SAMB for "UPt2Si2"

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- Group: No. 129 D_{4h}^{7} $P4/nmm$ [tetragonal]
- Associated point group: No. 15 D_{4h} $4/mmm$ [tetragonal]

- Generation condition
  - model type: `tight_binding`
  - time-reversal type: `electric`
  - irrep: `[A1g]`
  - `spinless`

- Unit cell:
  $a = 4.1972,\ b = 4.1972,\ c = 9.6906,\ \alpha = 90.0,\ \beta = 90.0,\ \gamma = 90.0$
- Lattice vectors:
  $\boldsymbol{a}_1 = \begin{pmatrix} 4.1972 & 0 & 0 \end{pmatrix}$
  $\boldsymbol{a}_2 = \begin{pmatrix} 0 & 4.1972 & 0 \end{pmatrix}$
  $\boldsymbol{a}_3 = \begin{pmatrix} 0 & 0 & 9.6906 \end{pmatrix}$

Table 1: High-symmetry line: Γ-X.

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

- Kets: dimension = 46

Table 2: Hilbert space for full matrix.

No.	ket	No.	ket	No.	ket	No.	ket	No.	ket
1	f_{xyz}@U_1	2	f_{ax}@U_1	3	f_{ay}@U_1	4	f_{az}@U_1	5	f_{bx}@U_1
6	f_{by}@U_1	7	f_{bz}@U_1	8	f_{xyz}@U_2	9	f_{ax}@U_2	10	f_{ay}@U_2
11	f_{az}@U_2	12	f_{bx}@U_2	13	f_{by}@U_2	14	f_{bz}@U_2	15	d_u@$\mathrm{Pt1}_1$
16	d_v@$\mathrm{Pt1}_1$	17	d_{yz}@$\mathrm{Pt1}_1$	18	d_{zx}@$\mathrm{Pt1}_1$	19	d_{xy}@$\mathrm{Pt1}_1$	20	d_u@$\mathrm{Pt1}_2$
21	d_v@$\mathrm{Pt1}_2$	22	d_{yz}@$\mathrm{Pt1}_2$	23	d_{zx}@$\mathrm{Pt1}_2$	24	d_{xy}@$\mathrm{Pt1}_2$	25	d_u@$\mathrm{Pt2}_1$
26	d_v@$\mathrm{Pt2}_1$	27	d_{yz}@$\mathrm{Pt2}_1$	28	d_{zx}@$\mathrm{Pt2}_1$	29	d_{xy}@$\mathrm{Pt2}_1$	30	d_u@$\mathrm{Pt2}_2$
31	d_v@$\mathrm{Pt2}_2$	32	d_{yz}@$\mathrm{Pt2}_2$	33	d_{zx}@$\mathrm{Pt2}_2$	34	d_{xy}@$\mathrm{Pt2}_2$	35	p_x@$\mathrm{Si1}_1$
36	p_y@$\mathrm{Si1}_1$	37	p_z@$\mathrm{Si1}_1$	38	p_x@$\mathrm{Si1}_2$	39	p_y@$\mathrm{Si1}_2$	40	p_z@$\mathrm{Si1}_2$
41	p_x@$\mathrm{Si2}_1$	42	p_y@$\mathrm{Si2}_1$	43	p_z@$\mathrm{Si2}_1$	44	p_x@$\mathrm{Si2}_2$	45	p_y@$\mathrm{Si2}_2$
46	p_z@$\mathrm{Si2}_2$								

