B$_2$ [6n: .m.]	b$_4$	S$_1$	Mo$_1$	1	1	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0.12425 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{3} & \frac{1}{6} & 0.062125 \end{pmatrix}$	[1,8]
	b$_5$	S$_2$	Mo$_1$	1	1	$\begin{pmatrix} -\frac{1}{3} & \frac{1}{3} & -0.12425 \end{pmatrix}$ @ $\begin{pmatrix} \frac{5}{6} & \frac{1}{6} & 0.937875 \end{pmatrix}$	[2,12]
	b$_6$	S$_2$	Mo$_1$	1	1	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & -0.12425 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{3} & \frac{1}{6} & 0.937875 \end{pmatrix}$	[3,10]
	b$_7$	S$_2$	Mo$_1$	1	1	$\begin{pmatrix} -\frac{1}{3} & -\frac{2}{3} & -0.12425 \end{pmatrix}$ @ $\begin{pmatrix} \frac{5}{6} & \frac{2}{3} & 0.937875 \end{pmatrix}$	[4,11]

Table 4

	bond	tail	head	n	#	$\boldsymbol{b}@\boldsymbol{c}$	mapping
	b_8	S_1	Mo_1	1	1	$\left(-\frac{1}{3} \quad \frac{1}{3} \quad 0.12425\right) @ \left(\frac{5}{6} \quad \frac{1}{6} \quad 0.062125\right)$	[5,7]
	b_9	S_1	Mo_1	1	1	$\left(-\frac{1}{3} \quad -\frac{2}{3} \quad 0.12425\right) @ \left(\frac{5}{6} \quad \frac{2}{3} \quad 0.062125\right)$	[6,9]
B_3 [6n: .m.]	b_{10}	S_1	S_1	1	1	$\left(1 \quad 0 \quad 0\right) @ \left(\frac{1}{6} \quad \frac{1}{3} \quad 0.12425\right)$	[1,-7]
	b_{11}	S_2	S_2	1	1	$\left(1 \quad 0 \quad 0\right) @ \left(\frac{1}{6} \quad \frac{1}{3} \quad 0.87575\right)$	[-2,10]
	b_{12}	S_2	S_2	1	1	$\left(1 \quad 1 \quad 0\right) @ \left(\frac{1}{6} \quad \frac{5}{6} \quad 0.87575\right)$	[3,-11]
	b_{13}	S_2	S_2	1	1	$\left(0 \quad 1 \quad 0\right) @ \left(\frac{2}{3} \quad \frac{5}{6} \quad 0.87575\right)$	[-4,12]
	b_{14}	S_1	S_1	1	1	$\left(0 \quad 1 \quad 0\right) @ \left(\frac{2}{3} \quad \frac{5}{6} \quad 0.12425\right)$	[5,-9]
	b_{15}	S_1	S_1	1	1	$\left(1 \quad 1 \quad 0\right) @ \left(\frac{1}{6} \quad \frac{5}{6} \quad 0.12425\right)$	[-6,8]

- SAMB:

No. 1 $\hat{\mathbb{Q}}_0^{(A_1')} [M_1, S_1]$

$\hat{\mathbb{Z}}_1 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1')}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A_1')}]$

No. 2 $\hat{\mathbb{Q}}_2^{(A_1')} [M_1, S_1]$

$\hat{\mathbb{Z}}_2 = \mathbb{X}_2[\mathbb{Q}_2^{(a,A_1')}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A_1')}]$

No. 3 $\hat{\mathbb{Q}}_4^{(A_1')} [M_1, S_1]$

$\hat{\mathbb{Z}}_3 = \mathbb{X}_3[\mathbb{Q}_4^{(a,A_1')}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A_1')}]$

No. 4 $\hat{\mathbb{Q}}_0^{(A_1')} [M_2, S_2]$

$\hat{\mathbb{Z}}_4 = \mathbb{X}_{14}[\mathbb{Q}_0^{(a,A_1')}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s,A_1')}]$

No. 5 $\hat{\mathbb{Q}}_2^{(A_1')} [M_2, S_2]$

$\hat{\mathbb{Z}}_5 = \mathbb{X}_{15}[\mathbb{Q}_2^{(a,A_1')}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s,A_1')}]$

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No. 6 $\hat{\mathbb{Q}}_0^{(A_1')}$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_6 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1')}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A_1')}]$$

No. 7 $\hat{\mathbb{Q}}_2^{(A_1')}$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_7 = \mathbb{X}_2[\mathbb{Q}_2^{(a,A_1')}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A_1')}]$$

