SAMB for "CeCoSi"

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

 - time-reversal type: electric
 - irrep: [A1g]
 - spinful
- Unit cell:

$$a=4.057,\ b=4.057,\ c=6.987,\ \alpha=90.0,\ \beta=90.0,\ \gamma=90.0$$

• Lattice vectors:

$$\boldsymbol{a}_1 = \begin{pmatrix} 4.057 & 0 & 0 \end{pmatrix}$$

$$\mathbf{a}_2 = \begin{pmatrix} 0 & 4.057 & 0 \end{pmatrix}$$

$$a_3 = (0 \quad 0 \quad 6.987)$$

Table 1: High-symmetry line: Γ -X.

symbol	position	n	symbol	position		
Γ	$\begin{pmatrix} 0 & 0 \end{pmatrix}$	0)	X	$\left(\frac{1}{2}\right)$	0	0)

• Kets: dimension = 36

Table 2: Hilbert space for full matrix.

No	. ket	No.	ket	No.	ket	No.	ket	No.	ket
1	(p_x,\uparrow) @Ce ₁	2	(p_x,\downarrow) @Ce ₁	3	(p_y,\uparrow) @Ce ₁	4	(p_y,\downarrow) @Ce ₁	5	(p_z,\uparrow) @Ce ₁
6	(p_z,\downarrow) @Ce ₁	7	(p_x,\uparrow) @Ce ₂	8	(p_x,\downarrow) @Ce ₂	9	(p_y,\uparrow) @Ce ₂	10	(p_y,\downarrow) @Ce ₂
11	(p_z,\uparrow) @Ce ₂	12	(p_z,\downarrow) @Ce ₂	13	(p_x,\uparrow) @Co ₁	14	(p_x,\downarrow) @Co ₁	15	(p_y,\uparrow) @Co ₁
16	(p_y,\downarrow) @Co ₁	17	(p_z,\uparrow) @Co ₁	18	(p_z,\downarrow) @Co ₁	19	(p_x,\uparrow) @Co ₂	20	(p_x,\downarrow) @Co ₂
21	(p_y,\uparrow) @Co ₂	22	(p_y,\downarrow) @Co ₂	23	(p_z,\uparrow) @Co ₂	24	(p_z,\downarrow) @Co ₂	25	(p_x,\uparrow) @Si ₁
26	(p_x,\downarrow) @Si ₁	27	(p_y,\uparrow) @Si ₁	28	(p_y,\downarrow) @Si ₁	29	(p_z,\uparrow) @Si ₁	30	(p_z,\downarrow) @Si ₁
31	(p_x,\uparrow) @Si ₂	32	(p_x,\downarrow) @Si ₂	33	(p_y,\uparrow) @Si ₂	34	(p_y,\downarrow) @Si ₂	35	(p_z,\uparrow) @Si ₂
36	(p_z,\downarrow) @Si ₂								

• Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S ₁ [2c: 4mm]	Ce_1	$\begin{pmatrix} \frac{1}{4} & \frac{1}{4} & 0.678 \end{pmatrix}$	[1,2,7,8,11,12,13,14]
	Ce_2	$\begin{array}{ c c c c }\hline \begin{pmatrix} \frac{3}{4} & \frac{3}{4} & 0.322 \end{pmatrix}$	[3,4,5,6,9,10,15,16]
S ₂ [2a: -4m2]	Co_1	$\begin{pmatrix} \frac{1}{4} & \frac{3}{4} & 0 \end{pmatrix}$	[1,2,5,6,11,12,15,16]
	Co_2	$\left(\begin{array}{ccc} \frac{3}{4} & \frac{1}{4} & 0 \end{array}\right)$	[3,4,7,8,9,10,13,14]
S ₃ [2c: 4mm]	Si_1	$\begin{pmatrix} \frac{1}{4} & \frac{1}{4} & 0.178 \end{pmatrix}$	[1,2,7,8,11,12,13,14]
	Si_2	$ \left(\frac{3}{4} \frac{3}{4} 0.822 \right) $	[3,4,5,6,9,10,15,16]

