

# 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**
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- Unit cell:
  - $a = 4.1972$ ,  $b = 4.1972$ ,  $c = 9.6906$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 90.0$
- Lattice vectors:
  - $\mathbf{a}_1 = (4.1972 \ 0 \ 0)$
  - $\mathbf{a}_2 = (0 \ 4.1972 \ 0)$
  - $\mathbf{a}_3 = (0 \ 0 \ 9.6906)$

Table 1: High-symmetry line:  $\Gamma$ -X.

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

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- 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	$d_u@Pt1_1$
16	$d_v@Pt1_1$	17	$d_{yz}@Pt1_1$	18	$d_{zx}@Pt1_1$	19	$d_{xy}@Pt1_1$	20	$d_u@Pt1_2$
21	$d_v@Pt1_2$	22	$d_{yz}@Pt1_2$	23	$d_{zx}@Pt1_2$	24	$d_{xy}@Pt1_2$	25	$d_u@Pt2_1$
26	$d_v@Pt2_1$	27	$d_{yz}@Pt2_1$	28	$d_{zx}@Pt2_1$	29	$d_{xy}@Pt2_1$	30	$d_u@Pt2_2$
31	$d_v@Pt2_2$	32	$d_{yz}@Pt2_2$	33	$d_{zx}@Pt2_2$	34	$d_{xy}@Pt2_2$	35	$p_x@Si1_1$
36	$p_y@Si1_1$	37	$p_z@Si1_1$	38	$p_x@Si1_2$	39	$p_y@Si1_2$	40	$p_z@Si1_2$
41	$p_x@Si2_1$	42	$p_y@Si2_1$	43	$p_z@Si2_1$	44	$p_x@Si2_2$	45	$p_y@Si2_2$
46	$p_z@Si2_2$								

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S <sub>1</sub> [2c: 4mm]	U <sub>1</sub>	$\begin{pmatrix} \frac{1}{4} & \frac{1}{4} & 0.7484 \end{pmatrix}$	[1,2,7,8,11,12,13,14]
	U <sub>2</sub>	$\begin{pmatrix} \frac{3}{4} & \frac{3}{4} & 0.2516 \end{pmatrix}$	[3,4,5,6,9,10,15,16]
S <sub>2</sub> [2a: -4m2]	Pt1 <sub>1</sub>	$\begin{pmatrix} \frac{3}{4} & \frac{1}{4} & 0 \end{pmatrix}$	[1,2,5,6,11,12,15,16]
	Pt1 <sub>2</sub>	$\begin{pmatrix} \frac{1}{4} & \frac{3}{4} & 0 \end{pmatrix}$	[3,4,7,8,9,10,13,14]
S <sub>3</sub> [2c: 4mm]	Pt2 <sub>1</sub>	$\begin{pmatrix} \frac{1}{4} & \frac{1}{4} & 0.3785 \end{pmatrix}$	[1,2,7,8,11,12,13,14]
	Pt2 <sub>2</sub>	$\begin{pmatrix} \frac{3}{4} & \frac{3}{4} & 0.6215 \end{pmatrix}$	[3,4,5,6,9,10,15,16]
S <sub>4</sub> [2b: -4m2]	Si1 <sub>1</sub>	$\begin{pmatrix} \frac{3}{4} & \frac{1}{4} & \frac{1}{2} \end{pmatrix}$	[1,2,5,6,11,12,15,16]
	Si1 <sub>2</sub>	$\begin{pmatrix} \frac{1}{4} & \frac{3}{4} & \frac{1}{2} \end{pmatrix}$	[3,4,7,8,9,10,13,14]
S <sub>5</sub> [2c: 4mm]	Si2 <sub>1</sub>	$\begin{pmatrix} \frac{1}{4} & \frac{1}{4} & 0.133 \end{pmatrix}$	[1,2,7,8,11,12,13,14]
	Si2 <sub>2</sub>	$\begin{pmatrix} \frac{3}{4} & \frac{3}{4} & 0.867 \end{pmatrix}$	[3,4,5,6,9,10,15,16]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	$n$	#	$\mathbf{b@c}$	mapping
B <sub>1</sub> [8i: .m.]	b <sub>1</sub>	Si2 <sub>1</sub>	Pt1 <sub>1</sub>	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 <sub>2</sub>	Si2 <sub>1</sub>	Pt1 <sub>1</sub>	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 <sub>3</sub>	Si2 <sub>2</sub>	Pt1 <sub>2</sub>	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 <sub>4</sub>	Si2 <sub>2</sub>	Pt1 <sub>2</sub>	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 <sub>5</sub>	Si2 <sub>2</sub>	Pt1 <sub>1</sub>	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 <sub>6</sub>	Si2 <sub>2</sub>	Pt1 <sub>1</sub>	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 <sub>7</sub>	Si2 <sub>1</sub>	Pt1 <sub>2</sub>	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 <sub>8</sub>	Si2 <sub>1</sub>	Pt1 <sub>2</sub>	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 <sub>2</sub> [8i: .m.]	b <sub>9</sub>	Si1 <sub>1</sub>	Pt2 <sub>1</sub>	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 <sub>10</sub>	Si1 <sub>1</sub>	Pt2 <sub>1</sub>	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 <sub>11</sub>	Si1 <sub>2</sub>	Pt2 <sub>2</sub>	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 <sub>12</sub>	Si1 <sub>2</sub>	Pt2 <sub>2</sub>	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 <sub>13</sub>	Si1 <sub>1</sub>	Pt2 <sub>2</sub>	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 <sub>14</sub>	Si1 <sub>1</sub>	Pt2 <sub>2</sub>	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 <sub>15</sub>	Si1 <sub>2</sub>	Pt2 <sub>1</sub>	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 <sub>16</sub>	Si1 <sub>2</sub>	Pt2 <sub>1</sub>	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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 5: Atomic SAMB group.