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S_1 [2c: 4mm]	U_1	$\begin{pmatrix} \frac{1}{4} & \frac{1}{4} & 0.7484 \end{pmatrix}$	[1,2,7,8,11,12,13,14]
	U_2	$\begin{pmatrix} \frac{3}{4} & \frac{3}{4} & 0.2516 \end{pmatrix}$	[3,4,5,6,9,10,15,16]
S_2 [2a: -4m2]	$\mathrm{Pt1}_1$	$\begin{pmatrix} \frac{3}{4} & \frac{1}{4} & 0 \end{pmatrix}$	[1,2,5,6,11,12,15,16]
	$\mathrm{Pt1}_2$	$\begin{pmatrix} \frac{1}{4} & \frac{3}{4} & 0 \end{pmatrix}$	[3,4,7,8,9,10,13,14]
S_3 [2c: 4mm]	$\mathrm{Pt2}_1$	$\begin{pmatrix} \frac{1}{4} & \frac{1}{4} & 0.3785 \end{pmatrix}$	[1,2,7,8,11,12,13,14]
	$\mathrm{Pt2}_2$	$\begin{pmatrix} \frac{3}{4} & \frac{3}{4} & 0.6215 \end{pmatrix}$	[3,4,5,6,9,10,15,16]
S_4 [2b: -4m2]	$\mathrm{Si1}_1$	$\begin{pmatrix} \frac{3}{4} & \frac{1}{4} & \frac{1}{2} \end{pmatrix}$	[1,2,5,6,11,12,15,16]
	$\mathrm{Si1}_2$	$\begin{pmatrix} \frac{1}{4} & \frac{3}{4} & \frac{1}{2} \end{pmatrix}$	[3,4,7,8,9,10,13,14]
S_5 [2c: 4mm]	$\mathrm{Si2}_1$	$\begin{pmatrix} \frac{1}{4} & \frac{1}{4} & 0.133 \end{pmatrix}$	[1,2,7,8,11,12,13,14]
	$\mathrm{Si2}_2$	$\begin{pmatrix} \frac{3}{4} & \frac{3}{4} & 0.867 \end{pmatrix}$	[3,4,5,6,9,10,15,16]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	$\boldsymbol{b}$@$\boldsymbol{c}$	mapping
B_1 [8i: .m.]	b_1	$Si2_1$	$Pt1_1$	1	1	$\begin{pmatrix} \frac{1}{2} & 0 & 0.133 \end{pmatrix}$ @ $\begin{pmatrix} 0 & \frac{1}{4} & 0.0665 \end{pmatrix}$	[1,12]
	b_2	$Si2_1$	$Pt1_1$	1	1	$\begin{pmatrix} -\frac{1}{2} & 0 & 0.133 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{2} & \frac{1}{4} & 0.0665 \end{pmatrix}$	[2,11]
	b_3	$Si2_2$	$Pt1_2$	1	1	$\begin{pmatrix} \frac{1}{2} & 0 & -0.133 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{2} & \frac{3}{4} & 0.9335 \end{pmatrix}$	[3,10]
	b_4	$Si2_2$	$Pt1_2$	1	1	$\begin{pmatrix} -\frac{1}{2} & 0 & -0.133 \end{pmatrix}$ @ $\begin{pmatrix} 0 & \frac{3}{4} & 0.9335 \end{pmatrix}$	[4,9]
	b_5	$Si2_2$	$Pt1_1$	1	1	$\begin{pmatrix} 0 & \frac{1}{2} & -0.133 \end{pmatrix}$ @ $\begin{pmatrix} \frac{3}{4} & \frac{1}{2} & 0.9335 \end{pmatrix}$	[5,16]
	b_6	$Si2_2$	$Pt1_1$	1	1	$\begin{pmatrix} 0 & -\frac{1}{2} & -0.133 \end{pmatrix}$ @ $\begin{pmatrix} \frac{3}{4} & 0 & 0.9335 \end{pmatrix}$	[6,15]
	b_7	$Si2_1$	$Pt1_2$	1	1	$\begin{pmatrix} 0 & \frac{1}{2} & 0.133 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{4} & 0 & 0.0665 \end{pmatrix}$	[7,14]
	b_8	$Si2_1$	$Pt1_2$	1	1	$\begin{pmatrix} 0 & -\frac{1}{2} & 0.133 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{4} & \frac{1}{2} & 0.0665 \end{pmatrix}$	[8,13]
B_2 [8i: .m.]	b_9	$Si1_1$	$Pt2_1$	1	1	$\begin{pmatrix} -\frac{1}{2} & 0 & 0.1215 \end{pmatrix}$ @ $\begin{pmatrix} 0 & \frac{1}{4} & 0.43925 \end{pmatrix}$	[1,12]
	b_{10}	$Si1_1$	$Pt2_1$	1	1	$\begin{pmatrix} \frac{1}{2} & 0 & 0.1215 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{2} & \frac{1}{4} & 0.43925 \end{pmatrix}$	[2,11]
	b_{11}	$Si1_2$	$Pt2_2$	1	1	$\begin{pmatrix} -\frac{1}{2} & 0 & -0.1215 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{2} & \frac{3}{4} & 0.56075 \end{pmatrix}$	[3,10]
	b_{12}	$Si1_2$	$Pt2_2$	1	1	$\begin{pmatrix} \frac{1}{2} & 0 & -0.1215 \end{pmatrix}$ @ $\begin{pmatrix} 0 & \frac{3}{4} & 0.56075 \end{pmatrix}$	[4,9]
	b_{13}	$Si1_1$	$Pt2_2$	1	1	$\begin{pmatrix} 0 & -\frac{1}{2} & -0.1215 \end{pmatrix}$ @ $\begin{pmatrix} \frac{3}{4} & \frac{1}{2} & 0.56075 \end{pmatrix}$	[5,16]
	b_{14}	$Si1_1$	$Pt2_2$	1	1	$\begin{pmatrix} 0 & \frac{1}{2} & -0.1215 \end{pmatrix}$ @ $\begin{pmatrix} \frac{3}{4} & 0 & 0.56075 \end{pmatrix}$	[6,15]
	b_{15}	$Si1_2$	$Pt2_1$	1	1	$\begin{pmatrix} 0 & -\frac{1}{2} & 0.1215 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{4} & 0 & 0.43925 \end{pmatrix}$	[7,14]
	b_{16}	$Si1_2$	$Pt2_1$	1	1	$\begin{pmatrix} 0 & \frac{1}{2} & 0.1215 \end{pmatrix}$ @ $\begin{pmatrix} \frac{1}{4} & \frac{1}{2} & 0.43925 \end{pmatrix}$	[8,13]