 $\bullet\,$ Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	b@c	mapping
B ₁ [8i: .m.]	b ₁	Co_1	Ce_1	1	1	$\left(0 -\frac{1}{2} 0.322\right) @ \left(\frac{1}{4} 0 0.839\right)$	[1,11]
	b_2	Co_1	Ce_1	1	1	$\left(0 \frac{1}{2} 0.322\right) @ \left(\frac{1}{4} \frac{1}{2} 0.839\right)$	[2,12]
	b_3	Co_2	Ce_2	1	1	$ \begin{pmatrix} 0 & \frac{1}{2} & -0.322 \end{pmatrix} @ \begin{pmatrix} \frac{3}{4} & 0 & 0.161 \end{pmatrix} $	[3,9]
	b_4	Co_2	Ce_2	1	1	$ \begin{pmatrix} 0 & -\frac{1}{2} & -0.322 \end{pmatrix} @ \begin{pmatrix} \frac{3}{4} & \frac{1}{2} & 0.161 \end{pmatrix} $	[4,10]
	b_5	Co ₁	Ce_2	1	1	$ \begin{pmatrix} -\frac{1}{2} & 0 & -0.322 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{3}{4} & 0.161 \end{pmatrix} $	[5,15]
	b_6	Co_1	Ce_2	1	1	$\left(\begin{array}{cccc} \left(\frac{1}{2} & 0 & -0.322\right) & \left(\begin{array}{cccc} 0 & \frac{3}{4} & 0.161\end{array}\right) \end{array}\right)$	[6,16]
	b_7	Co_2	Ce_1	1	1	$\left(\begin{array}{cccccccccccccccccccccccccccccccccccc$	[7,13]
	b_8	Co_2	Ce_1	1	1	$\left(-\frac{1}{2} 0 0.322 \right) @ \left(0 \frac{1}{4} 0.839 \right)$	[8,14]
B ₂ [8j:m]	b ₉	Si_2	Ce_1	1	1	$\left(-\frac{1}{2} -\frac{1}{2} 0.144\right) @ \left(0 0 \frac{3}{4}\right)$	[1,14]
	b_{10}	Si_2	Ce_1	1	1	$\left(\begin{array}{cccccccccccccccccccccccccccccccccccc$	[2,13]
	b_{11}	Si_1	Ce_2	1	1	$\begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & -0.144 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{4} \end{pmatrix}$	[3,15]
	b_{12}	Si_1	Ce_2	1	1	$\left(\begin{array}{cccc} \frac{1}{2} & -\frac{1}{2} & -0.144 \end{array}\right) @ \left(\begin{array}{cccc} 0 & \frac{1}{2} & \frac{1}{4} \end{array}\right)$	[4,16]
	b_{13}	Si_1	Ce_2	1	1	$\left(\begin{array}{cccc} -\frac{1}{2} & -\frac{1}{2} & -0.144 \end{array} \right) @ \left(\begin{array}{cccc} \frac{1}{2} & \frac{1}{2} & \frac{1}{4} \end{array} \right)$	[5,10]
	b_{14}	Si_1	Ce_2	1	1	$\left(\begin{array}{cccccccccccccccccccccccccccccccccccc$	[6,9]
	b_{15}	Si_2	Ce_1	1	1	$\left(\begin{array}{cccc} \frac{1}{2} & -\frac{1}{2} & 0.144 \end{array}\right) @ \left(\begin{array}{cccc} \frac{1}{2} & 0 & \frac{3}{4} \end{array}\right)$	[7,11]
	b_{16}	Si_2	Ce_1	1	1	$\left(-\frac{1}{2} \frac{1}{2} 0.144\right) @ \left(0 \frac{1}{2} \frac{3}{4}\right)$	[8,12]
B ₃ [8i: .m.]	b ₁₇	Si_1	Co_1	1	1	$\left(0 \frac{1}{2} 0.178\right) @ \left(\frac{1}{4} 0 0.089\right)$	[1,11]
	b_{18}	Si_1	Co_1	1	1	$\begin{pmatrix} 0 & -\frac{1}{2} & 0.178 \end{pmatrix} @ \begin{pmatrix} \frac{1}{4} & \frac{1}{2} & 0.089 \end{pmatrix}$	[2,12]
	b_{19}	Si_2	Co_2	1	1	$\left(\begin{array}{cccccccccccccccccccccccccccccccccccc$	[3,9]
	b_{20}	Si_2	Co_2	1	1	$\left(0 \frac{1}{2} -0.178\right)^{\circ} \left(\frac{3}{4} \frac{1}{2} 0.911\right)^{\circ}$	[4,10]
	b_{21}	Si_2	Co_1	1	1	$\left(\begin{array}{cccc} \frac{1}{2} & 0 & -0.178 \end{array}\right) @ \left(\begin{array}{cccc} \frac{1}{2} & \frac{3}{4} & 0.911 \end{array}\right)$	[5,15]
	b_{22}	Si_2	Co_1	1	1	$\left(\begin{array}{cccc} -\frac{1}{2} & 0 & -0.178 \end{array} \right) @ \left(\begin{array}{ccccc} 0 & \frac{3}{4} & 0.911 \end{array} \right)$	[6,16]
	b_{23}	Si_1	Co_2	1	1	$\left(\begin{array}{cccccccccccccccccccccccccccccccccccc$	[7,13]
	b_{24}	Si_1	Co_2	1	1	$\left(\begin{array}{cccc} \left(\frac{1}{2} & 0 & 0.178\right) & \left(\begin{array}{cccc} 0 & \frac{1}{4} & 0.089\end{array}\right) \end{array}\right)$	[8,14]

No. 1
$$\hat{\mathbb{Q}}_0^{(A_{1g})}$$
 [M₁, S₁]

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

No. 2
$$\hat{\mathbb{Q}}_2^{(A_{1g})}$$
 [M₁, S₁]

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

No. 3
$$\hat{\mathbb{Q}}_0^{(A_{1g})}(1,1)$$
 [M₁, S₁]

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

No. 4
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$$
 [M₁, S₁]

$$\hat{\mathbb{Z}}_4 = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_{1g})}(1,-1)] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A_{1g})}]$$

No. 5
$$\hat{\mathbb{Q}}_0^{(A_{1g})}$$
 [M₁, S₂]

$$\hat{\mathbb{Z}}_5 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s,A_{1g})}]$$

$$\begin{tabular}{|c|c|c|c|c|}\hline No. \ 6 & \hat{\mathbb{Q}}_2^{(A_{1g})} \ [M_1,S_2] \\ \hline \end{tabular}$$

$$\hat{\mathbb{Z}}_6 = \mathbb{X}_2[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s,A_{1g})}]$$

No. 7
$$\hat{\mathbb{Q}}_0^{(A_{1g})}(1,1) [M_1, S_2]$$

$$\hat{\mathbb{Z}}_7 = \mathbb{X}_3[\mathbb{Q}_0^{(a,A_{1g})}(1,1)] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s,A_{1g})}]$$

No. 8
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$$
 [M₁, S₂]

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

No. 9
$$\hat{\mathbb{Q}}_0^{(A_{1g})}$$
 [M₁, S₃]

$$\hat{\mathbb{Z}}_9 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(s, A_{1g})}]$$

No. 10
$$\hat{\mathbb{Q}}_{2}^{(A_{1g})}$$
 [M₁, S₃]

$$\hat{\mathbb{Z}}_{10} = \mathbb{X}_2[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(s,A_{1g})}]$$

No. 11
$$\hat{\mathbb{Q}}_0^{(A_{1g})}(1,1)$$
 [M₁, S₃]

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

No. 12
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$$
 [M₁, S₃]

$$\hat{\mathbb{Z}}_{12} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_{1g})}(1,-1)] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(s,A_{1g})}]$$

No. 13
$$\hat{\mathbb{Q}}_0^{(A_{1g})}$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{13} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_{1g})}]$$

No. 14
$$\hat{\mathbb{Q}}_{2}^{(A_{1g})}$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{14} = \mathbb{X}_2[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_{1g})}]$$

