

SAMB for “Mn3Sn”

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- Group: No. 194 D_{6h}^4 $P6_3/mmc$ [hexagonal]
 - Associated point group: No. 27 D_{6h} $6/mmm$ [hexagonal]
 - Generation condition
 - model type: **tight_binding**
 - time-reversal type: **electric**
 - irrep: **[A1g]**
 - **spinless**
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- Unit cell:
 $a = 1.0$, $b = 1.0$, $c = 1.0$, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 120.0$
- Lattice vectors:
 $\mathbf{a}_1 = (1.0 \ 0 \ 0)$
 $\mathbf{a}_2 = (-0.5 \ 0.86602540378444 \ 0)$
 $\mathbf{a}_3 = (0 \ 0 \ 1.0)$

Table 1: High-symmetry line: Γ -X.

symbol	position	symbol	position
Γ	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	X	$\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$

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- Kets: dimension = 40

Table 2: Hilbert space for full matrix.

No.	ket	No.	ket	No.	ket	No.	ket	No.	ket
1	$d_u @ Mn_1$	2	$d_v @ Mn_1$	3	$d_{yz} @ Mn_1$	4	$d_{zx} @ Mn_1$	5	$d_{xy} @ Mn_1$
6	$d_u @ Mn_2$	7	$d_v @ Mn_2$	8	$d_{yz} @ Mn_2$	9	$d_{zx} @ Mn_2$	10	$d_{xy} @ Mn_2$
11	$d_u @ Mn_3$	12	$d_v @ Mn_3$	13	$d_{yz} @ Mn_3$	14	$d_{zx} @ Mn_3$	15	$d_{xy} @ Mn_3$
16	$d_u @ Mn_4$	17	$d_v @ Mn_4$	18	$d_{yz} @ Mn_4$	19	$d_{zx} @ Mn_4$	20	$d_{xy} @ Mn_4$
21	$d_u @ Mn_5$	22	$d_v @ Mn_5$	23	$d_{yz} @ Mn_5$	24	$d_{zx} @ Mn_5$	25	$d_{xy} @ Mn_5$
26	$d_u @ Mn_6$	27	$d_v @ Mn_6$	28	$d_{yz} @ Mn_6$	29	$d_{zx} @ Mn_6$	30	$d_{xy} @ Mn_6$
31	$d_u @ Sn_1$	32	$d_v @ Sn_1$	33	$d_{yz} @ Sn_1$	34	$d_{zx} @ Sn_1$	35	$d_{xy} @ Sn_1$
36	$d_u @ Sn_2$	37	$d_v @ Sn_2$	38	$d_{yz} @ Sn_2$	39	$d_{zx} @ Sn_2$	40	$d_{xy} @ Sn_2$