- SAMB:

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

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

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

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

$\boxed{\text{No. 3}}$ $\hat{\mathbb{Q}}_4^{(A_{1g},1)}$ $[\mathrm{M}_1, \mathrm{S}_1]$

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

$\boxed{\text{No. 4}}$ $\hat{\mathbb{Q}}_4^{(A_{1g},2)}$ $[\mathrm{M}_1, \mathrm{S}_1]$

$\hat{\mathbb{Z}}_4 = \mathbb{X}_4[\mathbb{Q}_4^{(a,A_{1g},2)}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A_{1g})}]$

$\boxed{\text{No. 5}}$ $\hat{\mathbb{Q}}_6^{(A_{1g},1)}$ $[\mathrm{M}_1, \mathrm{S}_1]$

$\hat{\mathbb{Z}}_5 = \mathbb{X}_5[\mathbb{Q}_6^{(a,A_{1g},1)}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A_{1g})}]$

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

$\hat{\mathbb{Z}}_6 = \mathbb{X}_6[\mathbb{Q}_6^{(a,A_{1g},2)}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A_{1g})}]$

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

$\hat{\mathbb{Z}}_7 = \mathbb{X}_7[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s,A_{1g})}]$

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

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

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

$\hat{\mathbb{Z}}_9 = \mathbb{X}_9[\mathbb{Q}_4^{(a,A_{1g},1)}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s,A_{1g})}]$

$\boxed{\text{No. 10}}$ $\hat{\mathbb{Q}}_4^{(A_{1g},2)}$ $[\mathrm{M}_2, \mathrm{S}_2]$

$\hat{\mathbb{Z}}_{10} = \mathbb{X}_{10}[\mathbb{Q}_4^{(a,A_{1g},2)}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s,A_{1g})}]$

$\boxed{\text{No. 11}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_2, \mathrm{S}_3]$

$\hat{\mathbb{Z}}_{11} = \mathbb{X}_7[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(s,A_{1g})}]$

$\boxed{\text{No. 12}}$ $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_2, \mathrm{S}_3]$

$$\hat{\mathbb{Z}}_{12} = \mathbb{X}_8[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(s,A_{1g})}]$$

$\boxed{\text{No. 13}}$ $\hat{\mathbb{Q}}_4^{(A_{1g},1)}$ $[\mathrm{M}_2, \mathrm{S}_3]$

$$\hat{\mathbb{Z}}_{13} = \mathbb{X}_9[\mathbb{Q}_4^{(a,A_{1g},1)}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(s,A_{1g})}]$$

$\boxed{\text{No. 14}}$ $\hat{\mathbb{Q}}_4^{(A_{1g},2)}$ $[\mathrm{M}_2, \mathrm{S}_3]$

$$\hat{\mathbb{Z}}_{14} = \mathbb{X}_{10}[\mathbb{Q}_4^{(a,A_{1g},2)}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(s,A_{1g})}]$$

$\boxed{\text{No. 15}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_3, \mathrm{S}_4]$

$$\hat{\mathbb{Z}}_{15} = \mathbb{X}_{11}[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(s,A_{1g})}]$$

$\boxed{\text{No. 16}}$ $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_3, \mathrm{S}_4]$

$$\hat{\mathbb{Z}}_{16} = \mathbb{X}_{12}[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(s,A_{1g})}]$$

$\boxed{\text{No. 17}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_3, \mathrm{S}_5]$

$$\hat{\mathbb{Z}}_{17} = \mathbb{X}_{11}[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(s,A_{1g})}]$$

$\boxed{\text{No. 18}}$ $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_3, \mathrm{S}_5]$

$$\hat{\mathbb{Z}}_{18} = \mathbb{X}_{12}[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(s,A_{1g})}]$$

$\boxed{\text{No. 19}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_4, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{19} = \frac{\sqrt{3}\mathbb{X}_{13}[\mathbb{Q}_1^{(a,A_{2u})}] \otimes \mathbb{Y}_6[\mathbb{Q}_1^{(b,A_{2u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a,E_u)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{1,0}^{(b,E_u)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a,E_u)}] \otimes \mathbb{Y}_8[\mathbb{Q}_{1,1}^{(b,E_u)}]}{3}$$