No. 15
$$\hat{\mathbb{Q}}_0^{(A_{1g})}$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{15} = \frac{\sqrt{3}\mathbb{X}_{5}[\mathbb{Q}_{2}^{(a,B_{1g})}] \otimes \mathbb{Y}_{5}[\mathbb{Q}_{2}^{(b,B_{1g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{7}[\mathbb{Q}_{2,0}^{(a,E_{g})}] \otimes \mathbb{Y}_{6}[\mathbb{Q}_{2,0}^{(b,E_{g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{8}[\mathbb{Q}_{2,1}^{(a,E_{g})}] \otimes \mathbb{Y}_{7}[\mathbb{Q}_{2,1}^{(b,E_{g})}]}{3}$$

No. 16
$$\hat{\mathbb{Q}}_{2}^{(A_{1g})}$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{16} = -\frac{\sqrt{6}\mathbb{X}_{5}[\mathbb{Q}_{2}^{(a,B_{1g})}] \otimes \mathbb{Y}_{5}[\mathbb{Q}_{2}^{(b,B_{1g})}]}{3} + \frac{\sqrt{6}\mathbb{X}_{7}[\mathbb{Q}_{2,0}^{(a,E_{g})}] \otimes \mathbb{Y}_{6}[\mathbb{Q}_{2,0}^{(b,E_{g})}]}{6} + \frac{\sqrt{6}\mathbb{X}_{8}[\mathbb{Q}_{2,1}^{(a,E_{g})}] \otimes \mathbb{Y}_{7}[\mathbb{Q}_{2,1}^{(b,E_{g})}]}{6}$$

No. 17
$$\hat{\mathbb{Q}}_0^{(A_{1g})}(1,1)$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{17} = \mathbb{X}_{3}[\mathbb{Q}_{0}^{(a,A_{1g})}(1,1)] \otimes \mathbb{Y}_{4}[\mathbb{Q}_{0}^{(b,A_{1g})}]$$

No. 18
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{18} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_{1g})}(1,-1)] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_{1g})}]$$

No. 19
$$\hat{\mathbb{Q}}_0^{(A_{1g})}(1,-1)$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{19} = \frac{\sqrt{3}\mathbb{X}_{11}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{6}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{7}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{9}[\mathbb{Q}_{2}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{5}[\mathbb{Q}_{2}^{(b,B_{1g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{9}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{9}[\mathbb{Q}_{2,1}^{(b,E_g)}(1,-1)]}{3} + \frac{\sqrt{3}\mathbb{X}_{9}[\mathbb{Q}_{2,1}^{(b,E_g)}(1,-1)] \otimes \mathbb{Y}_{9}[\mathbb{Q}_{2,1}^{(b,E_g)}(1,-1)]}{3} + \frac{\sqrt{3}\mathbb{X}_{9}[\mathbb{Q}_{2,1}^{(b,E_g)}(1,-1)]}{3} + \frac{\sqrt{3}\mathbb{X}_{9}[\mathbb{Q}_{2,1}^{(b,E_g)}(1,-1)]}{3} + \frac{\sqrt{3}\mathbb{X$$

No. 20
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{20} = \frac{\sqrt{6}\mathbb{X}_{11}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{6}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{7}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{6}\mathbb{X}_{9}[\mathbb{Q}_{2}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{5}[\mathbb{Q}_{2}^{(b,B_{1g})}]}{3} + \frac{\sqrt{6}\mathbb{X}_{9}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{9}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)]}{6} + \frac{\sqrt{6}\mathbb{X}_{9}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)]}{6} + \frac{\sqrt{6}\mathbb{X}_{9}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)]}{6} + \frac{\sqrt{6}\mathbb{X$$

No. 21
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0)$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{21} = \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{G}_{1,0}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{6}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{14}[\mathbb{G}_{1,1}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{7}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{2}$$

No. 22
$$\hat{\mathbb{Q}}_2^{(A_{1g})}$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{22} = \frac{\sqrt{2}\mathbb{X}_{15}[\mathbb{M}_{1,0}^{(a,E_g)}] \otimes \mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{16}[\mathbb{M}_{1,1}^{(a,E_g)}] \otimes \mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 23
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,1)$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{23} = \frac{\sqrt{2}\mathbb{X}_{17}[\mathbb{M}_{1,0}^{(a,E_g)}(1,1)] \otimes \mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{M}_{1,1}^{(a,E_g)}(1,1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 24
$$\hat{\mathbb{Q}}_{2}^{(A_{1g})}(1,-1)$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{24} = \frac{\sqrt{2}\mathbb{X}_{19}[\mathbb{M}_{1,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{20}[\mathbb{M}_{1,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 25
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$$
 [M₁, B₁]

$$\begin{split} \hat{\mathbb{Z}}_{25} &= -\frac{\sqrt{3}\mathbb{X}_{21}[\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)] \otimes \mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{3}\mathbb{X}_{22}[\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{5}\mathbb{X}_{23}[\mathbb{M}_{3,0}^{(a,E_g,2)}(1,-1)] \otimes \mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} \\ &+ \frac{\sqrt{5}\mathbb{X}_{24}[\mathbb{M}_{3,1}^{(a,E_g,2)}(1,-1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{5}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{9}[\mathbb{T}_{2}^{(b,B_{1g})}]}{3} \end{split}$$

No. 26
$$\hat{\mathbb{Q}}_4^{(A_{1g},1)}(1,-1)$$
 [M₁, B₁]

$$\begin{split} \hat{\mathbb{Z}}_{26} &= \frac{\sqrt{195}\mathbb{X}_{21}[\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)] \otimes \mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{78} - \frac{\sqrt{195}\mathbb{X}_{22}[\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{78} - \frac{\sqrt{13}\mathbb{X}_{23}[\mathbb{M}_{3,0}^{(a,E_g,2)}(1,-1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} \\ &+ \frac{\sqrt{13}\mathbb{X}_{24}[\mathbb{M}_{3,1}^{(a,E_g,2)}(1,-1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} + \frac{5\sqrt{13}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{9}[\mathbb{T}_{2}^{(b,B_{1g})}]}{39} \end{split}$$