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S ₁ [6h: mm2]	Mn ₁	$\begin{pmatrix} 0.8388 & 0.6776 & \frac{1}{4} \end{pmatrix}$	[1,6,14,17]
	Mn ₂	$\begin{pmatrix} 0.1612 & 0.3224 & \frac{3}{4} \end{pmatrix}$	[2,3,13,18]
	Mn ₃	$\begin{pmatrix} 0.1612 & 0.8388 & \frac{3}{4} \end{pmatrix}$	[4,11,19,22]
	Mn ₄	$\begin{pmatrix} 0.6776 & 0.8388 & \frac{3}{4} \end{pmatrix}$	[5,12,20,21]
	Mn ₅	$\begin{pmatrix} 0.8388 & 0.1612 & \frac{1}{4} \end{pmatrix}$	[7,10,15,23]
	Mn ₆	$\begin{pmatrix} 0.3224 & 0.1612 & \frac{1}{4} \end{pmatrix}$	[8,9,16,24]
S ₂ [2c: -6m2]	Sn ₁	$\begin{pmatrix} \frac{1}{3} & \frac{2}{3} & \frac{1}{4} \end{pmatrix}$	[1,6,7,8,9,10,14,15,16,17,23,24]
	Sn ₂	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & \frac{3}{4} \end{pmatrix}$	[2,3,4,5,11,12,13,18,19,20,21,22]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	$\mathbf{b@c}$	mapping
B ₁ [6h: mm2]	b ₁	Mn ₅	Mn ₁	1	1	$\begin{pmatrix} 0 & 0.4836 & 0 \end{pmatrix} @ \begin{pmatrix} 0.8388 & 0.9194 & \frac{1}{4} \end{pmatrix}$	[1,-7,-15,17]
	b ₂	Mn ₃	Mn ₂	1	1	$\begin{pmatrix} 0 & -0.4836 & 0 \end{pmatrix} @ \begin{pmatrix} 0.1612 & 0.0806 & \frac{3}{4} \end{pmatrix}$	[2,-4,13,-19]
	b ₃	Mn ₄	Mn ₂	1	1	$\begin{pmatrix} -0.4836 & -0.4836 & 0 \end{pmatrix} @ \begin{pmatrix} 0.9194 & 0.0806 & \frac{3}{4} \end{pmatrix}$	[3,-12,18,-21]
	b ₄	Mn ₄	Mn ₃	1	1	$\begin{pmatrix} -0.4836 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} 0.9194 & 0.8388 & \frac{3}{4} \end{pmatrix}$	[-5,11,-20,22]
	b ₅	Mn ₆	Mn ₁	1	1	$\begin{pmatrix} 0.4836 & 0.4836 & 0 \end{pmatrix} @ \begin{pmatrix} 0.0806 & 0.9194 & \frac{1}{4} \end{pmatrix}$	[6,-9,14,-24]
	b ₆	Mn ₆	Mn ₅	1	1	$\begin{pmatrix} 0.4836 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} 0.0806 & 0.1612 & \frac{1}{4} \end{pmatrix}$	[-8,10,-16,23]
B ₂ [6g: .2/m.]	b ₇	Sn ₂	Sn ₁	1	1	$\begin{pmatrix} \frac{1}{3} & \frac{2}{3} & -\frac{1}{2} \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[1,-3,-13,14]
	b ₈	Sn ₂	Sn ₁	1	1	$\begin{pmatrix} \frac{1}{3} & \frac{2}{3} & \frac{1}{2} \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$	[-2,6,17,-18]
	b ₉	Sn ₂	Sn ₁	1	1	$\begin{pmatrix} \frac{1}{3} & -\frac{1}{3} & -\frac{1}{2} \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[-4,10,15,-22]
	b ₁₀	Sn ₂	Sn ₁	1	1	$\begin{pmatrix} -\frac{2}{3} & -\frac{1}{3} & -\frac{1}{2} \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[-5,9,16,-21]
	b ₁₁	Sn ₂	Sn ₁	1	1	$\begin{pmatrix} \frac{1}{3} & -\frac{1}{3} & \frac{1}{2} \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$	[7,-11,-19,23]
	b ₁₂	Sn ₂	Sn ₁	1	1	$\begin{pmatrix} -\frac{2}{3} & -\frac{1}{3} & \frac{1}{2} \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$	[8,-12,-20,24]
B ₃ [12j: m..]	b ₁₃	Sn ₁	Mn ₁	1	1	$\begin{pmatrix} 0.4945333333333333 & -0.0109333333333333 & 0 \end{pmatrix} @ \begin{pmatrix} 0.0860666666666667 & 0.6721333333333333 & \frac{1}{4} \end{pmatrix}$	[1,17]
	b ₁₄	Sn ₂	Mn ₂	1	1	$\begin{pmatrix} -0.4945333333333333 & 0.0109333333333333 & 0 \end{pmatrix} @ \begin{pmatrix} 0.9139333333333333 & 0.3278666666666667 & \frac{3}{4} \end{pmatrix}$	[2,13]
	b ₁₅	Sn ₂	Mn ₂	1	1	$\begin{pmatrix} 0.5054666666666667 & 0.0109333333333333 & 0 \end{pmatrix} @ \begin{pmatrix} 0.4139333333333333 & 0.3278666666666667 & \frac{3}{4} \end{pmatrix}$	[3,18]
	b ₁₆	Sn ₂	Mn ₃	1	1	$\begin{pmatrix} -0.4945333333333333 & -0.5054666666666667 & 0 \end{pmatrix} @ \begin{pmatrix} 0.9139333333333333 & 0.5860666666666667 & \frac{3}{4} \end{pmatrix}$	[4,19]
	b ₁₇	Sn ₂	Mn ₄	1	1	$\begin{pmatrix} -0.0109333333333333 & 0.4945333333333333 & 0 \end{pmatrix} @ \begin{pmatrix} 0.6721333333333333 & 0.0860666666666667 & \frac{3}{4} \end{pmatrix}$	[5,20]
	b ₁₈	Sn ₁	Mn ₁	1	1	$\begin{pmatrix} -0.5054666666666667 & -0.0109333333333333 & 0 \end{pmatrix} @ \begin{pmatrix} 0.5860666666666667 & 0.6721333333333333 & \frac{1}{4} \end{pmatrix}$	[6,14]
	b ₁₉	Sn ₁	Mn ₅	1	1	$\begin{pmatrix} 0.4945333333333333 & 0.5054666666666667 & 0 \end{pmatrix} @ \begin{pmatrix} 0.0860666666666667 & 0.4139333333333333 & \frac{1}{4} \end{pmatrix}$	[7,15]
	b ₂₀	Sn ₁	Mn ₆	1	1	$\begin{pmatrix} 0.0109333333333333 & -0.4945333333333333 & 0 \end{pmatrix} @ \begin{pmatrix} 0.3278666666666667 & 0.9139333333333333 & \frac{1}{4} \end{pmatrix}$	[8,16]
	b ₂₁	Sn ₁	Mn ₆	1	1	$\begin{pmatrix} 0.0109333333333333 & 0.5054666666666667 & 0 \end{pmatrix} @ \begin{pmatrix} 0.3278666666666667 & 0.4139333333333333 & \frac{1}{4} \end{pmatrix}$	[9,24]
	b ₂₂	Sn ₁	Mn ₅	1	1	$\begin{pmatrix} -0.5054666666666667 & -0.4945333333333333 & 0 \end{pmatrix} @ \begin{pmatrix} 0.5860666666666667 & 0.9139333333333333 & \frac{1}{4} \end{pmatrix}$	[10,23]
	b ₂₃	Sn ₂	Mn ₃	1	1	$\begin{pmatrix} 0.5054666666666667 & 0.4945333333333333 & 0 \end{pmatrix} @ \begin{pmatrix} 0.4139333333333333 & 0.0860666666666667 & \frac{3}{4} \end{pmatrix}$	[11,22]
	b ₂₄	Sn ₂	Mn ₄	1	1	$\begin{pmatrix} -0.0109333333333333 & -0.5054666666666667 & 0 \end{pmatrix} @ \begin{pmatrix} 0.6721333333333333 & 0.5860666666666667 & \frac{3}{4} \end{pmatrix}$	[12,21]

- SAM:

$$\boxed{\text{No. 1}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{S}_1]$$

$$\hat{\mathbb{Z}}_1 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_{1g})}]$$

$$\boxed{\text{No. 2}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\text{M}_1, \text{S}_1]$$

$$\hat{\mathbb{Z}}_2 = \mathbb{X}_2[\mathbb{Q}_2^{(a, A_{1g})}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_{1g})}]$$

$$\boxed{\text{No. 3}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{S}_1]$$

$$\hat{\mathbb{Z}}_3 = \frac{\sqrt{2}\mathbb{X}_8[\mathbb{Q}_{2,0}^{(a, E_{2g})}] \otimes \mathbb{Y}_2[\mathbb{Q}_{2,0}^{(s, E_{2g})}]}{2} + \frac{\sqrt{2}\mathbb{X}_9[\mathbb{Q}_{2,1}^{(a, E_{2g})}] \otimes \mathbb{Y}_3[\mathbb{Q}_{2,1}^{(s, E_{2g})}]}{2}$$

$$\boxed{\text{No. 4}} \quad \hat{\mathbb{Q}}_4^{(A_{1g})} [\text{M}_1, \text{S}_1]$$