No. 8 $\hat{\mathbb{Q}}_3^{(A_1')}$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_8 = -\frac{\sqrt{2}\,\mathbb{X}_4[\mathbb{Q}_{2,0}^{(a,E')}] \otimes \mathbb{Y}_4[\mathbb{Q}_{1,0}^{(b,E')}]}{2} - \frac{\sqrt{2}\,\mathbb{X}_5[\mathbb{Q}_{2,1}^{(a,E')}] \otimes \mathbb{Y}_5[\mathbb{Q}_{1,1}^{(b,E')}]}{2}$$

No. 9 $\hat{\mathbb{Q}}_4^{(A_1')}$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_9 = \mathbb{X}_3[\mathbb{Q}_4^{(a,A_1')}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A_1')}]$$

No. 10 $\hat{\mathbb{Q}}_3^{(A_1')}$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{10} = \frac{\sqrt{406}\,\mathbb{X}_6[\mathbb{Q}_{4,0}^{(a,E',1)}] \otimes \mathbb{Y}_4[\mathbb{Q}_{1,0}^{(b,E')}]}{29} + \frac{\sqrt{406}\,\mathbb{X}_7[\mathbb{Q}_{4,1}^{(a,E',1)}] \otimes \mathbb{Y}_5[\mathbb{Q}_{1,1}^{(b,E')}]}{29} + \frac{\sqrt{58}\,\mathbb{X}_8[\mathbb{Q}_{4,0}^{(a,E',2)}] \otimes \mathbb{Y}_4[\mathbb{Q}_{1,0}^{(b,E')}]}{58} + \frac{\sqrt{58}\,\mathbb{X}_9[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{Y}_5[\mathbb{Q}_{1,1}^{(b,E')}]}{58}$$

No. 11 $\hat{\mathbb{G}}_4^{(A_1')}$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{11} = -\frac{\sqrt{58}\,\mathbb{X}_6[\mathbb{Q}_{4,0}^{(a,E',1)}] \otimes \mathbb{Y}_4[\mathbb{Q}_{1,0}^{(b,E')}]}{58} - \frac{\sqrt{58}\,\mathbb{X}_7[\mathbb{Q}_{4,1}^{(a,E',1)}] \otimes \mathbb{Y}_5[\mathbb{Q}_{1,1}^{(b,E')}]}{58} + \frac{\sqrt{406}\,\mathbb{X}_8[\mathbb{Q}_{4,0}^{(a,E',2)}] \otimes \mathbb{Y}_4[\mathbb{Q}_{1,0}^{(b,E')}]}{29} + \frac{\sqrt{406}\,\mathbb{X}_9[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{Y}_5[\mathbb{Q}_{1,1}^{(b,E')}]}{29}$$

No. 12 $\hat{\mathbb{Q}}_3^{(A_1')}$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{12} = \mathbb{X}_{10}[\mathbb{M}_1^{(a,A_2')}] \otimes \mathbb{Y}_8[\mathbb{T}_3^{(b,A_2')}]$$

No. 13 $\hat{\mathbb{Q}}_3^{(A_1')}$ $[\mathrm{M}_1, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{13} = \frac{\sqrt{2}\,\mathbb{X}_{12}[\mathbb{M}_{3,0}^{(a,E')}] \otimes \mathbb{Y}_6[\mathbb{T}_{1,0}^{(b,E')}]}{2} + \frac{\sqrt{2}\,\mathbb{X}_{13}[\mathbb{M}_{3,1}^{(a,E')}] \otimes \mathbb{Y}_7[\mathbb{T}_{1,1}^{(b,E')}]}{2}$$

No. 14 $\hat{\mathbb{Q}}_3^{(A_1')}[M_1, B_1]$

$$\hat{\mathbb{Z}}_{14} = -\mathbb{X}_{11}[\mathbb{M}_3^{(a,A_2')}] \otimes \mathbb{Y}_8[\mathbb{T}_3^{(b,A_2')}]$$

No. 15 $\hat{\mathbb{Q}}_0^{(A_1')}[M_3, B_2]$

$$\hat{\mathbb{Z}}_{15} = \frac{\sqrt{3}\mathbb{X}_{23}[\mathbb{Q}_1^{(a,A_2'')}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_1^{(b,A_2'')}]}{3} + \frac{\sqrt{3}\mathbb{X}_{25}[\mathbb{Q}_{1,0}^{(a,E')}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E')}]}{3} + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E')}]}{3}$$