No. 27
$$\hat{\mathbb{Q}}_{4}^{(A_{1g},2)}(1,-1)$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{27} = -\frac{\sqrt{65}\mathbb{X}_{21}[\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{13} + \frac{\sqrt{65}\mathbb{X}_{22}[\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)]\otimes\mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{13} + \frac{\sqrt{39}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g})}(1,-1)]\otimes\mathbb{Y}_{9}[\mathbb{T}_{2}^{(b,B_{1g})}]}{13} + \frac{\sqrt{39}\mathbb{X}_{10}[\mathbb{T}_{2,1}^{(a,B_{1g})}(1,-1)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,1}^{(b,B_{1g})}]}{13} + \frac{\sqrt{39}\mathbb{X}_{10}[\mathbb{T}_{2,1}^{(b,B_{1g})}(1,-1)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,1}^{(b,B_{1g})}]}{13} + \frac{\sqrt{39}\mathbb{X}_{10}[\mathbb{T}_{2,1}^{(b,B_{1g})}(1,-1)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,1}^{(b,B_{1g})}]}{13} + \frac{\sqrt{39}\mathbb{X}_{10}[\mathbb{T}_{2,1}^{(b,B_{1g})}(1,-1)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,1}^{(b,B_{1g})}]}{13} + \frac{\sqrt{39}\mathbb{X}_{10}[\mathbb{T}_{2,1}^{(b,B_{1g})}(1,-1)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,1}^{(b,B_{1g})}]}{13} + \frac{\sqrt{39}\mathbb{X}_{10}[\mathbb{T}_{2,1}^{(b,B_{1g})}(1,-1)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,1}^{(b,B_{1g})}]}{13} + \frac{\sqrt{39}\mathbb{X}_{10}[\mathbb{T}_{2,1}^{(b,B_{1g})}(1,-1)]\otimes\mathbb{Y}_{10}[\mathbb{T}_{2,1}^{(b,B_{1g})}]}{13} + \frac{\sqrt{39}\mathbb{X}_{10}[\mathbb{T}_{2,1}^{(b,B_{1g})}(1,-1)]\otimes\mathbb{Y}_{10}[\mathbb{T$$

No. 28
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0)$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{28} = \mathbb{X}_{31}[\mathbb{T}_2^{(a,A_{1g})}(1,0)] \otimes \mathbb{Y}_8[\mathbb{T}_0^{(b,A_{1g})}]$$

No. 29
$$\hat{\mathbb{Q}}_0^{(A_{1g})}(1,0)$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{29} = \frac{\sqrt{3}\mathbb{X}_{25}[\mathbb{T}_{2,0}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{T}_{2,1}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{28}[\mathbb{T}_{2}^{(a,B_{1g})}(1,0)] \otimes \mathbb{Y}_{9}[\mathbb{T}_{2}^{(b,B_{1g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{28}[\mathbb{T}_{2}^{(b,B_{1g})}(1,0)] \otimes \mathbb{Y}_{9}[\mathbb{T}_{2}^{(b,B_{1g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{28}$$

No. 30
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0)$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{30} = \frac{\sqrt{6}\mathbb{X}_{25}[\mathbb{T}_{2,0}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{10}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_{26}[\mathbb{T}_{2,1}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{11}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{6}\mathbb{X}_{28}[\mathbb{T}_{2}^{(a,B_{1g})}(1,0)] \otimes \mathbb{Y}_{9}[\mathbb{T}_{2}^{(b,B_{1g})}]}{3} - \frac{\sqrt{6}\mathbb{X}_{28}[\mathbb{T}_{2}^{(a,B_{1g})}(1,0)] \otimes \mathbb{Y}_{9}[\mathbb{T}_{2}^{(a,B_{1g})}]}{3} - \frac{\sqrt{6}\mathbb{X}_{28}$$

No. 31
$$\hat{\mathbb{Q}}_0^{(A_{1g})}$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{31} = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_0^{(b,A_{1g})}]$$

No. 32
$$\hat{\mathbb{Q}}_{2}^{(A_{1g})}$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{32} = \mathbb{X}_2[\mathbb{Q}_2^{(a, A_{1g})}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_0^{(b, A_{1g})}]$$

No. 33
$$\hat{\mathbb{Q}}_0^{(A_{1g})}$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{33} = \frac{\sqrt{3}\mathbb{X}_{6}[\mathbb{Q}_{2}^{(a,B_{2g})}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_{2}^{(b,B_{2g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{7}[\mathbb{Q}_{2,0}^{(a,E_{g})}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b,E_{g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{8}[\mathbb{Q}_{2,1}^{(a,E_{g})}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{8}[\mathbb{Q}_{2,1}^{(b,E_{g})}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}]}{3} + \frac{\sqrt{3}\mathbb{Z}_{8}[\mathbb{Q}_{2,1}^{(b,E_{g})}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}]}{3} + \frac{\sqrt{3}\mathbb{Z}_{8}[\mathbb{Q}_{2,1}^{(b,E_{g})}] \otimes \mathbb{Z}_{8}[\mathbb{Q}_{2,1}^{(b,E_{g})}]}{3} + \frac{\sqrt{3}\mathbb{Z}_{8}[\mathbb{Q}_{2,1}^{(b,E_{g})}] \otimes \mathbb{Z}_{8}[\mathbb{Q}_{2,1}^{(b,E_{g})}]}{3} + \frac{\sqrt{3}\mathbb{Z}_{8}[\mathbb{Q}_{2,1}^{(b,E_{g})}]}{3} + \frac{\sqrt{3}\mathbb{Z}_{8}[\mathbb{Q}_{2,1}^{(b,E_{g})}]}{3} +$$

No. 34
$$\hat{\mathbb{Q}}_{2}^{(A_{1g})}$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{34} = -\frac{\sqrt{6}\mathbb{X}_{6}[\mathbb{Q}_{2}^{(a,B_{2g})}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_{2}^{(b,B_{2g})}]}{3} + \frac{\sqrt{6}\mathbb{X}_{7}[\mathbb{Q}_{2,0}^{(a,E_{g})}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b,E_{g})}]}{6} + \frac{\sqrt{6}\mathbb{X}_{8}[\mathbb{Q}_{2,1}^{(a,E_{g})}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}]}{6}$$

No. 35
$$\hat{\mathbb{Q}}_0^{(A_{1g})}(1,1)$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{35} = \mathbb{X}_3[\mathbb{Q}_0^{(a, A_{1g})}(1, 1)] \otimes \mathbb{Y}_{12}[\mathbb{Q}_0^{(b, A_{1g})}]$$