$$\hat{\mathbb{Z}}_4 = \mathbb{X}_3[\mathbb{Q}_4^{(a, A_{1g})}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_{1g})}]$$

$$\boxed{\text{No. 5}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\text{M}_1, \text{S}_1]$$

$$\hat{\mathbb{Z}}_5 = \frac{\sqrt{2}\mathbb{X}_{12}[\mathbb{Q}_{4,0}^{(a, E_{2g}, 2)}] \otimes \mathbb{Y}_2[\mathbb{Q}_{2,0}^{(s, E_{2g})}]}{2} + \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{Q}_{4,1}^{(a, E_{2g}, 2)}] \otimes \mathbb{Y}_3[\mathbb{Q}_{2,1}^{(s, E_{2g})}]}{2}$$

$$\boxed{\text{No. 6}} \quad \hat{\mathbb{Q}}_6^{(A_{1g}, 2)} [\text{M}_1, \text{S}_1]$$

$$\hat{\mathbb{Z}}_6 = \frac{\sqrt{2}\mathbb{X}_{10}[\mathbb{Q}_{4,0}^{(a, E_{2g}, 1)}] \otimes \mathbb{Y}_2[\mathbb{Q}_{2,0}^{(s, E_{2g})}]}{2} + \frac{\sqrt{2}\mathbb{X}_{11}[\mathbb{Q}_{4,1}^{(a, E_{2g}, 1)}] \otimes \mathbb{Y}_3[\mathbb{Q}_{2,1}^{(s, E_{2g})}]}{2}$$

$$\boxed{\text{No. 7}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{S}_2]$$

$$\hat{\mathbb{Z}}_7 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(s, A_{1g})}]$$

$$\boxed{\text{No. 8}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\text{M}_1, \text{S}_2]$$

$$\hat{\mathbb{Z}}_8 = \mathbb{X}_2[\mathbb{Q}_2^{(a, A_{1g})}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(s, A_{1g})}]$$

$$\boxed{\text{No. 9}} \quad \hat{\mathbb{Q}}_4^{(A_{1g})} [\text{M}_1, \text{S}_2]$$

$$\hat{\mathbb{Z}}_9 = \mathbb{X}_3[\mathbb{Q}_4^{(a, A_{1g})}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(s, A_{1g})}]$$

$$\boxed{\text{No. 10}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{10} = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 11}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\text{M}_1, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{11} = \mathbb{X}_2[\mathbb{Q}_2^{(a, A_{1g})}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 12}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{12} = \frac{\sqrt{2}\mathbb{X}_8[\mathbb{Q}_{2,0}^{(a, E_{2g})}] \otimes \mathbb{Y}_6[\mathbb{Q}_{2,0}^{(b, E_{2g})}]}{2} + \frac{\sqrt{2}\mathbb{X}_9[\mathbb{Q}_{2,1}^{(a, E_{2g})}] \otimes \mathbb{Y}_7[\mathbb{Q}_{2,1}^{(b, E_{2g})}]}{2}$$

$$\boxed{\text{No. 13}} \quad \hat{\mathbb{Q}}_4^{(A_{1g})} [\text{M}_1, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{13} = \mathbb{X}_3[\mathbb{Q}_4^{(a, A_{1g})}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b, A_{1g})}]$$

$$\boxed{\text{No. 14}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\text{M}_1, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{14} = \frac{\sqrt{2}\mathbb{X}_{12}[\mathbb{Q}_{4,0}^{(a, E_{2g}, 2)}] \otimes \mathbb{Y}_6[\mathbb{Q}_{2,0}^{(b, E_{2g})}]}{2} + \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{Q}_{4,1}^{(a, E_{2g}, 2)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{2,1}^{(b, E_{2g})}]}{2}$$

$$\boxed{\text{No. 15}} \quad \hat{\mathbb{Q}}_6^{(A_{1g}, 2)} [\text{M}_1, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{15} = \frac{\sqrt{2}\mathbb{X}_{10}[\mathbb{Q}_{4,0}^{(a, E_{2g}, 1)}] \otimes \mathbb{Y}_6[\mathbb{Q}_{2,0}^{(b, E_{2g})}]}{2} + \frac{\sqrt{2}\mathbb{X}_{11}[\mathbb{Q}_{4,1}^{(a, E_{2g}, 1)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{2,1}^{(b, E_{2g})}]}{2}$$

$$\boxed{\text{No. 16}} \quad \hat{\mathbb{Q}}_6^{(A_{1g}, 2)} [\text{M}_1, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{16} = -\mathbb{X}_{15}[\text{M}_1^{(a, A_{2g})}] \otimes \mathbb{Y}_{10}[\mathbb{T}_6^{(b, A_{2g})}]$$

$$\boxed{\text{No. 17}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\text{M}_1, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{17} = -\frac{\sqrt{2}\mathbb{X}_{17}[\mathbb{M}_{3,0}^{(a,E_{2g})}] \otimes \mathbb{Y}_8[\mathbb{T}_{2,0}^{(b,E_{2g})}]}{2} - \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{M}_{3,1}^{(a,E_{2g})}] \otimes \mathbb{Y}_9[\mathbb{T}_{2,1}^{(b,E_{2g})}]}{2}$$

$$\boxed{\text{No. 18}} \quad \hat{\mathbb{Q}}_6^{(A_{1g},2)} [\text{M}_1, \text{B}_1]$$

$$\hat{\mathbb{Z}}_{18} = \mathbb{X}_{16}[\mathbb{M}_3^{(a,A_{2g})}] \otimes \mathbb{Y}_{10}[\mathbb{T}_6^{(b,A_{2g})}]$$

$$\boxed{\text{No. 19}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{19} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\boxed{\text{No. 20}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\text{M}_1, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{20} = \mathbb{X}_2[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\boxed{\text{No. 21}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{21} = \frac{\mathbb{X}_4[\mathbb{Q}_{2,0}^{(a,E_{1g})}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{2,0}^{(b,E_{1g})}]}{2} + \frac{\mathbb{X}_5[\mathbb{Q}_{2,1}^{(a,E_{1g})}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_{2,1}^{(b,E_{1g})}]}{2} + \frac{\mathbb{X}_8[\mathbb{Q}_{2,0}^{(a,E_{2g})}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b,E_{2g})}]}{2} + \frac{\mathbb{X}_9[\mathbb{Q}_{2,1}^{(a,E_{2g})}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{2g})}]}{2}$$