$\boxed{\text{No. 20}}$ $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_4, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{20} = \frac{\sqrt{6}\mathbb{X}_{13}[\mathbb{Q}_1^{(a,A_{2u})}] \otimes \mathbb{Y}_6[\mathbb{Q}_1^{(b,A_{2u})}]}{3} - \frac{\sqrt{6}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a,E_u)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{1,0}^{(b,E_u)}]}{6} - \frac{\sqrt{6}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a,E_u)}] \otimes \mathbb{Y}_8[\mathbb{Q}_{1,1}^{(b,E_u)}]}{6}$$

$\boxed{\text{No. 21}}$ $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_4, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{21} = \frac{\sqrt{21}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{Y}_6[\mathbb{Q}_1^{(b,A_{2u})}]}{7} - \frac{\sqrt{21}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{1,0}^{(b,E_u)}]}{14} - \frac{\sqrt{21}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{Y}_8[\mathbb{Q}_{1,1}^{(b,E_u)}]}{14} - \frac{\sqrt{35}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{1,0}^{(b,E_u)}]}{14} - \frac{\sqrt{35}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{Y}_8[\mathbb{Q}_{1,1}^{(b,E_u)}]}{14}$$

$\boxed{\text{No. 22}}$ $\hat{\mathbb{Q}}_4^{(A_{1g},1)}$ $[\mathrm{M}_4, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{22} = \frac{\sqrt{3}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{Y}_6[\mathbb{Q}_1^{(b,A_{2u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{1,0}^{(b,E_u)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{Y}_8[\mathbb{Q}_{1,1}^{(b,E_u)}]}{3}$$

$\boxed{\text{No. 23}}$ $\hat{\mathbb{Q}}_4^{(A_{1g},2)}$ $[\mathrm{M}_4, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{23} = \frac{\sqrt{105}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{Y}_6[\mathbb{Q}_1^{(b,A_{2u})}]}{21} - \frac{\sqrt{105}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{1,0}^{(b,E_u)}]}{42} - \frac{\sqrt{105}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{Y}_8[\mathbb{Q}_{1,1}^{(b,E_u)}]}{42} + \frac{3\sqrt{7}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{1,0}^{(b,E_u)}]}{14} + \frac{3\sqrt{7}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{Y}_8[\mathbb{Q}_{1,1}^{(b,E_u)}]}{14}$$

$\boxed{\text{No. 24}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_4, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{24} = \mathbb{X}_{23}[\mathbb{Q}_3^{(a,B_{2u})}] \otimes \mathbb{Y}_9[\mathbb{Q}_3^{(b,B_{2u})}]$$

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

$$\hat{\mathbb{Z}}_{25} = -\frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{G}_{2,0}^{(a,E_u)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{1,0}^{(b,E_u)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{G}_{2,1}^{(a,E_u)}] \otimes \mathbb{Y}_8[\mathbb{Q}_{1,1}^{(b,E_u)}]}{2}$$

$\boxed{\text{No. 26}}$ $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_4, \mathrm{B}_1]$

$$\hat{\mathbb{Z}}_{26} = -\mathbb{X}_{24}[\mathbb{G}_2^{(a,B_{2u})}] \otimes \mathbb{Y}_9[\mathbb{Q}_3^{(b,B_{2u})}]$$

$\boxed{\text{No. 27}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_4, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{27} = \frac{\sqrt{3}\mathbb{X}_{13}[\mathbb{Q}_1^{(a,A_{2u})}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_1^{(b,A_{2u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a,E_u)}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E_u)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a,E_u)}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E_u)}]}{3}$$

$\boxed{\text{No. 28}}$ $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_4, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{28} = \frac{\sqrt{6}\mathbb{X}_{13}[\mathbb{Q}_1^{(a,A_{2u})}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_1^{(b,A_{2u})}]}{3} - \frac{\sqrt{6}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a,E_u)}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E_u)}]}{6} - \frac{\sqrt{6}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a,E_u)}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E_u)}]}{6}$$

$\boxed{\text{No. 29}}$ $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_4, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{29} = \frac{\sqrt{21}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_1^{(b,A_{2u})}]}{7} - \frac{\sqrt{21}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E_u)}]}{14} - \frac{\sqrt{21}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E_u)}]}{14} - \frac{\sqrt{35}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E_u)}]}{14} - \frac{\sqrt{35}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E_u)}]}{14}$$

$\boxed{\text{No. 30}}$ $\hat{\mathbb{Q}}_4^{(A_{1g},1)}$ $[\mathrm{M}_4, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{30} = \frac{\sqrt{3}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_1^{(b,A_{2u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E_u)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E_u)}]}{3}$$

$\boxed{\text{No. 31}}$ $\hat{\mathbb{Q}}_4^{(A_{1g},2)}$ $[\mathrm{M}_4, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{31} = \frac{\sqrt{105}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_1^{(b,A_{2u})}]}{21} - \frac{\sqrt{105}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E_u)}]}{42} - \frac{\sqrt{105}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E_u)}]}{42} + \frac{3\sqrt{7}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E_u)}]}{14} + \frac{3\sqrt{7}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E_u)}]}{14}$$