No. 36
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{36} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_{1g})}(1,-1)] \otimes \mathbb{Y}_{12}[\mathbb{Q}_0^{(b,A_{1g})}]$$

No. 37
$$\hat{\mathbb{Q}}_0^{(A_{1g})}(1,-1)$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{37} = \frac{\sqrt{3}\mathbb{X}_{10}[\mathbb{Q}_{2}^{(a,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{13}[\mathbb{Q}_{2}^{(b,B_{2g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{11}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)]\otimes\mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(b,E_g)}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(b,E_g)}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2$$

No. 38
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{38} = -\frac{\sqrt{6}\mathbb{X}_{10}[\mathbb{Q}_{2}^{(a,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{13}[\mathbb{Q}_{2}^{(b,B_{2g})}]}{3} + \frac{\sqrt{6}\mathbb{X}_{11}[\mathbb{Q}_{2,0}^{(a,E_{g})}(1,-1)]\otimes\mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b,E_{g})}]}{6} + \frac{\sqrt{6}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}]}{6} + \frac{\sqrt{6}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}]}{6} + \frac{\sqrt{6}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(b,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_{g})}(1,-1)]\otimes\mathbb{Y}_{15$$

No. 39
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0)$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{39} = \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{G}_{1,0}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{14}[\mathbb{G}_{1,1}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{2}$$

No. 40
$$\hat{\mathbb{Q}}_{2}^{(A_{1g})}$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{40} = \frac{\sqrt{2}\mathbb{X}_{15}[\mathbb{M}_{1,0}^{(a,E_g)}] \otimes \mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{16}[\mathbb{M}_{1,1}^{(a,E_g)}] \otimes \mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 41
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,1)$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{41} = \frac{\sqrt{2}\mathbb{X}_{17}[\mathbb{M}_{1,0}^{(a,E_g)}(1,1)] \otimes \mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{M}_{1,1}^{(a,E_g)}(1,1)] \otimes \mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 42
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{42} = \frac{\sqrt{2}\mathbb{X}_{19}[\mathbb{M}_{1,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{20}[\mathbb{M}_{1,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 43
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$$
 [M₁, B₂]

$$\begin{split} \hat{\mathbb{Z}}_{43} &= -\frac{\sqrt{3}\mathbb{X}_{21}[\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)] \otimes \mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{3}\mathbb{X}_{22}[\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)] \otimes \mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{5}\mathbb{X}_{23}[\mathbb{M}_{3,0}^{(a,E_g,2)}(1,-1)] \otimes \mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} \\ &+ \frac{\sqrt{5}\mathbb{X}_{24}[\mathbb{M}_{3,1}^{(a,E_g,2)}(1,-1)] \otimes \mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} + \frac{\sqrt{5}\mathbb{X}_{29}[\mathbb{M}_{3}^{(a,B_{2g})}(1,-1)] \otimes \mathbb{Y}_{17}[\mathbb{T}_{2}^{(b,B_{2g})}]}{3} \end{split}$$

No. 44
$$\hat{\mathbb{Q}}_{4}^{(A_{1g},1)}(1,-1)$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{44} = -\frac{\sqrt{3}\mathbb{X}_{23}[\mathbb{M}_{3,0}^{(a,E_g,2)}(1,-1)]\otimes\mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{24}[\mathbb{M}_{3,1}^{(a,E_g,2)}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{3} - \frac{\sqrt{3}\mathbb{X}_{29}[\mathbb{M}_{3}^{(a,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{17}[\mathbb{T}_{2}^{(b,B_{2g})}]}{3} - \frac{\sqrt{3}\mathbb{X}_{29}[\mathbb{M}_{3}^{(a,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}]}{3} - \frac{\sqrt{3}\mathbb{X}_{29}[\mathbb{M}_{3}^{(a,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}]}{3} - \frac{\sqrt{3}\mathbb{X}_{29}[\mathbb{M}_{3}^{(a,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}]}{3} - \frac{\sqrt{3}\mathbb{X}_{29}[\mathbb{M}_{3}^{(a,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}]}{3} - \frac{\sqrt{3}\mathbb{X}_{29}[\mathbb{M}_{3}^{(a,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}]}{3} - \frac{\sqrt{3}\mathbb{X}_{29}[\mathbb{M}_{3}^{(a,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}]}{3} - \frac{\mathbb{X}_{29}[\mathbb{M}_{3}^{(a,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}]}{3} - \frac{\mathbb{X}_{29}[\mathbb{M}_{3}^{(a,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{M}_{3}^{(a,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,B_{2g})$$

No. 45
$$\hat{\mathbb{Q}}_4^{(A_{1g},2)}(1,-1)$$
 [M₁, B₂]

$$\begin{split} \hat{\mathbb{Z}}_{45} &= -\frac{\sqrt{15}\mathbb{X}_{21}[\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)]\otimes\mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{15}\mathbb{X}_{22}[\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} \\ &+ \frac{\mathbb{X}_{23}[\mathbb{M}_{3,0}^{(a,E_g,2)}(1,-1)]\otimes\mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} - \frac{\mathbb{X}_{24}[\mathbb{M}_{3,1}^{(a,E_g,2)}(1,-1)]\otimes\mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} - \frac{\mathbb{X}_{29}[\mathbb{M}_{3}^{(a,B_{2g})}(1,-1)]\otimes\mathbb{Y}_{17}[\mathbb{T}_{2}^{(b,B_{2g})}]}{3} \end{split}$$

No. 46
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0)$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{46} = \mathbb{X}_{31}[\mathbb{T}_2^{(a,A_{1g})}(1,0)] \otimes \mathbb{Y}_{16}[\mathbb{T}_0^{(b,A_{1g})}]$$