No. 16 $\hat{\mathbb{Q}}_2^{(A_1')}[M_3, B_2]$

$$\hat{\mathbb{Z}}_{16} = \frac{\sqrt{6}\mathbb{X}_{23}[\mathbb{Q}_1^{(a,A_2'')}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_1^{(b,A_2'')}]}{3} - \frac{\sqrt{6}\mathbb{X}_{25}[\mathbb{Q}_{1,0}^{(a,E')}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E')}]}{6} - \frac{\sqrt{6}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E')}]}{6}$$

No. 17 $\hat{\mathbb{Q}}_3^{(A_1')}[M_3, B_2]$

$$\hat{\mathbb{Z}}_{17} = \mathbb{X}_{31}[\mathbb{Q}_3^{(a,A_1')}] \otimes \mathbb{Y}_9[\mathbb{Q}_0^{(b,A_1')}]$$

No. 18 $\hat{\mathbb{Q}}_2^{(A_1')}[M_3, B_2]$

$$\hat{\mathbb{Z}}_{18} = \frac{\sqrt{21}\mathbb{X}_{24}[\mathbb{Q}_3^{(a,A_2'')}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_1^{(b,A_2'')}]}{7} + \frac{\sqrt{14}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E')}]}{7} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E')}]}{7}$$

No. 19 $\hat{\mathbb{Q}}_4^{(A_1')}[M_3, B_2]$

$$\hat{\mathbb{Z}}_{19} = \frac{2\sqrt{7}\mathbb{X}_{24}[\mathbb{Q}_3^{(a,A_2'')}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_1^{(b,A_2'')}]}{7} - \frac{\sqrt{42}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E')}]}{14} - \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E')}]}{14}$$

No. 20 $\hat{\mathbb{Q}}_3^{(A_1')}[M_3, B_2]$

$$\hat{\mathbb{Z}}_{20} = -\frac{\sqrt{2}\mathbb{X}_{32}[\mathbb{Q}_{3,0}^{(a,E'')}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_{2,0}^{(b,E'')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,1}^{(b,E'')}]}{2}$$

No. 21 $\hat{\mathbb{Q}}_2^{(A_1')}[M_3, B_2]$

$$\hat{\mathbb{Z}}_{21} = \frac{\sqrt{2}\mathbb{X}_{29}[\mathbb{G}_{2,0}^{(a,E')}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{30}[\mathbb{G}_{2,1}^{(a,E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E')}]}{2}$$

No. 22 $\hat{\mathbb{Q}}_3^{(A'_1)}$ [M$_3$, B$_2$]

$$\hat{\mathbb{Z}}_{22} = -\frac{\sqrt{2}\mathbb{X}_{34}[\mathbb{G}_{2,0}^{(a,E'')}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_{2,0}^{(b,E'')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{35}[\mathbb{G}_{2,1}^{(a,E'')}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,1}^{(b,E'')}]}{2}$$

No. 23 $\hat{\mathbb{Q}}_0^{(A'_1)}$ [M$_2$, B$_3$]

$$\hat{\mathbb{Z}}_{23} = \mathbb{X}_{14}[\mathbb{Q}_0^{(a,A'_1)}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_0^{(b,A'_1)}]$$

No. 24 $\hat{\mathbb{Q}}_2^{(A'_1)}$ [M$_2$, B$_3$]

$$\hat{\mathbb{Z}}_{24} = \mathbb{X}_{15}[\mathbb{Q}_2^{(a,A'_1)}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_0^{(b,A'_1)}]$$

No. 25 $\hat{\mathbb{Q}}_3^{(A'_1)}$ [M$_2$, B$_3$]

$$\hat{\mathbb{Z}}_{25} = -\frac{\sqrt{2}\mathbb{X}_{16}[\mathbb{Q}_{2,0}^{(a,E')}] \otimes \mathbb{Y}_{16}[\mathbb{Q}_{1,0}^{(b,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{17}[\mathbb{Q}_{2,1}^{(a,E')}] \otimes \mathbb{Y}_{17}[\mathbb{Q}_{1,1}^{(b,E')}]}{2}$$

No. 26 $\hat{\mathbb{Q}}_0^{(A'_1)}$ [M$_2$, B$_3$]

$$\hat{\mathbb{Z}}_{26} = \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{Q}_{2,0}^{(a,E'')}] \otimes \mathbb{Y}_{18}[\mathbb{Q}_{2,0}^{(b,E'')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{19}[\mathbb{Q}_{2,1}^{(a,E'')}] \otimes \mathbb{Y}_{19}[\mathbb{Q}_{2,1}^{(b,E'')}]}{2}$$

