

SAMB for “MoS2”

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- 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:
 $\mathbf{a}_1 = (3.1661 \ 0 \ 0)$
 $\mathbf{a}_2 = (-1.58305 \ 2.74192303092191 \ 0)$
 $\mathbf{a}_3 = (0 \ 0 \ 20.0)$

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	#	$b@c$	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]

continued ...

Table 4

	bond	tail	head	n	#	$\mathbf{b@c}$	mapping
	b ₈	S ₁	Mo ₁	1	1	$\begin{pmatrix} -\frac{1}{3} & \frac{1}{3} & 0.12425 \end{pmatrix} @ \begin{pmatrix} \frac{5}{6} & \frac{1}{6} & 0.062125 \end{pmatrix}$	[5,7]
	b ₉	S ₁	Mo ₁	1	1	$\begin{pmatrix} -\frac{1}{3} & -\frac{2}{3} & 0.12425 \end{pmatrix} @ \begin{pmatrix} \frac{5}{6} & \frac{2}{3} & 0.062125 \end{pmatrix}$	[6,9]
B ₃ [6n: .m.]	b ₁₀	S ₁	S ₁	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & \frac{1}{3} & 0.12425 \end{pmatrix}$	[1,-7]
	b ₁₁	S ₂	S ₂	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & \frac{1}{3} & 0.87575 \end{pmatrix}$	[-2,10]
	b ₁₂	S ₂	S ₂	1	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & \frac{5}{6} & 0.87575 \end{pmatrix}$	[3,-11]
	b ₁₃	S ₂	S ₂	1	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{2}{3} & \frac{5}{6} & 0.87575 \end{pmatrix}$	[-4,12]
	b ₁₄	S ₁	S ₁	1	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{2}{3} & \frac{5}{6} & 0.12425 \end{pmatrix}$	[5,-9]
	b ₁₅	S ₁	S ₁	1	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & \frac{5}{6} & 0.12425 \end{pmatrix}$	[-6,8]

- SAMB:

$$\boxed{\text{No. 1}} \quad \hat{Q}_0^{(A'_1)} [M_1, S_1]$$

$$\hat{Z}_1 = \mathbb{X}_1[Q_0^{(a, A'_1)}] \otimes \mathbb{Y}_1[Q_0^{(s, A'_1)}]$$

$$\boxed{\text{No. 2}} \quad \hat{Q}_2^{(A'_1)} [M_1, S_1]$$

$$\hat{Z}_2 = \mathbb{X}_2[Q_2^{(a, A'_1)}] \otimes \mathbb{Y}_1[Q_0^{(s, A'_1)}]$$

$$\boxed{\text{No. 3}} \quad \hat{Q}_4^{(A'_1)} [M_1, S_1]$$

$$\hat{Z}_3 = \mathbb{X}_3[Q_4^{(a, A'_1)}] \otimes \mathbb{Y}_1[Q_0^{(s, A'_1)}]$$

$$\boxed{\text{No. 4}} \quad \hat{Q}_0^{(A'_1)} [M_2, S_2]$$

$$\hat{Z}_4 = \mathbb{X}_{14}[Q_0^{(a, A'_1)}] \otimes \mathbb{Y}_2[Q_0^{(s, A'_1)}]$$

$$\boxed{\text{No. 5}} \quad \hat{Q}_2^{(A'_1)} [M_2, S_2]$$

$$\hat{Z}_5 = \mathbb{X}_{15}[Q_2^{(a, A'_1)}] \otimes \mathbb{Y}_2[Q_0^{(s, A'_1)}]$$

$$\boxed{\text{No. 6}} \quad \hat{\mathbb{Q}}_0^{(A'_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

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

$$\boxed{\text{No. 7}} \quad \hat{\mathbb{Q}}_2^{(A'_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbb{Z}}_7 = \mathbb{X}_2[\mathbb{Q}_2^{(a,A'_1)}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A'_1)}]$$

$$\boxed{\text{No. 8}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

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

$$\boxed{\text{No. 9}} \quad \hat{\mathbb{Q}}_4^{(A'_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbb{Z}}_9 = \mathbb{X}_3[\mathbb{Q}_4^{(a,A'_1)}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A'_1)}]$$

$$\boxed{\text{No. 10}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

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

$$\boxed{\text{No. 11}} \quad \hat{\mathbb{G}}_4^{(A'_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

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

$$\boxed{\text{No. 12}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbb{Z}}_{12} = \mathbb{X}_{10}[\mathbb{M}_1^{(a,A'_2)}] \otimes \mathbb{Y}_8[\mathbb{T}_3^{(b,A'_2)}]$$

$$\boxed{\text{No. 13}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

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

$$\boxed{\text{No. 14}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\text{M}_1, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{14} = -\mathbb{X}_{11}[\text{M}_3^{(a, A'_2)}] \otimes \mathbb{Y}_8[\text{T}_3^{(b, A'_2)}]$$

$$\boxed{\text{No. 15}} \quad \hat{\mathbb{Q}}_0^{(A'_1)} [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{15} = \frac{\sqrt{3}\mathbb{X}_{23}[\mathbb{Q}_1^{(a, A'_2'')}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_1^{(b, A'_2')}] }{3} + \frac{\sqrt{3}\mathbb{X}_{25}[\mathbb{Q}_{1,0}^{(a, E')}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b, E')}] }{3} + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a, E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b, E')}] }{3}$$

$$\boxed{\text{No. 16}} \quad \hat{\mathbb{Q}}_2^{(A'_1)} [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{16} = \frac{\sqrt{6}\mathbb{X}_{23}[\mathbb{Q}_1^{(a, A'_2'')}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_1^{(b, A'_2')}] }{3} - \frac{\sqrt{6}\mathbb{X}_{25}[\mathbb{Q}_{1,0}^{(a, E')}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b, E')}] }{6} - \frac{\sqrt{6}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a, E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b, E')}] }{6}$$