No. 47
$$\hat{\mathbb{Q}}_0^{(A_{1g})}(1,0)$$
 [M₁, B₂]

$$\hat{\mathbb{Z}}_{47} = \frac{\sqrt{3}\mathbb{X}_{25}[\mathbb{T}_{2,0}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{T}_{2,1}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{30}[\mathbb{T}_{2}^{(a,B_{2g})}(1,0)] \otimes \mathbb{Y}_{17}[\mathbb{T}_{2}^{(b,B_{2g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{30}[\mathbb{T}_{2}^{(a,B_{2g})}(1,0)] \otimes \mathbb{Y}_{3}[\mathbb{T}_{2}^{(b,B_{2g})}(1,0)]}{3} + \frac{\sqrt{3}\mathbb{X}_{30}[\mathbb{T}_{2}^{(a,B_{2g})}(1,0)] \otimes \mathbb{Y}_{3}[\mathbb{T}_{2}^{(b,B_{2g})}(1,0)]}{3} + \frac{\sqrt{3}\mathbb{X}_{30}[\mathbb{T}_{2}^{(a,B_{2g})}(1,0)] \otimes \mathbb{Y}_{3}[\mathbb{T}_{2}^{(b,B_{2g})}(1,0)]}{3} + \frac{\sqrt{3}\mathbb{X}_{30}[\mathbb{T}_{2}^{(b,B_{2g})}(1,0)]}{3} + \frac{\sqrt{3}\mathbb{X}_{30}[\mathbb{T}_{2}^{(b,B_{2g})}(1,0)]}{3$$

No. 48
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0) [M_1, B_2]$$

$$\hat{\mathbb{Z}}_{48} = \frac{\sqrt{6}\mathbb{X}_{25}[\mathbb{T}_{2,0}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{18}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_{26}[\mathbb{T}_{2,1}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{19}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{6}\mathbb{X}_{30}[\mathbb{T}_{2}^{(a,B_{2g})}(1,0)] \otimes \mathbb{Y}_{17}[\mathbb{T}_{2}^{(b,B_{2g})}]}{3}$$

No. 49
$$\hat{\mathbb{Q}}_0^{(A_{1g})}$$
 [M₁, B₃]

$$\hat{\mathbb{Z}}_{49} = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_{20}[\mathbb{Q}_0^{(b, A_{1g})}]$$

No. 50
$$\hat{\mathbb{Q}}_{2}^{(A_{1g})}$$
 [M₁, B₃]

$$\hat{\mathbb{Z}}_{50} = \mathbb{X}_2[\mathbb{Q}_2^{(a,A_{1g})}] \otimes \mathbb{Y}_{20}[\mathbb{Q}_0^{(b,A_{1g})}]$$

No. 51
$$\hat{\mathbb{Q}}_0^{(A_{1g})}$$
 [M₁, B₃]

$$\hat{\mathbb{Z}}_{51} = \frac{\sqrt{3}\mathbb{X}_{5}[\mathbb{Q}_{2}^{(a,B_{1g})}] \otimes \mathbb{Y}_{21}[\mathbb{Q}_{2}^{(b,B_{1g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{7}[\mathbb{Q}_{2,0}^{(a,E_{g})}] \otimes \mathbb{Y}_{22}[\mathbb{Q}_{2,0}^{(b,E_{g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{8}[\mathbb{Q}_{2,1}^{(a,E_{g})}] \otimes \mathbb{Y}_{23}[\mathbb{Q}_{2,1}^{(b,E_{g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{8}[\mathbb{Q}_{2,1}^{(b,E_{g})}] \otimes \mathbb{Y}_{23}[\mathbb{Q}_{2,1}^{(b,E_{g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{8}[\mathbb{Q}_{2,1}^{(b,E_{g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{8}[\mathbb{Q}_{2,1$$

No. 52
$$\hat{\mathbb{Q}}_{2}^{(A_{1g})}$$
 [M₁, B₃]

$$\hat{\mathbb{Z}}_{52} = -\frac{\sqrt{6}\mathbb{X}_{5}[\mathbb{Q}_{2}^{(a,B_{1g})}] \otimes \mathbb{Y}_{21}[\mathbb{Q}_{2}^{(b,B_{1g})}]}{3} + \frac{\sqrt{6}\mathbb{X}_{7}[\mathbb{Q}_{2,0}^{(a,E_{g})}] \otimes \mathbb{Y}_{22}[\mathbb{Q}_{2,0}^{(b,E_{g})}]}{6} + \frac{\sqrt{6}\mathbb{X}_{8}[\mathbb{Q}_{2,1}^{(a,E_{g})}] \otimes \mathbb{Y}_{23}[\mathbb{Q}_{2,1}^{(b,E_{g})}]}{6}$$

No. 53
$$\hat{\mathbb{Q}}_0^{(A_{1g})}(1,1) [M_1, B_3]$$

$$\hat{\mathbb{Z}}_{53} = \mathbb{X}_{3}[\mathbb{Q}_{0}^{(a,A_{1g})}(1,1)] \otimes \mathbb{Y}_{20}[\mathbb{Q}_{0}^{(b,A_{1g})}]$$

No. 54
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$$
 [M₁, B₃]

$$\hat{\mathbb{Z}}_{54} = \mathbb{X}_4[\mathbb{Q}_2^{(a,A_{1g})}(1,-1)] \otimes \mathbb{Y}_{20}[\mathbb{Q}_0^{(b,A_{1g})}]$$

No. 55
$$\hat{\mathbb{Q}}_0^{(A_{1g})}(1,-1)$$
 [M₁, B₃]

$$\hat{\mathbb{Z}}_{55} = \frac{\sqrt{3}\mathbb{X}_{11}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{22}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{23}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{9}[\mathbb{Q}_{2}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{21}[\mathbb{Q}_{2}^{(b,B_{1g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{9}[\mathbb{Q}_{2,1}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{21}[\mathbb{Q}_{2,1}^{(b,B_{1g})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{9}[\mathbb{Q}_{2,1}^{(b,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{21}[\mathbb{Q}_{2,1}^{(b,B_{1g})}]}{3$$