$\boxed{\text{No. 32}}$ $\hat{\mathbb{Q}}_0^{(A_{1g})}$ $[\mathrm{M}_4, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{32} = \mathbb{X}_{23}[\mathbb{Q}_3^{(a,B_{2u})}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_3^{(b,B_{2u})}]$$

$\boxed{\text{No. 33}}$ $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_4, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{33} = -\frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{G}_{2,0}^{(a,E_u)}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E_u)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{G}_{2,1}^{(a,E_u)}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E_u)}]}{2}$$

$\boxed{\text{No. 34}}$ $\hat{\mathbb{Q}}_2^{(A_{1g})}$ $[\mathrm{M}_4, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_{34} = -\mathbb{X}_{24}[\mathbb{G}_2^{(a,B_{2u})}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_3^{(b,B_{2u})}]$$

Table 5: Atomic SAMB group.

group	bra	ket
M_1	$f_{xyz}, f_{ax}, f_{ay}, f_{az}, f_{bx}, f_{by}, f_{bz}$	$f_{xyz}, f_{ax}, f_{ay}, f_{az}, f_{bx}, f_{by}, f_{bz}$
M_2	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$
M_3	p_x, p_y, p_z	p_x, p_y, p_z
M_4	p_x, p_y, p_z	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$

Table 6: Atomic SAMB.

symbol	type	group	form
$\mathbb{X}_1$	$\mathbb{Q}_0^{(a,A_{1g})}$	M_1	$\begin{pmatrix} \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} \end{pmatrix}$
$\mathbb{X}_2$	$\mathbb{Q}_2^{(a,A_{1g})}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{21}}{21} & 0 & 0 & \frac{\sqrt{35}}{14} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{21}}{21} & 0 & 0 & -\frac{\sqrt{35}}{14} & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{21}}{21} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_3$	$\mathbb{Q}_4^{(a,A_{1g},1)}$	M_1	$\begin{pmatrix} -\frac{\sqrt{66}}{11} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_4$	$\mathbb{Q}_4^{(a,A_{1g},2)}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2310}}{308} & 0 & 0 & -\frac{3\sqrt{154}}{308} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2310}}{308} & 0 & 0 & \frac{3\sqrt{154}}{308} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2310}}{154} & 0 & 0 & 0 \\ 0 & -\frac{3\sqrt{154}}{308} & 0 & 0 & \frac{\sqrt{2310}}{132} & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{154}}{308} & 0 & 0 & \frac{\sqrt{2310}}{132} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2310}}{66} \end{pmatrix}$
$\mathbb{X}_5$	$\mathbb{Q}_6^{(a,A_{1g},1)}$	M_1	$\begin{pmatrix} \frac{2\sqrt{462}}{77} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{5\sqrt{462}}{462} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{5\sqrt{462}}{462} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{5\sqrt{462}}{462} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} \end{pmatrix}$
$\mathbb{X}_6$	$\mathbb{Q}_6^{(a,A_{1g},2)}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{5\sqrt{66}}{132} & 0 & 0 & -\frac{\sqrt{110}}{44} & 0 & 0 \\ 0 & 0 & -\frac{5\sqrt{66}}{132} & 0 & 0 & \frac{\sqrt{110}}{44} & 0 \\ 0 & 0 & 0 & \frac{5\sqrt{66}}{66} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{110}}{44} & 0 & 0 & -\frac{\sqrt{66}}{44} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{110}}{44} & 0 & 0 & -\frac{\sqrt{66}}{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{66}}{22} \end{pmatrix}$
$\mathbb{X}_7$	$\mathbb{Q}_0^{(a,A_{1g})}$	M_2	$\begin{pmatrix} \frac{\sqrt{5}}{5} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{5}}{5} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{5}}{5} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{5}}{5} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{5}}{5} \end{pmatrix}$
$\mathbb{X}_8$	$\mathbb{Q}_2^{(a,A_{1g})}$	M_2	$\begin{pmatrix} \frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{7} \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_9$	$\mathbb{Q}_4^{(a,A_{1g},1)}$	M_2	$\begin{pmatrix} \frac{\sqrt{30}}{10} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{30}}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{30}}{15} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{15} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{30}}{15} \end{pmatrix}$
$\mathbb{X}_{10}$	$\mathbb{Q}_4^{(a,A_{1g},2)}$	M_2	$\begin{pmatrix} \frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{21} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{21} & 0 \\ 0 & 0 & 0 & 0 & \frac{2\sqrt{42}}{21} \end{pmatrix}$
$\mathbb{X}_{11}$	$\mathbb{Q}_0^{(a,A_{1g})}$	M_3	$\begin{pmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$
$\mathbb{X}_{12}$	$\mathbb{Q}_2^{(a,A_{1g})}$	M_3	$\begin{pmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{pmatrix}$
$\mathbb{X}_{13}$	$\mathbb{Q}_1^{(a,A_{2u})}$	M_4	$\begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{30}}{10} & 0 \\ 0 & 0 & \frac{\sqrt{30}}{10} & 0 & 0 \\ \frac{\sqrt{10}}{5} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{14}$	$\mathbb{Q}_3^{(a,A_{2u})}$	M_4	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{5}}{5} & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{5} & 0 & 0 \\ \frac{\sqrt{15}}{5} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{15}$	$\mathbb{Q}_{1,0}^{(a,E_u)}$	M_4	$\begin{pmatrix} -\frac{\sqrt{10}}{10} & \frac{\sqrt{30}}{10} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{10} \\ 0 & 0 & 0 & \frac{\sqrt{30}}{10} & 0 \end{pmatrix}$
$\mathbb{X}_{16}$	$\mathbb{Q}_{1,1}^{(a,E_u)}$	M_4	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{10} \\ -\frac{\sqrt{10}}{10} & -\frac{\sqrt{30}}{10} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{30}}{10} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{17}$	$\mathbb{Q}_{3,0}^{(a,E_u,1)}$	M_4	$\begin{pmatrix} -\frac{\sqrt{15}}{10} & \frac{3\sqrt{5}}{10} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{5} \\ 0 & 0 & 0 & -\frac{\sqrt{5}}{5} & 0 \end{pmatrix}$