$$\boxed{\text{No. 22}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\text{M}_1, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{22} = \frac{\mathbb{X}_4[\mathbb{Q}_{2,0}^{(a,E_{1g})}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{2,0}^{(b,E_{1g})}]}{2} + \frac{\mathbb{X}_5[\mathbb{Q}_{2,1}^{(a,E_{1g})}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_{2,1}^{(b,E_{1g})}]}{2} - \frac{\mathbb{X}_8[\mathbb{Q}_{2,0}^{(a,E_{2g})}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b,E_{2g})}]}{2} - \frac{\mathbb{X}_9[\mathbb{Q}_{2,1}^{(a,E_{2g})}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{2g})}]}{2}$$

$$\boxed{\text{No. 23}} \quad \hat{\mathbb{Q}}_4^{(A_{1g})} [\text{M}_1, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{23} = \mathbb{X}_3[\mathbb{Q}_4^{(a,A_{1g})}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\boxed{\text{No. 24}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\text{M}_1, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{24} = \frac{\sqrt{6}\mathbb{X}_{12}[\mathbb{Q}_{4,0}^{(a,E_{2g},2)}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b,E_{2g})}]}{6} + \frac{\sqrt{6}\mathbb{X}_{13}[\mathbb{Q}_{4,1}^{(a,E_{2g},2)}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{2g})}]}{6} + \frac{\sqrt{3}\mathbb{X}_6[\mathbb{Q}_{4,0}^{(a,E_{1g})}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{2,0}^{(b,E_{1g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_7[\mathbb{Q}_{4,1}^{(a,E_{1g})}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_{2,1}^{(b,E_{1g})}]}{3}$$

$$\boxed{\text{No. 25}} \quad \hat{\mathbb{Q}}_4^{(A_{1g})} [\text{M}_1, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{25} = -\frac{\sqrt{3}\mathbb{X}_{12}[\mathbb{Q}_{4,0}^{(a,E_{2g},2)}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b,E_{2g})}]}{3} - \frac{\sqrt{3}\mathbb{X}_{13}[\mathbb{Q}_{4,1}^{(a,E_{2g},2)}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{2g})}]}{3} + \frac{\sqrt{6}\mathbb{X}_6[\mathbb{Q}_{4,0}^{(a,E_{1g})}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{2,0}^{(b,E_{1g})}]}{6} + \frac{\sqrt{6}\mathbb{X}_7[\mathbb{Q}_{4,1}^{(a,E_{1g})}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_{2,1}^{(b,E_{1g})}]}{6}$$

$$\boxed{\text{No. 26}} \quad \hat{\mathbb{Q}}_6^{(A_{1g},2)} [\text{M}_1, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{26} = \frac{\sqrt{2}\mathbb{X}_{10}[\mathbb{Q}_{4,0}^{(a,E_{2g},1)}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b,E_{2g})}]}{2} + \frac{\sqrt{2}\mathbb{X}_{11}[\mathbb{Q}_{4,1}^{(a,E_{2g},1)}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{2g})}]}{2}$$

$$\boxed{\text{No. 27}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{27} = \mathbb{X}_{14}[\mathbb{Q}_4^{(a,B_{2g})}] \otimes \mathbb{Y}_{16}[\mathbb{Q}_4^{(b,B_{2g})}]$$

$$\boxed{\text{No. 28}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{28} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_{17}[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\boxed{\text{No. 29}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\text{M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{29} = \mathbb{X}_2[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{Y}_{17}[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\boxed{\text{No. 30}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{30} = \frac{\sqrt{2}\mathbb{X}_8[\mathbb{Q}_{2,0}^{(a,E_{2g})}] \otimes \mathbb{Y}_{18}[\mathbb{Q}_{2,0}^{(b,E_{2g})}]}{2} + \frac{\sqrt{2}\mathbb{X}_9[\mathbb{Q}_{2,1}^{(a,E_{2g})}] \otimes \mathbb{Y}_{19}[\mathbb{Q}_{2,1}^{(b,E_{2g})}]}{2}$$

$$\boxed{\text{No. 31}} \quad \hat{\mathbb{Q}}_6^{(A_{1g},2)} [\text{M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{31} = \frac{\sqrt{2}\mathbb{X}_8[\mathbb{Q}_{2,0}^{(a,E_{2g})}] \otimes \mathbb{Y}_{20}[\mathbb{Q}_{4,0}^{(b,E_{2g},1)}]}{2} + \frac{\sqrt{2}\mathbb{X}_9[\mathbb{Q}_{2,1}^{(a,E_{2g})}] \otimes \mathbb{Y}_{21}[\mathbb{Q}_{4,1}^{(b,E_{2g},1)}]}{2}$$

$$\boxed{\text{No. 32}} \quad \hat{\mathbb{Q}}_4^{(A_{1g})} [\text{M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{32} = \mathbb{X}_3[\mathbb{Q}_4^{(a,A_{1g})}] \otimes \mathbb{Y}_{17}[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\boxed{\text{No. 33}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\text{M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{33} = \frac{\sqrt{2}\mathbb{X}_{12}[\mathbb{Q}_{4,0}^{(a,E_{2g},2)}] \otimes \mathbb{Y}_{18}[\mathbb{Q}_{2,0}^{(b,E_{2g})}]}{2} + \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{Q}_{4,1}^{(a,E_{2g},2)}] \otimes \mathbb{Y}_{19}[\mathbb{Q}_{2,1}^{(b,E_{2g})}]}{2}$$