No. 27 $\hat{\mathbb{Q}}_2^{(A'_1)}$ [M$_2$, B$_3$]

$$\hat{\mathbb{Z}}_{27} = \frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{M}_{1,0}^{(a,E'')}] \otimes \mathbb{Y}_{20}[\mathbb{T}_{2,0}^{(b,E'')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{M}_{1,1}^{(a,E'')}] \otimes \mathbb{Y}_{21}[\mathbb{T}_{2,1}^{(b,E'')}]}{2}$$

No. 28 $\hat{\mathbb{Q}}_3^{(A'_1)}$ [M$_2$, B$_3$]

$$\hat{\mathbb{Z}}_{28} = \mathbb{X}_{20}[\mathbb{M}_1^{(a,A'_2)}] \otimes \mathbb{Y}_{22}[\mathbb{T}_3^{(b,A'_2)}]$$

Table 5: Atomic SAMB group.

group	bra	ket
M_1	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$
M_2	p_x, p_y, p_z	p_x, p_y, p_z
M_3	p_x, p_y, p_z	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$

Table 6: Atomic SAMB.

symbol	type	group	form
$\mathbb{X}_1$	$\mathbb{Q}_0^{(a,A_1')}$	M_1	$\begin{pmatrix} \frac{\sqrt{5}}{5} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{5}}{5} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{5}}{5} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{5}}{5} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{5}}{5} \end{pmatrix}$
$\mathbb{X}_2$	$\mathbb{Q}_2^{(a,A_1')}$	M_1	$\begin{pmatrix} \frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{7} \end{pmatrix}$
$\mathbb{X}_3$	$\mathbb{Q}_4^{(a,A_1')}$	M_1	$\begin{pmatrix} \frac{3\sqrt{70}}{35} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{70}}{70} & 0 & 0 & 0 \\ 0 & 0 & -\frac{2\sqrt{70}}{35} & 0 & 0 \\ 0 & 0 & 0 & -\frac{2\sqrt{70}}{35} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{70}}{70} \end{pmatrix}$
$\mathbb{X}_4$	$\mathbb{Q}_{2,0}^{(a,E')}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{7} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \\ \frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \end{pmatrix}$

Table 6

symbol	type	group	form
$\mathbb{X}_5$	$\mathbb{Q}_{2,1}^{(a,E')}$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ \frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_6$	$\mathbb{Q}_{4,0}^{(a,E',1)}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_7$	$\mathbb{Q}_{4,1}^{(a,E',1)}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{X}_8$	$\mathbb{Q}_{4,0}^{(a,E',2)}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0 \\ 0 & 0 & -\frac{\sqrt{14}}{7} & 0 & 0 \\ -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_9$	$\mathbb{Q}_{4,1}^{(a,E',2)}$	M_1	$\begin{pmatrix} 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{10}$	$\mathbb{M}_1^{(a,A_2')}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{10}i}{5} \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{5} & 0 & 0 & 0 \end{pmatrix}$

continued ...

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Table 6

symbol	type	group	form
$\mathbb{X}_{11}$	$\mathbb{M}_3^{(a,A_2')}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{10}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{5} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 \\ 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{12}$	$\mathbb{M}_{3,0}^{(a,E')}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{13}$	$\mathbb{M}_{3,1}^{(a,E')}$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{2}i}{2} & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{14}$	$\mathbb{Q}_0^{(a,A_1')}$	M_2	$\begin{pmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$
$\mathbb{X}_{15}$	$\mathbb{Q}_2^{(a,A_1')}$	M_2	$\begin{pmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{pmatrix}$
$\mathbb{X}_{16}$	$\mathbb{Q}_{2,0}^{(a,E')}$	M_2	$\begin{pmatrix} 0 & -\frac{\sqrt{2}}{2} & 0 \\ -\frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{17}$	$\mathbb{Q}_{2,1}^{(a,E')}$	M_2	$\begin{pmatrix} -\frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{18}$	$\mathbb{Q}_{2,0}^{(a,E'')}$	M_2	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \end{pmatrix}$

continued ...