continued …

Table 6

symbol	type	group	form
$\mathbb{X}_{18}$	$\mathbb{Q}_{3,1}^{(a,E_u,1)}$	M_4	$\begin{pmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{5} \\ -\frac{\sqrt{15}}{10} & -\frac{3\sqrt{5}}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{5} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{19}$	$\mathbb{Q}_{3,0}^{(a,E_u,2)}$	M_4	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{3} & 0 \end{pmatrix}$
$\mathbb{X}_{20}$	$\mathbb{Q}_{3,1}^{(a,E_u,2)}$	M_4	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \\ -\frac{1}{2} & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{3} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{21}$	$\mathbb{G}_{2,0}^{(a,E_u)}$	M_4	$\begin{pmatrix} -\frac{\sqrt{2}}{2} & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \end{pmatrix}$
$\mathbb{X}_{22}$	$\mathbb{G}_{2,1}^{(a,E_u)}$	M_4	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \\ \frac{\sqrt{2}}{2} & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{23}$	$\mathbb{Q}_{3}^{(a,B_{2u})}$	M_4	$\begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{24}$	$\mathbb{G}_{2}^{(a,B_{2u})}$	M_4	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & \frac{\sqrt{6}}{3} & 0 & 0 & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
$\mathbb{Y}_1$	$\mathbb{Q}_0^{(s,A_{1g})}$	S_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_2$	$\mathbb{Q}_0^{(s,A_{1g})}$	S_2	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_3$	$\mathbb{Q}_0^{(s,A_{1g})}$	S_3	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$

continued ...

Table 7

symbol	type	cluster	form
$\mathbb{Y}_4$	$\mathbb{Q}_0^{(s,A_{1g})}$	S_4	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_5$	$\mathbb{Q}_0^{(s,A_{1g})}$	S_5	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_6$	$\mathbb{Q}_1^{(b,A_{2u})}$	B_1	$\begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} \end{pmatrix}$
$\mathbb{Y}_7$	$\mathbb{Q}_{1,0}^{(b,E_u)}$	B_1	$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{Y}_8$	$\mathbb{Q}_{1,1}^{(b,E_u)}$	B_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$
$\mathbb{Y}_9$	$\mathbb{Q}_3^{(b,B_{2u})}$	B_1	$\begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} \end{pmatrix}$
$\mathbb{Y}_{10}$	$\mathbb{Q}_1^{(b,A_{2u})}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} \end{pmatrix}$
$\mathbb{Y}_{11}$	$\mathbb{Q}_{1,0}^{(b,E_u)}$	B_2	$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{Y}_{12}$	$\mathbb{Q}_{1,1}^{(b,E_u)}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$
$\mathbb{Y}_{13}$	$\mathbb{Q}_3^{(b,B_{2u})}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} \end{pmatrix}$