$$\boxed{\text{No. 34}} \quad \hat{\mathbb{Q}}_6^{(A_{1g},2)} [\text{M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{34} = \frac{\sqrt{2}\mathbb{X}_{10}[\mathbb{Q}_{4,0}^{(a,E_{2g},1)}] \otimes \mathbb{Y}_{18}[\mathbb{Q}_{2,0}^{(b,E_{2g})}]}{2} + \frac{\sqrt{2}\mathbb{X}_{11}[\mathbb{Q}_{4,1}^{(a,E_{2g},1)}] \otimes \mathbb{Y}_{19}[\mathbb{Q}_{2,1}^{(b,E_{2g})}]}{2}$$

$$\boxed{\text{No. 35}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{35} = \frac{\sqrt{2}\mathbb{X}_{10}[\mathbb{Q}_{4,0}^{(a,E_{2g},1)}] \otimes \mathbb{Y}_{20}[\mathbb{Q}_{4,0}^{(b,E_{2g},1)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{11}[\mathbb{Q}_{4,1}^{(a,E_{2g},1)}] \otimes \mathbb{Y}_{21}[\mathbb{Q}_{4,1}^{(b,E_{2g},1)}]}{2}$$

$$\boxed{\text{No. 36}} \quad \hat{\mathbb{Q}}_6^{(A_{1g},2)} [\text{M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{36} = -\frac{\sqrt{2}\mathbb{X}_{12}[\mathbb{Q}_{4,0}^{(a,E_{2g},2)}] \otimes \mathbb{Y}_{20}[\mathbb{Q}_{4,0}^{(b,E_{2g},1)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{Q}_{4,1}^{(a,E_{2g},2)}] \otimes \mathbb{Y}_{21}[\mathbb{Q}_{4,1}^{(b,E_{2g},1)}]}{2}$$

$$\boxed{\text{No. 37}} \quad \hat{\mathbb{Q}}_6^{(A_{1g},2)} [\text{M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{37} = -\mathbb{X}_{15}[\text{M}_1^{(a,A_{2g})}] \otimes \mathbb{Y}_{26}[\mathbb{T}_6^{(b,A_{2g})}]$$

$$\boxed{\text{No. 38}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [\text{M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{38} = -\frac{\sqrt{2}\mathbb{X}_{17}[\mathbb{M}_{3,0}^{(a,E_{2g})}] \otimes \mathbb{Y}_{22}[\mathbb{T}_{2,0}^{(b,E_{2g})}]}{2} - \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{M}_{3,1}^{(a,E_{2g})}] \otimes \mathbb{Y}_{23}[\mathbb{T}_{2,1}^{(b,E_{2g})}]}{2}$$

$$\boxed{\text{No. 39}} \quad \hat{\mathbb{Q}}_6^{(A_{1g},2)} [\text{M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{39} = -\frac{\sqrt{2}\mathbb{X}_{17}[\mathbb{M}_{3,0}^{(a,E_{2g})}] \otimes \mathbb{Y}_{24}[\mathbb{T}_{4,0}^{(b,E_{2g},1)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{M}_{3,1}^{(a,E_{2g})}] \otimes \mathbb{Y}_{25}[\mathbb{T}_{4,1}^{(b,E_{2g},1)}]}{2}$$

$$\boxed{\text{No. 40}} \quad \hat{\mathbb{Q}}_6^{(A_{1g},2)} [\text{M}_1, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{40} = \mathbb{X}_{16}[\text{M}_3^{(a,A_{2g})}] \otimes \mathbb{Y}_{26}[\mathbb{T}_6^{(b,A_{2g})}]$$

Table 5: Atomic SAMB group.

group	bra	ket
M ₁	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$

Table 6: Atomic SAMB.

symbol	type	group	form
\mathbb{X}_1	$\mathbb{Q}_0^{(a, A_{1g})}$	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	$\mathbb{Q}_2^{(a, A_{1g})}$	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	$\mathbb{Q}_4^{(a, A_{1g})}$	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	$\mathbb{Q}_{2,0}^{(a, E_{1g})}$	M ₁	$\begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \\ \frac{\sqrt{14}}{14} & \frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
\mathbb{X}_5	$\mathbb{Q}_{2,1}^{(a,E_{1g})}$	M_1	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \\ \frac{\sqrt{14}}{14} & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 \end{pmatrix}$
\mathbb{X}_6	$\mathbb{Q}_{4,0}^{(a,E_{1g})}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{21}}{7} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{7}}{14} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{7}}{14} \\ \frac{\sqrt{21}}{7} & -\frac{\sqrt{7}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{7}}{14} & 0 & 0 \end{pmatrix}$
\mathbb{X}_7	$\mathbb{Q}_{4,1}^{(a,E_{1g})}$	M_1	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{21}}{7} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{7}}{14} & 0 & 0 \\ \frac{\sqrt{21}}{7} & \frac{\sqrt{7}}{14} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{7}}{14} \\ 0 & 0 & 0 & -\frac{\sqrt{7}}{14} & 0 \end{pmatrix}$
\mathbb{X}_8	$\mathbb{Q}_{2,0}^{(a,E_{2g})}$	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}_9	$\mathbb{Q}_{2,1}^{(a,E_{2g})}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{7} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \\ \frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{10}	$\mathbb{Q}_{4,0}^{(a,E_{2g},1)}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{2} \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
\mathbb{X}_{11}	$\mathbb{Q}_{4,1}^{(a,E_{2g},1)}$	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}_{12}	$\mathbb{Q}_{4,0}^{(a,E_{2g},2)}$	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}_{13}	$\mathbb{Q}_{4,1}^{(a,E_{2g},2)}$	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}_{14}	$\mathbb{Q}_4^{(a,B_{2g})}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & \frac{1}{2} & 0 \end{pmatrix}$
\mathbb{X}_{15}	$\mathbb{M}_1^{(a,A_{2g})}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{10}i}{5} \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{5} & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{16}	$\mathbb{M}_3^{(a,A_{2g})}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{10}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{5} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 \\ 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
\mathbb{X}_{17}	$\mathbb{M}_{3,0}^{(a,E_{2g})}$	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}_{18}	$\mathbb{M}_{3,1}^{(a,E_{2g})}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
\mathbb{Y}_1	$\mathbb{Q}_0^{(s,A_{1g})}$	S_1	$\begin{pmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{Y}_2	$\mathbb{Q}_{2,0}^{(s,E_{2g})}$	S_1	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} \end{pmatrix}$
\mathbb{Y}_3	$\mathbb{Q}_{2,1}^{(s,E_{2g})}$	S_1	$\begin{pmatrix} 0 & 0 & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$
\mathbb{Y}_4	$\mathbb{Q}_0^{(s,A_{1g})}$	S_2	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{Y}_5	$\mathbb{Q}_0^{(b,A_{1g})}$	B_1	$\begin{pmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{Y}_6	$\mathbb{Q}_{2,0}^{(b,E_{2g})}$	B_1	$\begin{pmatrix} \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{Y}_7	$\mathbb{Q}_{2,1}^{(b,E_{2g})}$	B_1	$\begin{pmatrix} -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} & 0 \end{pmatrix}$
\mathbb{Y}_8	$\mathbb{T}_{2,0}^{(b,E_{2g})}$	B_1	$\begin{pmatrix} \frac{i}{2} & \frac{i}{2} & \frac{i}{2} & 0 & \frac{i}{2} & 0 \end{pmatrix}$
\mathbb{Y}_9	$\mathbb{T}_{2,1}^{(b,E_{2g})}$	B_1	$\begin{pmatrix} \frac{\sqrt{3}i}{6} & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{3} & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{3} \end{pmatrix}$
\mathbb{Y}_{10}	$\mathbb{T}_6^{(b,A_{2g})}$	B_1	$\begin{pmatrix} \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{6} \end{pmatrix}$
\mathbb{Y}_{11}	$\mathbb{Q}_0^{(b,A_{1g})}$	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}_{12}	$\mathbb{Q}_{2,0}^{(b,E_{1g})}$	B_2	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$
\mathbb{Y}_{13}	$\mathbb{Q}_{2,1}^{(b,E_{1g})}$	B_2	$\begin{pmatrix} \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} \end{pmatrix}$