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Table 6

symbol	type	group	form
$\mathbb{X}_{19}$	$\mathbb{Q}_{2,1}^{(a,E'')}$	M$_2$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
$\mathbb{X}_{20}$	$\mathbb{M}_{1}^{(a,A_2')}$	M$_2$	$\begin{pmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{21}$	$\mathbb{M}_{1,0}^{(a,E'')}$	M$_2$	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{22}$	$\mathbb{M}_{1,1}^{(a,E'')}$	M$_2$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & \frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$
$\mathbb{X}_{23}$	$\mathbb{Q}_{1}^{(a,A_2'')}$	M$_3$	$\begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{30}}{10} & 0 \\ 0 & 0 & \frac{\sqrt{30}}{10} & 0 & 0 \\ \frac{\sqrt{10}}{5} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{24}$	$\mathbb{Q}_{3}^{(a,A_2'')}$	M$_3$	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{5}}{5} & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{5} & 0 & 0 \\ \frac{\sqrt{15}}{5} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{25}$	$\mathbb{Q}_{1,0}^{(a,E')}$	M$_3$	$\begin{pmatrix} -\frac{\sqrt{10}}{10} & \frac{\sqrt{30}}{10} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{10} \\ 0 & 0 & 0 & \frac{\sqrt{30}}{10} & 0 \end{pmatrix}$
$\mathbb{X}_{26}$	$\mathbb{Q}_{1,1}^{(a,E')}$	M$_3$	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{10} \\ -\frac{\sqrt{10}}{10} & -\frac{\sqrt{30}}{10} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{30}}{10} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{27}$	$\mathbb{Q}_{3,0}^{(a,E')}$	M$_3$	$\begin{pmatrix} \frac{\sqrt{10}}{5} & -\frac{\sqrt{30}}{30} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{30}}{30} \\ 0 & 0 & 0 & \frac{2\sqrt{30}}{15} & 0 \end{pmatrix}$
$\mathbb{X}_{28}$	$\mathbb{Q}_{3,1}^{(a,E')}$	M$_3$	$\begin{pmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{30}}{30} \\ \frac{\sqrt{10}}{5} & \frac{\sqrt{30}}{30} & 0 & 0 & 0 \\ 0 & 0 & \frac{2\sqrt{30}}{15} & 0 & 0 \end{pmatrix}$

Table 6

symbol	type	group	form
$\mathbb{X}_{29}$	$\mathbb{G}_{2,0}^{(a,E')}$	M$_3$	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \end{pmatrix}$
$\mathbb{X}_{30}$	$\mathbb{G}_{2,1}^{(a,E')}$	M$_3$	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \\ \frac{\sqrt{2}}{2} & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{31}$	$\mathbb{Q}_{3}^{(a,A_1')}$	M$_3$	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{32}$	$\mathbb{Q}_{3,0}^{(a,E'')}$	M$_3$	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{3} \end{pmatrix}$
$\mathbb{X}_{33}$	$\mathbb{Q}_{3,1}^{(a,E'')}$	M$_3$	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{3} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{34}$	$\mathbb{G}_{2,0}^{(a,E'')}$	M$_3$	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{3} \end{pmatrix}$
$\mathbb{X}_{35}$	$\mathbb{G}_{2,1}^{(a,E'')}$	M$_3$	$\begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{3} & 0 & 0 & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
$\mathbb{Y}_1$	$\mathbb{Q}_0^{(s,A_1')}$	S$_1$	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_2$	$\mathbb{Q}_0^{(s,A_1')}$	S$_2$	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_3$	$\mathbb{Q}_0^{(b,A_1')}$	B$_1$	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \end{pmatrix}$