Table 8: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_{1g})}$	0	A_{1g}	–	–	1
2	$\mathbb{Q}_1^{(A_{2u})}$	1	A_{2u}	–	–	z
3	$\mathbb{Q}_{1,0}^{(E_u)}$	1	E_u	–	0	x
4	$\mathbb{Q}_{1,1}^{(E_u)}$	1	E_u	–	1	y
5	$\mathbb{Q}_2^{(A_{1g})}$	2	A_{1g}	–	–	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
6	$\mathbb{Q}_3^{(A_{2u})}$	3	A_{2u}	–	–	$-\frac{z\left(3x^2+3y^2-2z^2\right)}{2}$
7	$\mathbb{Q}_3^{(B_{2u})}$	3	B_{2u}	–	–	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
8	$\mathbb{Q}_{3,0}^{(E_u,1)}$	3	E_u	1	0	$\frac{x\left(2x^2-3y^2-3z^2\right)}{2}$
9	$\mathbb{Q}_{3,1}^{(E_u,1)}$	3	E_u	1	1	$-\frac{y\left(3x^2-2y^2+3z^2\right)}{2}$
10	$\mathbb{Q}_{3,0}^{(E_u,2)}$	3	E_u	2	0	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
11	$\mathbb{Q}_{3,1}^{(E_u,2)}$	3	E_u	2	1	$\frac{\sqrt{15}y(x-z)(x+z)}{2}$

continued …

Table 8

No.	symbol	rank	irrep.	mul.	comp.	form
12	$\mathbb{Q}_4^{(A_{1g},1)}$	4	A_{1g}	1	–	$\frac{\sqrt{21}\left(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4\right)}{6}$
13	$\mathbb{Q}_4^{(A_{1g},2)}$	4	A_{1g}	2	–	$-\frac{\sqrt{15}\left(x^4-12x^2y^2+6x^2z^2+y^4+6y^2z^2-2z^4\right)}{12}$
14	$\mathbb{Q}_6^{(A_{1g},1)}$	6	A_{1g}	1	–	$\frac{\sqrt{2}\cdot\left(2x^6-15x^4y^2-15x^4z^2-15x^2y^4+180x^2y^2z^2-15x^2z^4+2y^6-15y^4z^2-15y^2z^4+2z^6\right)}{8}$
15	$\mathbb{Q}_6^{(A_{1g},2)}$	6	A_{1g}	2	–	$-\frac{\sqrt{14}\left(x^6-15x^4z^2+15x^2z^4+y^6-15y^4z^2+15y^2z^4-2z^6\right)}{8}$

Table 9: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_2^{(B_{2u})}$	2	B_{2u}	–	–	$\sqrt{3}XY$
2	$\mathbb{G}_{2,0}^{(E_u)}$	2	E_u	–	0	$\sqrt{3}YZ$
3	$\mathbb{G}_{2,1}^{(E_u)}$	2	E_u	–	1	$\sqrt{3}XZ$

- Group info.: Generator = $\{2_{001}|\frac{1}{2}\frac{1}{2}0\}$, $\{4^+_{001}|\frac{1}{2}00\}$, $\{2_{010}|0\frac{1}{2}0\}$, $\{-1|0\}$

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

rep. SO	symmetry operations
$\{1|0\}$	$\{1|0\}$
$\{2_{001}|\frac{1}{2}\frac{1}{2}0\}$	$\{2_{001}|\frac{1}{2}\frac{1}{2}0\}$
$\{2_{100}|\frac{1}{2}00\}$	$\{2_{100}|\frac{1}{2}00\}$, $\{2_{010}|0\frac{1}{2}0\}$
$\{2_{110}|\frac{1}{2}\frac{1}{2}0\}$	$\{2_{110}|\frac{1}{2}\frac{1}{2}0\}$, $\{2_{1-10}|0\}$
$\{4^+_{001}|\frac{1}{2}00\}$	$\{4^+_{001}|\frac{1}{2}00\}$, $\{4^-_{001}|0\frac{1}{2}0\}$
$\{-1|0\}$	$\{-1|0\}$
$\{m_{001}|\frac{1}{2}\frac{1}{2}0\}$	$\{m_{001}|\frac{1}{2}\frac{1}{2}0\}$

continued ...

Table 10

rep. SO	symmetry operations
$\{m_{100}\|\frac{1}{2}00\}$	$\{m_{100}\|\frac{1}{2}00\}$, $\{m_{010}\|0\frac{1}{2}0\}$
$\{m_{110}\|\frac{1}{2}\frac{1}{2}0\}$	$\{m_{110}\|\frac{1}{2}\frac{1}{2}0\}$, $\{m_{1-10}\|0\}$
$\{-4^{+}_{001}\|\frac{1}{2}00\}$	$\{-4^{+}_{001}\|\frac{1}{2}00\}$, $\{-4^{-}_{001}\|0\frac{1}{2}0\}$

Table 11: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1\|0\}$	2	$\{2_{001}\|\frac{1}{2}\frac{1}{2}0\}$	3	$\{2_{100}\|\frac{1}{2}00\}$	4	$\{2_{010}\|0\frac{1}{2}0\}$	5	$\{2_{110}\|\frac{1}{2}\frac{1}{2}0\}$
6	$\{2_{1-10}\|0\}$	7	$\{4^{+}_{001}\|\frac{1}{2}00\}$	8	$\{4^{-}_{001}\|0\frac{1}{2}0\}$	9	$\{-1\|0\}$	10	$\{m_{001}\|\frac{1}{2}\frac{1}{2}0\}$
11	$\{m_{100}\|\frac{1}{2}00\}$	12	$\{m_{010}\|0\frac{1}{2}0\}$	13	$\{m_{110}\|\frac{1}{2}\frac{1}{2}0\}$	14	$\{m_{1-10}\|0\}$	15	$\{-4^{+}_{001}\|\frac{1}{2}00\}$
16	$\{-4^{-}_{001}\|0\frac{1}{2}0\}$								