continued ...

Table 7

symbol	type	cluster	form
Y ₁₄	$\mathbb{Q}_{2,0}^{(b,E_{2g})}$	B ₂	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} \end{pmatrix}$
Y ₁₅	$\mathbb{Q}_{2,1}^{(b,E_{2g})}$	B ₂	$\begin{pmatrix} 0 & 0 & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$
Y ₁₆	$\mathbb{Q}_4^{(b,B_{2g})}$	B ₂	$\begin{pmatrix} \frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} \end{pmatrix}$
Y ₁₇	$\mathbb{Q}_0^{(b,A_{1g})}$	B ₃	$\begin{pmatrix} \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} \end{pmatrix}$
Y ₁₈	$\mathbb{Q}_{2,0}^{(b,E_{2g})}$	B ₃	$\begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & 0 \end{pmatrix}$
Y ₁₉	$\mathbb{Q}_{2,1}^{(b,E_{2g})}$	B ₃	$\begin{pmatrix} -\frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{6} \end{pmatrix}$
Y ₂₀	$\mathbb{Q}_{4,0}^{(b,E_{2g},1)}$	B ₃	$\begin{pmatrix} \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}}{12} & -\frac{\sqrt{6}}{6} \end{pmatrix}$
Y ₂₁	$\mathbb{Q}_{4,1}^{(b,E_{2g},1)}$	B ₃	$\begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & 0 \end{pmatrix}$
Y ₂₂	$\mathbb{T}_{2,0}^{(b,E_{2g})}$	B ₃	$\begin{pmatrix} \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & 0 \end{pmatrix}$
Y ₂₃	$\mathbb{T}_{2,1}^{(b,E_{2g})}$	B ₃	$\begin{pmatrix} -\frac{\sqrt{6}i}{12} & -\frac{\sqrt{6}i}{12} & \frac{\sqrt{6}i}{12} & -\frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}i}{12} & -\frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{12} & -\frac{\sqrt{6}i}{12} & \frac{\sqrt{6}i}{6} \end{pmatrix}$
Y ₂₄	$\mathbb{T}_{4,0}^{(b,E_{2g},1)}$	B ₃	$\begin{pmatrix} \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}i}{12} & -\frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}i}{12} & -\frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{12} & -\frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}i}{12} & -\frac{\sqrt{6}i}{6} \end{pmatrix}$
Y ₂₅	$\mathbb{T}_{4,1}^{(b,E_{2g},1)}$	B ₃	$\begin{pmatrix} \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & 0 \end{pmatrix}$
Y ₂₆	$\mathbb{T}_6^{(b,A_{2g})}$	B ₃	$\begin{pmatrix} \frac{\sqrt{3}i}{6} & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} & \frac{\sqrt{3}i}{6} & \frac{\sqrt{3}i}{6} & \frac{\sqrt{3}i}{6} & \frac{\sqrt{3}i}{6} \end{pmatrix}$

Table 8: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_{1g})}$	0	A_{1g}	—	—	1
2	$\mathbb{Q}_2^{(A_{1g})}$	2	A_{1g}	—	—	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
3	$\mathbb{Q}_{2,0}^{(E_{1g})}$	2	E_{1g}	—	0	$\sqrt{3}xz$
4	$\mathbb{Q}_{2,1}^{(E_{1g})}$	2	E_{1g}	—	1	$\sqrt{3}yz$
5	$\mathbb{Q}_{2,0}^{(E_{2g})}$	2	E_{2g}	—	0	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
6	$\mathbb{Q}_{2,1}^{(E_{2g})}$	2	E_{2g}	—	1	$-\sqrt{3}xy$
7	$\mathbb{Q}_4^{(A_{1g})}$	4	A_{1g}	—	—	$\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$
8	$\mathbb{Q}_4^{(B_{2g})}$	4	B_{2g}	—	—	$\frac{\sqrt{70}yz(3x^2-y^2)}{4}$

continued ...