Table 7

symbol	type	cluster	form
$\mathbb{Y}_4$	$\mathbb{Q}_{1,0}^{(b,E')}$	B$_1$	$\left(-\frac{\sqrt{2}}{2} \quad \frac{\sqrt{2}}{2} \quad 0\right)$
$\mathbb{Y}_5$	$\mathbb{Q}_{1,1}^{(b,E')}$	B$_1$	$\left(-\frac{\sqrt{6}}{6} \quad -\frac{\sqrt{6}}{6} \quad \frac{\sqrt{6}}{3}\right)$
$\mathbb{Y}_6$	$\mathbb{T}_{1,0}^{(b,E')}$	B$_1$	$\left(\frac{\sqrt{6}i}{6} \quad -\frac{\sqrt{6}i}{6} \quad -\frac{\sqrt{6}i}{3}\right)$
$\mathbb{Y}_7$	$\mathbb{T}_{1,1}^{(b,E')}$	B$_1$	$\left(-\frac{\sqrt{2}i}{2} \quad -\frac{\sqrt{2}i}{2} \quad 0\right)$
$\mathbb{Y}_8$	$\mathbb{T}_{3}^{(b,A'_2)}$	B$_1$	$\left(\frac{\sqrt{3}i}{3} \quad -\frac{\sqrt{3}i}{3} \quad \frac{\sqrt{3}i}{3}\right)$
$\mathbb{Y}_9$	$\mathbb{Q}_{0}^{(b,A'_1)}$	B$_2$	$\left(\frac{\sqrt{6}}{6} \quad \frac{\sqrt{6}}{6} \quad \frac{\sqrt{6}}{6} \quad \frac{\sqrt{6}}{6} \quad \frac{\sqrt{6}}{6} \quad \frac{\sqrt{6}}{6}\right)$
$\mathbb{Y}_{10}$	$\mathbb{Q}_{1}^{(b,A''_2)}$	B$_2$	$\left(\frac{\sqrt{6}}{6} \quad -\frac{\sqrt{6}}{6} \quad -\frac{\sqrt{6}}{6} \quad -\frac{\sqrt{6}}{6} \quad \frac{\sqrt{6}}{6} \quad \frac{\sqrt{6}}{6}\right)$
$\mathbb{Y}_{11}$	$\mathbb{Q}_{1,0}^{(b,E')}$	B$_2$	$\left(-\frac{1}{2} \quad \frac{1}{2} \quad -\frac{1}{2} \quad 0 \quad \frac{1}{2} \quad 0\right)$
$\mathbb{Y}_{12}$	$\mathbb{Q}_{1,1}^{(b,E')}$	B$_2$	$\left(-\frac{\sqrt{3}}{6} \quad -\frac{\sqrt{3}}{6} \quad -\frac{\sqrt{3}}{6} \quad \frac{\sqrt{3}}{3} \quad -\frac{\sqrt{3}}{6} \quad \frac{\sqrt{3}}{3}\right)$
$\mathbb{Y}_{13}$	$\mathbb{Q}_{2,0}^{(b,E'')}$	B$_2$	$\left(-\frac{1}{2} \quad -\frac{1}{2} \quad \frac{1}{2} \quad 0 \quad \frac{1}{2} \quad 0\right)$
$\mathbb{Y}_{14}$	$\mathbb{Q}_{2,1}^{(b,E'')}$	B$_2$	$\left(-\frac{\sqrt{3}}{6} \quad \frac{\sqrt{3}}{6} \quad \frac{\sqrt{3}}{6} \quad -\frac{\sqrt{3}}{3} \quad -\frac{\sqrt{3}}{6} \quad \frac{\sqrt{3}}{3}\right)$
$\mathbb{Y}_{15}$	$\mathbb{Q}_{0}^{(b,A'_1)}$	B$_3$	$\left(\frac{\sqrt{6}}{6} \quad \frac{\sqrt{6}}{6} \quad \frac{\sqrt{6}}{6} \quad \frac{\sqrt{6}}{6} \quad \frac{\sqrt{6}}{6} \quad \frac{\sqrt{6}}{6}\right)$
$\mathbb{Y}_{16}$	$\mathbb{Q}_{1,0}^{(b,E')}$	B$_3$	$\left(0 \quad 0 \quad -\frac{1}{2} \quad \frac{1}{2} \quad \frac{1}{2} \quad -\frac{1}{2}\right)$
$\mathbb{Y}_{17}$	$\mathbb{Q}_{1,1}^{(b,E')}$	B$_3$	$\left(-\frac{\sqrt{3}}{3} \quad -\frac{\sqrt{3}}{3} \quad \frac{\sqrt{3}}{6} \quad \frac{\sqrt{3}}{6} \quad \frac{\sqrt{3}}{6} \quad \frac{\sqrt{3}}{6}\right)$
$\mathbb{Y}_{18}$	$\mathbb{Q}_{2,0}^{(b,E'')}$	B$_3$	$\left(0 \quad 0 \quad \frac{1}{2} \quad -\frac{1}{2} \quad \frac{1}{2} \quad -\frac{1}{2}\right)$
$\mathbb{Y}_{19}$	$\mathbb{Q}_{2,1}^{(b,E'')}$	B$_3$	$\left(-\frac{\sqrt{3}}{3} \quad \frac{\sqrt{3}}{3} \quad -\frac{\sqrt{3}}{6} \quad -\frac{\sqrt{3}}{6} \quad \frac{\sqrt{3}}{6} \quad \frac{\sqrt{3}}{6}\right)$
$\mathbb{Y}_{20}$	$\mathbb{T}_{2,0}^{(b,E'')}$	B$_3$	$\left(-\frac{\sqrt{3}i}{3} \quad \frac{\sqrt{3}i}{3} \quad \frac{\sqrt{3}i}{6} \quad -\frac{\sqrt{3}i}{6} \quad \frac{\sqrt{3}i}{6} \quad -\frac{\sqrt{3}i}{6}\right)$
$\mathbb{Y}_{21}$	$\mathbb{T}_{2,1}^{(b,E'')}$	B$_3$	$\left(0 \quad 0 \quad \frac{i}{2} \quad \frac{i}{2} \quad -\frac{i}{2} \quad -\frac{i}{2}\right)$
$\mathbb{Y}_{22}$	$\mathbb{T}_{3}^{(b,A'_2)}$	B$_3$	$\left(\frac{\sqrt{6}i}{6} \quad \frac{\sqrt{6}i}{6} \quad -\frac{\sqrt{6}i}{6} \quad \frac{\sqrt{6}i}{6} \quad \frac{\sqrt{6}i}{6} \quad -\frac{\sqrt{6}i}{6}\right)$