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

	1	2_{001}	2_{100}	2_{110}	4^{+}_{001}	-1	m_{001}	m_{100}	m_{110}	-4^{+}_{001}
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	-1	-1	1	1	1	-1	-1	1
B_{1g}	1	1	1	-1	-1	1	1	1	-1	-1
B_{2g}	1	1	-1	1	-1	1	1	-1	1	-1
E_g	2	-2	0	0	0	2	-2	0	0	0
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	-1	-1	1	-1	-1	1	1	-1
B_{1u}	1	1	1	-1	-1	-1	-1	-1	1	1
B_{2u}	1	1	-1	1	-1	-1	-1	1	-1	1
E_u	2	-2	0	0	0	-2	2	0	0	0

Table 13: Parity conversion.

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

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

	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_g	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_u
A_{1g}	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_g	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_u
A_{2g}		A_{1g}	B_{2g}	B_{1g}	E_g	A_{2u}	A_{1u}	B_{2u}	B_{1u}	E_u
B_{1g}			A_{1g}	A_{2g}	E_g	B_{1u}	B_{2u}	A_{1u}	A_{2u}	E_u
B_{2g}				A_{1g}	E_g	B_{2u}	B_{1u}	A_{2u}	A_{1u}	E_u
E_g					$A_{1g} + B_{1g} + B_{2g}$	E_u	E_u	E_u	E_u	$A_{1u} + A_{2u} + B_{1u} + B_{2u}$
A_{1u}						A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_g
A_{2u}							A_{1g}	B_{2g}	B_{1g}	E_g
B_{1u}								A_{1g}	A_{2g}	E_g
B_{2u}									A_{1g}	E_g
E_u										$A_{1g} + B_{1g} + B_{2g}$

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

A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_g	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_u
–	–	–	–	A_{2g}	–	–	–	–	A_{2g}

Table 16: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix}2 & 1 & 1\end{pmatrix}$	2	$\begin{pmatrix}-2 & -1 & 1\end{pmatrix}$	3	$\begin{pmatrix}2 & -1 & -1\end{pmatrix}$	4	$\begin{pmatrix}-2 & 1 & -1\end{pmatrix}$
5	$\begin{pmatrix}1 & 2 & -1\end{pmatrix}$	6	$\begin{pmatrix}-1 & -2 & -1\end{pmatrix}$	7	$\begin{pmatrix}-1 & 2 & 1\end{pmatrix}$	8	$\begin{pmatrix}1 & -2 & 1\end{pmatrix}$
9	$\begin{pmatrix}-2 & -1 & -1\end{pmatrix}$	10	$\begin{pmatrix}2 & 1 & -1\end{pmatrix}$	11	$\begin{pmatrix}-2 & 1 & 1\end{pmatrix}$	12	$\begin{pmatrix}2 & -1 & 1\end{pmatrix}$
13	$\begin{pmatrix}-1 & -2 & 1\end{pmatrix}$	14	$\begin{pmatrix}1 & 2 & 1\end{pmatrix}$	15	$\begin{pmatrix}1 & -2 & -1\end{pmatrix}$	16	$\begin{pmatrix}-1 & 2 & -1\end{pmatrix}$

Table 17: Virtual-cluster basis.

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_{0}^{(A_{1g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$				
$\mathbb{Q}_{1}^{(A_{2u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$				
$\mathbb{Q}_{1,0}^{(E_{u})}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$
	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$				
$\mathbb{Q}_{1,1}^{(E_{u})}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$
	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$				
$\mathbb{Q}_{2}^{(B_{1g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$				
$\mathbb{Q}_{2}^{(B_{2g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$				
$\mathbb{Q}_{2,0}^{(E_{g})}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$
	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$				
$\mathbb{Q}_{2,1}^{(E_{g})}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$
	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$				
$\mathbb{Q}_{3}^{(B_{1u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$				

continued ...

Table 17

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_{3}^{(B_{2u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$				
$\mathbb{Q}_{3,0}^{(E_{u},1)}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$
	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$				
$\mathbb{Q}_{3,1}^{(E_{u},1)}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$
	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$				
$\mathbb{Q}_{4}^{(A_{2g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$				
$\mathbb{Q}_{4,0}^{(E_{g},1)}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$
	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$				
$\mathbb{Q}_{4,1}^{(E_{g},1)}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$
	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$				
$\mathbb{Q}_{5}^{(A_{1u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$				