No. 56
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$$
 [M₁, B₃]

$$\hat{\mathbb{Z}}_{56} = \frac{\sqrt{6}\mathbb{X}_{11}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{22}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_{12}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{23}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{6}\mathbb{X}_{9}[\mathbb{Q}_{2}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{21}[\mathbb{Q}_{2}^{(b,B_{1g})}]}{3} - \frac{\sqrt{6}\mathbb{X}_{9}[\mathbb{Q}_{2}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{21}[\mathbb{Q}_{2}^{(b,B_{1g})}(1,-1)]}{3} - \frac{\sqrt{6}\mathbb{X}_{9}[\mathbb{Q}_{2}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{21}[\mathbb{Q}_{2}^{(b,B_{1g})}(1,-1)]}{3} - \frac{\sqrt{6}\mathbb{X}_{9}[\mathbb{Q}_{2}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{21}[\mathbb{Q}_{2}^{(b,B_{1g})}(1,-1)]}{3} - \frac{\sqrt{6}\mathbb{X}_{9}[\mathbb{Q}_{2}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{21}[\mathbb{Q}_{2}^{(b,B_{1g})}(1,-1)]}{3} - \frac{\sqrt{6}\mathbb{X}_{9}[\mathbb{Q}_{2}^{(a,B_{1g})}(1,-1)]}{3} - \frac{\sqrt{6}\mathbb{X}_{9}[\mathbb{Q}_{2}^{(a,B_{1g})}(1,-1)]}{3}$$

No. 57
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0)$$
 [M₁, B₃]

$$\hat{\mathbb{Z}}_{57} = \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{G}_{1,0}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{22}[\mathbb{Q}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{14}[\mathbb{G}_{1,1}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{23}[\mathbb{Q}_{2,1}^{(b,E_g)}]}{2}$$

No. 58
$$\hat{\mathbb{Q}}_{2}^{(A_{1g})}$$
 [M₁, B₃]

$$\hat{\mathbb{Z}}_{58} = \frac{\sqrt{2}\mathbb{X}_{15}[\mathbb{M}_{1,0}^{(a,E_g)}] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{16}[\mathbb{M}_{1,1}^{(a,E_g)}] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 59
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,1)$$
 [M₁, B₃]

$$\hat{\mathbb{Z}}_{59} = \frac{\sqrt{2}\mathbb{X}_{17}[\mathbb{M}_{1,0}^{(a,E_g)}(1,1)] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{M}_{1,1}^{(a,E_g)}(1,1)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 60
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$$
 [M₁, B₃]

$$\hat{\mathbb{Z}}_{60} = \frac{\sqrt{2}\mathbb{X}_{19}[\mathbb{M}_{1,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{2} - \frac{\sqrt{2}\mathbb{X}_{20}[\mathbb{M}_{1,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{2}$$

No. 61
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,-1)$$
 [M₁, B₃]

$$\begin{split} \hat{\mathbb{Z}}_{61} &= -\frac{\sqrt{3}\mathbb{X}_{21}[\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{3}\mathbb{X}_{22}[\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{5}\mathbb{X}_{23}[\mathbb{M}_{3,0}^{(a,E_g,2)}(1,-1)] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} \\ &+ \frac{\sqrt{5}\mathbb{X}_{24}[\mathbb{M}_{3,1}^{(a,E_g,2)}(1,-1)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{5}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{25}[\mathbb{T}_{2}^{(b,B_{1g})}]}{3} \end{split}$$

No. 62
$$\hat{\mathbb{Q}}_4^{(A_{1g},1)}(1,-1)$$
 [M₁, B₃]

$$\hat{\mathbb{Z}}_{62} = \frac{\sqrt{195}\mathbb{X}_{21}[\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}}{78} - \frac{\sqrt{195}\mathbb{X}_{22}[\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}}{78} - \frac{\sqrt{13}\mathbb{X}_{23}[\mathbb{M}_{3,0}^{(a,E_g,2)}(1,-1)] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}}{6} + \frac{\sqrt{13}\mathbb{X}_{24}[\mathbb{M}_{3,1}^{(a,E_g,2)}(1,-1)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}}{6} + \frac{5\sqrt{13}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{25}[\mathbb{T}_{2}^{(b,B_{1g})}]}}{39} + \frac{\sqrt{13}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{25}[\mathbb{T}_{2}^{(b,B_{1g})}]}}{39} + \frac{\sqrt{13}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g})}(1,-1)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,B_{1g})}]}}{39} + \frac{\sqrt{13}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g},2)}(1,-1)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,B_{1g})}]}}{6} + \frac{\sqrt{13}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g},2)}(1,-1)] \otimes \mathbb{Y}_{27}[\mathbb{M}_{3}^{(a,B_{1g},2)}(1,-1)]}}{6} + \frac{\sqrt{13}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g},2)}(1,-1)] \otimes \mathbb{Y}_{27}[\mathbb{M}_{3}^{(a,B_{1g},2)}(1,-1)]}}{6} + \frac{\sqrt{13}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g},2)}(1,-1)]}{6} + \frac{\sqrt{13}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g},2)}(1,-1)]}{6} + \frac{\sqrt{13}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g},2)}(1,-1)]}{6} + \frac{\sqrt{13}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_$$

No. 63
$$\hat{\mathbb{Q}}_{4}^{(A_{1g},2)}(1,-1)$$
 [M₁, B₃]

$$\hat{\mathbb{Z}}_{63} = -\frac{\sqrt{65}\mathbb{X}_{21}[\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)]\otimes\mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{13} + \frac{\sqrt{65}\mathbb{X}_{22}[\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)]\otimes\mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{13} + \frac{\sqrt{39}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g})}(1,-1)]\otimes\mathbb{Y}_{25}[\mathbb{T}_{2}^{(b,B_{1g})}]}{13} + \frac{\sqrt{39}\mathbb{X}_{27}[\mathbb{M}_{3}^{(a,B_{1g})}(1,-1)]\otimes\mathbb{Y}_{$$

No. 64
$$\hat{\mathbb{Q}}_{2}^{(A_{1g})}(1,0)$$
 [M₁, B₃]
 $\hat{\mathbb{Z}}_{64} = \mathbb{X}_{31}[\mathbb{T}_{2}^{(a,A_{1g})}(1,0)] \otimes \mathbb{Y}_{24}[\mathbb{T}_{0}^{(b,A_{1g})}]$

No. 65
$$\hat{\mathbb{Q}}_0^{(A_{1g})}(1,0)$$
 [M₁, B₃]

$$\hat{\mathbb{Z}}_{65} = \frac{\sqrt{3}\mathbb{X}_{25}[\mathbb{T}_{2,0}^{(a,E_g)}(1,0)]\otimes\mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{T}_{2,1}^{(a,E_g)}(1,0)]\otimes\mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{28}[\mathbb{T}_{2}^{(a,B_{1g})}(1,0)]\otimes\mathbb{Y}_{25}[\mathbb{T}_{2}^{(b,B_{1g})}]}{3}$$