Table 8: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_1')}$	0	A_1'	–	–	1
2	$\mathbb{Q}_1^{(A_2'')}$	1	A_2''	–	–	z
3	$\mathbb{Q}_{1,0}^{(E')}$	1	E'	–	0	x
4	$\mathbb{Q}_{1,1}^{(E')}$	1	E'	–	1	y
5	$\mathbb{Q}_2^{(A_1')}$	2	A_1'	–	–	$-\frac{x^2}{2}-\frac{y^2}{2}+z^2$
6	$\mathbb{Q}_{2,0}^{(E'')}$	2	E''	–	0	$\sqrt{3}xz$
7	$\mathbb{Q}_{2,1}^{(E'')}$	2	E''	–	1	$\sqrt{3}yz$
8	$\mathbb{Q}_{2,0}^{(E')}$	2	E'	–	0	$-\sqrt{3}xy$
9	$\mathbb{Q}_{2,1}^{(E')}$	2	E'	–	1	$-\frac{\sqrt{3}(x-y)(x+y)}{2}$
10	$\mathbb{Q}_3^{(A_1')}$	3	A_1'	–	–	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$
11	$\mathbb{Q}_3^{(A_2'')}$	3	A_2''	–	–	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
12	$\mathbb{Q}_3^{(A_2')}$	3	A_2'	–	–	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$
13	$\mathbb{Q}_{3,0}^{(E'')}$	3	E''	–	0	$-\sqrt{15}xyz$
14	$\mathbb{Q}_{3,1}^{(E'')}$	3	E''	–	1	$-\frac{\sqrt{15}z(x-y)(x+y)}{2}$
15	$\mathbb{Q}_{3,0}^{(E')}$	3	E'	–	0	$-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$
16	$\mathbb{Q}_{3,1}^{(E')}$	3	E'	–	1	$-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$
17	$\mathbb{Q}_4^{(A_1')}$	4	A_1'	–	–	$\frac{3x^4}{8}+\frac{3x^2y^2}{4}-3x^2z^2+\frac{3y^4}{8}-3y^2z^2+z^4$
18	$\mathbb{Q}_{4,0}^{(E',1)}$	4	E'	1	0	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
19	$\mathbb{Q}_{4,1}^{(E',1)}$	4	E'	1	1	$-\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$
20	$\mathbb{Q}_{4,0}^{(E',2)}$	4	E'	2	0	$\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$
21	$\mathbb{Q}_{4,1}^{(E',2)}$	4	E'	2	1	$\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$

Table 9: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_1^{(A_2')}$	1	A_2'	–	–	Z

continued …

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Table 9

No.	symbol	rank	irrep.	mul.	comp.	form
2	$\mathbb{G}_{1,0}^{(E'')}$	1	E''	–	0	$-Y$
3	$\mathbb{G}_{1,1}^{(E'')}$	1	E''	–	1	X
4	$\mathbb{G}_{2,0}^{(E'')}$	2	E''	–	0	$\frac{\sqrt{3}(X-Y)(X+Y)}{2}$
5	$\mathbb{G}_{2,1}^{(E'')}$	2	E''	–	1	$-\sqrt{3}XY$
6	$\mathbb{G}_{2,0}^{(E')}$	2	E'	–	0	$-\sqrt{3}YZ$
7	$\mathbb{G}_{2,1}^{(E')}$	2	E'	–	1	$\sqrt{3}XZ$
8	$\mathbb{G}_{3}^{(A'_2)}$	3	A'_2	–	–	$-\frac{Z(3X^2+3Y^2-2Z^2)}{2}$
9	$\mathbb{G}_{3,0}^{(E')}$	3	E'	–	0	$\frac{\sqrt{15}Z(X-Y)(X+Y)}{2}$
10	$\mathbb{G}_{3,1}^{(E')}$	3	E'	–	1	$-\sqrt{15}XYZ$

- Group info.: Generator = $\{3^+_{001}|0\}$, $\{m_{001}|0\}$, $\{m_{110}|0\}$

Table 10: Conjugacy class (point-group part).