group	bra	ket
M <sub>1</sub>	$f_{xyz}, f_{ax}, f_{ay}, f_{az}, f_{bx}, f_{by}, f_{bz}$	$f_{xyz}, f_{ax}, f_{ay}, f_{az}, f_{bx}, f_{by}, f_{bz}$
M <sub>2</sub>	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$
M <sub>3</sub>	$p_x, p_y, p_z$	$p_x, p_y, p_z$
M <sub>4</sub>	$p_x, p_y, p_z$	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$

Table 6: Atomic SAMB.

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

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	$A_{2u}$	—	—	$\frac{z(3x^2+3y^2-2z^2)}{2}$
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	$\frac{x(2x^2-3y^2-3z^2)}{2}$
9	$\mathbb{Q}_{3,1}^{(E_u,1)}$	3	$E_u$	1	1	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
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	—	$\sqrt{21}(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4)$
13	$\mathbb{Q}_4^{(A_{1g},2)}$	4	$A_{1g}$	2	—	$-\frac{6}{\sqrt{15}}(x^4-12x^2y^2+6x^2z^2+y^4+6y^2z^2-2z^4)$
14	$\mathbb{Q}_6^{(A_{1g},1)}$	6	$A_{1g}$	1	—	$\frac{12}{\sqrt{2}}(2x^6-15x^4y^2-15x^4z^2-15x^2y^4+180x^2y^2z^2-15x^2z^4+2y^6-15y^4z^2-15y^2z^4+2z^6)$
15	$\mathbb{Q}_6^{(A_{1g},2)}$	6	$A_{1g}$	2	—	$-\frac{8}{\sqrt{14}}(x^6-15x^4z^2+15x^2z^4+y^6-15y^4z^2+15y^2z^4-2z^6)$

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
$\{\mathbf{m}_{100} \frac{1}{2}00\}$	$\{\mathbf{m}_{100} \frac{1}{2}00\}, \{\mathbf{m}_{010} 0\frac{1}{2}0\}$
$\{\mathbf{m}_{110} \frac{1}{2}\frac{1}{2}0\}$	$\{\mathbf{m}_{110} \frac{1}{2}\frac{1}{2}0\}, \{\mathbf{m}_{1-10} 0\}$
$\{-4_{001}^+ \frac{1}{2}00\}$	$\{-4_{001}^+ \frac{1}{2}00\}, \{-4_{001}^- 0\frac{1}{2}0\}$

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	$\{\mathbf{m}_{001} \frac{1}{2}\frac{1}{2}0\}$
11	$\{\mathbf{m}_{100} \frac{1}{2}00\}$	12	$\{\mathbf{m}_{010} 0\frac{1}{2}0\}$	13	$\{\mathbf{m}_{110} \frac{1}{2}\frac{1}{2}0\}$	14	$\{\mathbf{m}_{1-10} 0\}$	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	$\mathbf{m}_{001}$	$\mathbf{m}_{100}$	$\mathbf{m}_{110}$	$-4_{001}^+$
$A_{1g}$	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
$\mathbb{Q}_3^{(B_{2u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
$\mathbb{Q}_{3,0}^{(E_u,1)}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
$\mathbb{Q}_{3,1}^{(E_u,1)}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$
$\mathbb{Q}_4^{(A_{2g})}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$
$\mathbb{Q}_{4,0}^{(E_g,1)}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$
$\mathbb{Q}_{4,1}^{(E_g,1)}$	$-\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
$\mathbb{Q}_5^{(A_{1u})}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$