Table 8

No.	symbol	rank	irrep.	mul.	comp.	form
9	$\mathbb{Q}_{4,0}^{(E_{1g})}$	4	E_{1g}	—	0	$-\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{8}$
10	$\mathbb{Q}_{4,1}^{(E_{1g})}$	4	E_{1g}	—	1	$-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{8}$
11	$\mathbb{Q}_{4,0}^{(E_{2g},1)}$	4	E_{2g}	1	0	$\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$
12	$\mathbb{Q}_{4,1}^{(E_{2g},1)}$	4	E_{2g}	1	1	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
13	$\mathbb{Q}_{4,0}^{(E_{2g},2)}$	4	E_{2g}	2	0	$-\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{2}$
14	$\mathbb{Q}_{4,1}^{(E_{2g},2)}$	4	E_{2g}	2	1	$\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$
15	$\mathbb{Q}_6^{(A_{2g})}$	6	A_{2g}	—	—	$\frac{\sqrt{462}xy(x^2-3y^2)(3x^2-y^2)}{16}$

Table 9: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_1^{(A_{2g})}$	1	A_{2g}	—	—	Z
2	$\mathbb{G}_3^{(A_{2g})}$	3	A_{2g}	—	—	$-\frac{Z(3X^2+3Y^2-2Z^2)}{2}$
3	$\mathbb{G}_{3,0}^{(E_{2g})}$	3	E_{2g}	—	0	$\sqrt{15}XYZ$
4	$\mathbb{G}_{3,1}^{(E_{2g})}$	3	E_{2g}	—	1	$\frac{\sqrt{15}Z(X-Y)(X+Y)}{2}$

-
- Group info.: Generator = $\{3_{001}^+|0\}$, $\{2_{001}|00\frac{1}{2}\}$, $\{2_{110}|0\}$, $\{-1|0\}$

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

rep. SO	symmetry operations
$\{1 0\}$	$\{1 0\}$
$\{2_{001} 00\frac{1}{2}\}$	$\{2_{001} 00\frac{1}{2}\}$

continued ...

Table 10

rep. SO	symmetry operations
$\{2_{100} 0\}$	$\{2_{100} 0\}, \{2_{010} 0\}, \{2_{110} 0\}$
$\{2_{120} 00\frac{1}{2}\}$	$\{2_{120} 00\frac{1}{2}\}, \{2_{210} 00\frac{1}{2}\}, \{2_{1-10} 00\frac{1}{2}\}$
$\{3_{001}^+ 0\}$	$\{3_{001}^+ 0\}, \{3_{001}^- 0\}$
$\{6_{001}^+ 00\frac{1}{2}\}$	$\{6_{001}^+ 00\frac{1}{2}\}, \{6_{001}^- 00\frac{1}{2}\}$
$\{-1 0\}$	$\{-1 0\}$
$\{m_{100} 0\}$	$\{m_{100} 0\}, \{m_{010} 0\}, \{m_{110} 0\}$
$\{m_{001} 00\frac{1}{2}\}$	$\{m_{001} 00\frac{1}{2}\}$
$\{m_{120} 00\frac{1}{2}\}$	$\{m_{120} 00\frac{1}{2}\}, \{m_{210} 00\frac{1}{2}\}, \{m_{1-10} 00\frac{1}{2}\}$
$\{-3_{001}^+ 0\}$	$\{-3_{001}^+ 0\}, \{-3_{001}^- 0\}$
$\{-6_{001}^+ 00\frac{1}{2}\}$	$\{-6_{001}^+ 00\frac{1}{2}\}, \{-6_{001}^- 00\frac{1}{2}\}$

Table 11: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1 0\}$	2	$\{2_{001} 00\frac{1}{2}\}$	3	$\{2_{100} 0\}$	4	$\{2_{010} 0\}$	5	$\{2_{110} 0\}$
6	$\{2_{120} 00\frac{1}{2}\}$	7	$\{2_{210} 00\frac{1}{2}\}$	8	$\{2_{1-10} 00\frac{1}{2}\}$	9	$\{3_{001}^+ 0\}$	10	$\{3_{001}^- 0\}$
11	$\{6_{001}^+ 00\frac{1}{2}\}$	12	$\{6_{001}^- 00\frac{1}{2}\}$	13	$\{-1 0\}$	14	$\{m_{100} 0\}$	15	$\{m_{010} 0\}$
16	$\{m_{110} 0\}$	17	$\{m_{001} 00\frac{1}{2}\}$	18	$\{m_{120} 00\frac{1}{2}\}$	19	$\{m_{210} 00\frac{1}{2}\}$	20	$\{m_{1-10} 00\frac{1}{2}\}$
21	$\{-3_{001}^+ 0\}$	22	$\{-3_{001}^- 0\}$	23	$\{-6_{001}^+ 00\frac{1}{2}\}$	24	$\{-6_{001}^- 00\frac{1}{2}\}$		

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

	1	2 ₀₀₁	2 ₁₀₀	2 ₁₂₀	3 ₀₀₁ ⁺	6 ₀₀₁ ⁺	-1	m ₁₀₀	m ₀₀₁	m ₁₂₀	-3 ₀₀₁ ⁺	-6 ₀₀₁ ⁺
<i>A</i> _{1g}	1	1	1	1	1	1	1	1	1	1	1	1
<i>A</i> _{2g}	1	1	-1	-1	1	1	1	-1	1	-1	1	1
<i>B</i> _{1g}	1	-1	-1	1	1	-1	1	-1	-1	1	1	-1
<i>B</i> _{2g}	1	-1	1	-1	1	-1	1	1	-1	-1	1	-1

continued ...

Table 12

	1	2 ₀₀₁	2 ₁₀₀	2 ₁₂₀	3 ₀₀₁ ⁺	6 ₀₀₁ ⁺	-1	m ₁₀₀	m ₀₀₁	m ₁₂₀	-3 ₀₀₁ ⁺	-6 ₀₀₁ ⁺
E_{1g}	2	-2	0	0	-1	1	2	0	-2	0	-1	1
E_{2g}	2	2	0	0	-1	-1	2	0	2	0	-1	-1
A_{1u}	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
A_{2u}	1	1	-1	-1	1	1	-1	1	-1	1	-1	-1
B_{1u}	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1
B_{2u}	1	-1	1	-1	1	-1	-1	-1	1	1	-1	1
E_{1u}	2	-2	0	0	-1	1	-2	0	2	0	1	-1
E_{2u}	2	2	0	0	-1	-1	-2	0	-2	0	1	1

Table 13: Parity conversion.