rep. SO	symmetry operations
$\{1|0\}$	$\{1|0\}$
$\{2_{120}|0\}$	$\{2_{120}|0\}$, $\{2_{210}|0\}$, $\{2_{1-10}|0\}$
$\{3^+_{001}|0\}$	$\{3^+_{001}|0\}$, $\{3^-_{001}|0\}$
$\{m_{100}|0\}$	$\{m_{100}|0\}$, $\{m_{010}|0\}$, $\{m_{110}|0\}$
$\{m_{001}|0\}$	$\{m_{001}|0\}$
$\{-6^+_{001}|0\}$	$\{-6^+_{001}|0\}$, $\{-6^-_{001}|0\}$

Table 11: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1\|0\}$	2	$\{2_{120}\|0\}$	3	$\{2_{210}\|0\}$	4	$\{2_{1-10}\|0\}$	5	$\{3^+_{001}\|0\}$
6	$\{3^-_{001}\|0\}$	7	$\{m_{100}\|0\}$	8	$\{m_{010}\|0\}$	9	$\{m_{110}\|0\}$	10	$\{m_{001}\|0\}$
11	$\{-6^+_{001}\|0\}$	12	$\{-6^-_{001}\|0\}$							

Table 12: Character table (point-group part).

	1	2_{120}	3^+_{001}	m_{100}	m_{001}	-6^+_{001}
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	0	2	-1
E''	2	0	-1	0	-2	1

Table 13: Parity conversion.

$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$
$A'_1\ (A''_1)$	$A'_2\ (A''_2)$	$A''_1\ (A'_1)$	$A''_2\ (A'_2)$	$E''\ (E')$
$E'\ (E'')$				

Table 14: Symmetric product, $[\Gamma \otimes \Gamma']_+$.

	A'_1	A'_2	A''_1	A''_2	E'	E''
A'_1	A'_1	A'_2	A''_1	A''_2	E'	E''
A'_2		A'_1	A''_2	A''_1	E'	E''
A''_1			A'_1	A'_2	E''	E'

continued ...

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Table 14

	A_1'	A_2'	A_1''	A_2''	E'	E''
A_2''				A_1'	E''	E'
E'					$A_1' + E'$	$A_1'' + A_2'' + E''$
E''						$A_1' + E'$

Table 15: Anti-symmetric product, $[\Gamma \otimes \Gamma]_-$.

A_1'	A_2'	A_1''	A_2''	E'	E''
$-$	$-$	$-$	$-$	A_2'	A_2'

Table 16: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix} -1 & -1 & 1 \end{pmatrix}$	2	$\begin{pmatrix} 0 & -1 & -1 \end{pmatrix}$	3	$\begin{pmatrix} -1 & 0 & -1 \end{pmatrix}$	4	$\begin{pmatrix} 1 & 1 & -1 \end{pmatrix}$
5	$\begin{pmatrix} 1 & 0 & 1 \end{pmatrix}$	6	$\begin{pmatrix} 0 & 1 & 1 \end{pmatrix}$	7	$\begin{pmatrix} 0 & -1 & 1 \end{pmatrix}$	8	$\begin{pmatrix} -1 & 0 & 1 \end{pmatrix}$
9	$\begin{pmatrix} 1 & 1 & 1 \end{pmatrix}$	10	$\begin{pmatrix} -1 & -1 & -1 \end{pmatrix}$	11	$\begin{pmatrix} 0 & 1 & -1 \end{pmatrix}$	12	$\begin{pmatrix} 1 & 0 & -1 \end{pmatrix}$

Table 17: Virtual-cluster basis.

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_0^{(A_1')}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$
	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$								

Table 17

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_1^{(A_2'')}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$
	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$								
$\mathbb{Q}_{1,0}^{(E')}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$								
$\mathbb{Q}_{1,1}^{(E')}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$
	$\frac{\sqrt{2}}{4}$	0								
$\mathbb{Q}_{2,0}^{(E')}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	0	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	0	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$
	$\frac{\sqrt{2}}{4}$	0								
$\mathbb{Q}_{2,1}^{(E')}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$								
$\mathbb{Q}_{2,0}^{(E'')}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$								
$\mathbb{Q}_{2,1}^{(E'')}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	0	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
	$-\frac{\sqrt{2}}{4}$	0								
$\mathbb{Q}_3^{(A_2')}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$
	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$								
$\mathbb{Q}_{3,0}^{(E'')}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	0	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
	$-\frac{\sqrt{2}}{4}$	0								
$\mathbb{Q}_{3,1}^{(E'')}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$								
$\mathbb{Q}_4^{(A_1'')}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$
	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$								