$$\boxed{\text{No. 17}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{17} = \mathbb{X}_{31}[\mathbb{Q}_3^{(a, A'_1)}] \otimes \mathbb{Y}_9[\mathbb{Q}_0^{(b, A'_1)}]$$

$$\boxed{\text{No. 18}} \quad \hat{\mathbb{Q}}_2^{(A'_1)} [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{18} = \frac{\sqrt{21}\mathbb{X}_{24}[\mathbb{Q}_3^{(a, A'_2'')}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_1^{(b, A'_2')}] }{7} + \frac{\sqrt{14}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a, E')}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b, E')}] }{7} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a, E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b, E')}] }{7}$$

$$\boxed{\text{No. 19}} \quad \hat{\mathbb{Q}}_4^{(A'_1)} [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{19} = \frac{2\sqrt{7}\mathbb{X}_{24}[\mathbb{Q}_3^{(a, A'_2'')}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_1^{(b, A'_2')}] }{7} - \frac{\sqrt{42}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a, E')}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b, E')}] }{14} - \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a, E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b, E')}] }{14}$$

$$\boxed{\text{No. 20}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\text{M}_3, \text{B}_2]$$

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

$$\boxed{\text{No. 21}} \quad \hat{\mathbb{Q}}_2^{(A'_1)} [\text{M}_3, \text{B}_2]$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{7} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \\ \frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \end{pmatrix}$

continued ...

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}	$M_1^{(a,A'_2)}$	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 ...

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 ...

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	$\begin{pmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{30}}{30} \\ \frac{\sqrt{10}}{5} & \frac{\sqrt{30}}{30} & 0 & 0 & 0 \\ 0 & 0 & \frac{2\sqrt{30}}{15} & 0 & 0 \end{pmatrix}$

continued ...

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	(1)
\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	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \end{pmatrix}$

continued ...

Table 7

symbol	type	cluster	form
\mathbb{Y}_4	$\mathbb{Q}_{1,0}^{(b,E')}$	B_1	$\begin{pmatrix} -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
\mathbb{Y}_5	$\mathbb{Q}_{1,1}^{(b,E')}$	B_1	$\begin{pmatrix} -\frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{3} \end{pmatrix}$
\mathbb{Y}_6	$\mathbb{T}_{1,0}^{(b,E')}$	B_1	$\begin{pmatrix} \frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{3} \end{pmatrix}$
\mathbb{Y}_7	$\mathbb{T}_{1,1}^{(b,E')}$	B_1	$\begin{pmatrix} -\frac{\sqrt{2}i}{2} & -\frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$
\mathbb{Y}_8	$\mathbb{T}_3^{(b,A'_2)}$	B_1	$\begin{pmatrix} \frac{\sqrt{3}i}{3} & -\frac{\sqrt{3}i}{3} & \frac{\sqrt{3}i}{3} \end{pmatrix}$
\mathbb{Y}_9	$\mathbb{Q}_0^{(b,A'_1)}$	B_2	$\begin{pmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{Y}_{10}	$\mathbb{Q}_1^{(b,A'_2)}$	B_2	$\begin{pmatrix} \frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{Y}_{11}	$\mathbb{Q}_{1,0}^{(b,E')}$	B_2	$\begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & \frac{1}{2} & 0 \end{pmatrix}$
\mathbb{Y}_{12}	$\mathbb{Q}_{1,1}^{(b,E')}$	B_2	$\begin{pmatrix} -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{Y}_{13}	$\mathbb{Q}_{2,0}^{(b,E'')}$	B_2	$\begin{pmatrix} -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} & 0 \end{pmatrix}$
\mathbb{Y}_{14}	$\mathbb{Q}_{2,1}^{(b,E'')}$	B_2	$\begin{pmatrix} -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{Y}_{15}	$\mathbb{Q}_0^{(b,A'_1)}$	B_3	$\begin{pmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{Y}_{16}	$\mathbb{Q}_{1,0}^{(b,E')}$	B_3	$\begin{pmatrix} 0 & 0 & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$
\mathbb{Y}_{17}	$\mathbb{Q}_{1,1}^{(b,E')}$	B_3	$\begin{pmatrix} -\frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} \end{pmatrix}$
\mathbb{Y}_{18}	$\mathbb{Q}_{2,0}^{(b,E'')}$	B_3	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$
\mathbb{Y}_{19}	$\mathbb{Q}_{2,1}^{(b,E'')}$	B_3	$\begin{pmatrix} -\frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} \end{pmatrix}$
\mathbb{Y}_{20}	$\mathbb{T}_{2,0}^{(b,E'')}$	B_3	$\begin{pmatrix} -\frac{\sqrt{3}i}{3} & \frac{\sqrt{3}i}{3} & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} \end{pmatrix}$
\mathbb{Y}_{21}	$\mathbb{T}_{2,1}^{(b,E'')}$	B_3	$\begin{pmatrix} 0 & 0 & \frac{i}{2} & \frac{i}{2} & -\frac{i}{2} & -\frac{i}{2} \end{pmatrix}$
\mathbb{Y}_{22}	$\mathbb{T}_3^{(b,A'_2)}$	B_3	$\begin{pmatrix} \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{6} \end{pmatrix}$

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	—	—	$-\frac{z(3x^2+3y^2-2z^2)}{4}$
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 ...

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 ...

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
$\mathbb{Q}_0^{(A'_1)}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$
	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$								

continued ...

Table 17

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