\leftrightarrow	\leftrightarrow	\leftrightarrow	\leftrightarrow	\leftrightarrow
$A_{1g} (A_{1u})$	$A_{2g} (A_{2u})$	$B_{1g} (B_{1u})$	$B_{2g} (B_{2u})$	$E_{1g} (E_{1u})$
$E_{2g} (E_{2u})$	$A_{1u} (A_{1g})$	$A_{2u} (A_{2g})$	$B_{1u} (B_{1g})$	$B_{2u} (B_{2g})$
$E_{1u} (E_{1g})$	$E_{2u} (E_{2g})$			

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

	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_{1g}	E_{2g}	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_{1u}	E_{2u}
A_{1g}	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_{1g}	E_{2g}	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_{1u}	E_{2u}
A_{2g}		A_{1g}	B_{2g}	B_{1g}	E_{1g}	E_{2g}	A_{2u}	A_{1u}	B_{2u}	B_{1u}	E_{1u}	E_{2u}
B_{1g}			A_{1g}	A_{2g}	E_{2g}	E_{1g}	B_{1u}	B_{2u}	A_{1u}	A_{2u}	E_{2u}	E_{1u}
B_{2g}				A_{1g}	E_{2g}	E_{1g}	B_{2u}	B_{1u}	A_{2u}	A_{1u}	E_{2u}	E_{1u}
E_{1g}					$A_{1g} + E_{2g}$	$B_{1g} + B_{2g} + E_{1g}$	E_{1u}	E_{1u}	E_{2u}	E_{2u}	$A_{1u} + A_{2u} + E_{2u}$	$B_{1u} + B_{2u} + E_{1u}$
E_{2g}						$A_{1g} + E_{2g}$	E_{2u}	E_{2u}	E_{1u}	E_{1u}	$B_{1u} + B_{2u} + E_{1u}$	$A_{1u} + A_{2u} + E_{2u}$
A_{1u}							A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_{1g}	E_{2g}
A_{2u}								A_{1g}	B_{2g}	B_{1g}	E_{1g}	E_{2g}
B_{1u}									A_{1g}	A_{2g}	E_{2g}	E_{1g}
B_{2u}										A_{1g}	E_{2g}	E_{1g}
E_{1u}											$A_{1g} + E_{2g}$	$B_{1g} + B_{2g} + E_{1g}$
E_{2u}												$A_{1g} + E_{2g}$

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

A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_{1g}	E_{2g}	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_{1u}	E_{2u}
—	—	—	—	A_{2g}	A_{2g}	—	—	—	—	A_{2g}	A_{2g}

Table 16: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix} 1 + \sqrt{3} & -1 + \sqrt{3} & 1 \end{pmatrix}$	2	$\begin{pmatrix} -\sqrt{3} - 1 & 1 - \sqrt{3} & 1 \end{pmatrix}$	3	$\begin{pmatrix} 2 & 1 - \sqrt{3} & -1 \end{pmatrix}$	4	$\begin{pmatrix} -\sqrt{3} - 1 & -2 & -1 \end{pmatrix}$
5	$\begin{pmatrix} -1 + \sqrt{3} & 1 + \sqrt{3} & -1 \end{pmatrix}$	6	$\begin{pmatrix} -2 & -1 + \sqrt{3} & -1 \end{pmatrix}$	7	$\begin{pmatrix} 1 + \sqrt{3} & 2 & -1 \end{pmatrix}$	8	$\begin{pmatrix} 1 - \sqrt{3} & -\sqrt{3} - 1 & -1 \end{pmatrix}$
9	$\begin{pmatrix} 1 - \sqrt{3} & 2 & 1 \end{pmatrix}$	10	$\begin{pmatrix} -2 & -\sqrt{3} - 1 & 1 \end{pmatrix}$	11	$\begin{pmatrix} 2 & 1 + \sqrt{3} & 1 \end{pmatrix}$	12	$\begin{pmatrix} -1 + \sqrt{3} & -2 & 1 \end{pmatrix}$
13	$\begin{pmatrix} -\sqrt{3} - 1 & 1 - \sqrt{3} & -1 \end{pmatrix}$	14	$\begin{pmatrix} -2 & -1 + \sqrt{3} & 1 \end{pmatrix}$	15	$\begin{pmatrix} 1 + \sqrt{3} & 2 & 1 \end{pmatrix}$	16	$\begin{pmatrix} 1 - \sqrt{3} & -\sqrt{3} - 1 & 1 \end{pmatrix}$
17	$\begin{pmatrix} 1 + \sqrt{3} & -1 + \sqrt{3} & -1 \end{pmatrix}$	18	$\begin{pmatrix} 2 & 1 - \sqrt{3} & 1 \end{pmatrix}$	19	$\begin{pmatrix} -\sqrt{3} - 1 & -2 & 1 \end{pmatrix}$	20	$\begin{pmatrix} -1 + \sqrt{3} & 1 + \sqrt{3} & 1 \end{pmatrix}$
21	$\begin{pmatrix} -1 + \sqrt{3} & -2 & -1 \end{pmatrix}$	22	$\begin{pmatrix} 2 & 1 + \sqrt{3} & -1 \end{pmatrix}$	23	$\begin{pmatrix} -2 & -\sqrt{3} - 1 & -1 \end{pmatrix}$	24	$\begin{pmatrix} 1 - \sqrt{3} & 2 & -1 \end{pmatrix}$

Table 17: Virtual-cluster basis.

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_0^{(A_{1g})}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$						
$\mathbb{Q}_1^{(A_{2u})}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$						
$\mathbb{Q}_{1,0}^{(E_{1u})}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$
	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$

continued ...

Table 17

[illegible]

continued ...

Table 17

[illegible]

continued ...

Table 17

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_{6,1}^{(E_{1g},1)}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$
	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$
	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{12}$						
$\mathbb{Q}_7^{(A_{1u})}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$						