No. 66
$$\hat{\mathbb{Q}}_2^{(A_{1g})}(1,0)$$
 [M₁, B₃]

$$\hat{\mathbb{Z}}_{66} = \frac{\sqrt{6}\mathbb{X}_{25}[\mathbb{T}_{2,0}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{26}[\mathbb{T}_{2,0}^{(b,E_g)}]}{6} + \frac{\sqrt{6}\mathbb{X}_{26}[\mathbb{T}_{2,1}^{(a,E_g)}(1,0)] \otimes \mathbb{Y}_{27}[\mathbb{T}_{2,1}^{(b,E_g)}]}{6} - \frac{\sqrt{6}\mathbb{X}_{28}[\mathbb{T}_{2}^{(a,B_{1g})}(1,0)] \otimes \mathbb{Y}_{25}[\mathbb{T}_{2}^{(b,B_{1g})}]}{3}$$

Table 5: Atomic SAMB group.

group	bra	ket
M_1	$(p_x,\uparrow),(p_x,\downarrow),(p_y,\uparrow),(p_y,\downarrow),(p_z,\uparrow),(p_z,\downarrow)$	$(p_x,\uparrow),(p_x,\downarrow),(p_y,\uparrow),(p_y,\downarrow),(p_z,\uparrow),(p_z,\downarrow)$

Table 6: Atomic SAMB.

symbol	type	group	form
\mathbb{X}_1	$\mathbb{Q}_0^{(a,A_{1g})}$	$ m M_1$	$\begin{pmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \end{pmatrix}$

Table 6

symbol	type	group	form
\mathbb{X}_2	$\mathbb{Q}_2^{(a,A_{1g})}$	M_1	$\begin{pmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0\\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0\\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0\\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0\\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0\\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{X}_3	$\mathbb{Q}_0^{(a,A_{1g})}(1,1)$	$ m M_1$	$ \begin{pmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \end{pmatrix} $
\mathbb{X}_4	$\mathbb{Q}_2^{(a,A_{1g})}(1,-1)$	$ m M_1$	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_5	$\mathbb{Q}_2^{(a,B_{1g})}$	M_1	$ \begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 &$
\mathbb{X}_6	$\mathbb{Q}_2^{(a,B_{2g})}$	$ m M_1$	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0$

continued ...

Table 6

symbol	typo	group	form
	type $\mathbb{Q}_{2,0}^{(a,E_g)}$	group M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 &$
\mathbb{X}_8	$\mathbb{Q}_{2,1}^{(a,E_g)}$	$ m M_1$	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0$
\mathbb{X}_9	$\mathbb{Q}_2^{(a,B_{1g})}(1,-1)$	$ m M_1$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{10}	$\mathbb{Q}_2^{(a,B_{2g})}(1,-1)$	$ m M_1$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{pmatrix}$
X ₁₁	$\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)$	$ m M_1$	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0\\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4}\\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0\\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0\\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0\\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
\mathbb{X}_{12}	$\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)$	$ m M_1$	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0\\ 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0\\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0\\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & \frac{\sqrt{2}i}{4}\\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0\\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0\\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0\\ \end{pmatrix}$
\mathbb{X}_{13}	$\mathbb{G}_{1,0}^{(a,E_g)}(1,0)$	$ m M_1$	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$
\mathbb{X}_{14}	$\mathbb{G}_{1,1}^{(a,E_g)}(1,0)$	$ m M_1$	$\begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0\\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0\\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0\\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4}\\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0\\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{pmatrix}$
\mathbb{X}_{15}	$\mathbb{M}_{1,0}^{(a,E_g)}$	$ m M_1$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 &$
\mathbb{X}_{16}	$\mathbb{M}_{1,1}^{(a,E_g)}$	$ m M_1$	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0$

continued ...

Table 6

Table 6			
symbol	type	group	form
\mathbb{X}_{17}	$\mathbb{M}_{1,0}^{(a,E_g)}(1,1)$	M_1	$ \left(\begin{array}{cccccccccccccccccccccccccccccccccccc$
\mathbb{X}_{18}	$\mathbb{M}_{1,1}^{(a,E_g)}(1,1)$	M_1	$ \begin{bmatrix} \begin{pmatrix} 0 & -\frac{\sqrt{30}}{20} & 0 & 0 & -\frac{\sqrt{30}}{30} & 0 \\ 0 & \frac{\sqrt{30}i}{30} & 0 & \frac{\sqrt{30}}{20} & 0 & 0 \\ -\frac{\sqrt{30}i}{30} & 0 & \frac{\sqrt{30}}{20} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{15} & \frac{\sqrt{30}}{20} & 0 \\ \frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{15} & 0 & 0 & -\frac{\sqrt{30}}{20} \\ 0 & 0 & \frac{\sqrt{30}}{20} & 0 & 0 & \frac{\sqrt{30}i}{30} \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{20} & -\frac{\sqrt{30}i}{30} & 0 \end{bmatrix} $
\mathbb{X}_{19}	$\mathbb{M}_{1,0}^{(a,E_g)}(1,-1)$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \end{pmatrix}$
\mathbb{X}_{20}	$\mathbb{M}_{1,1}^{(a,E_g)}(1,-1)$	M_1	$\begin{pmatrix} 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0\\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0\\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6}\\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \end{pmatrix}$
\mathbb{X}_{21}	$\mathbb{M}_{3,0}^{(a,E_g,1)}(1,-1)$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{5}}{5} & 0 & \frac{\sqrt{5}i}{10} & -\frac{\sqrt{5}}{10} & 0\\ \frac{\sqrt{5}}{5} & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & \frac{\sqrt{5}}{10}\\ 0 & \frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0\\ -\frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0\\ -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{10}\\ 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \end{pmatrix}$

Table 6

Table 6			
symbol	type	group	form
\mathbb{X}_{22}	$\mathbb{M}_{3,1}^{(a,E_g,1)}(1,-1)$	$ m M_1$	$ \begin{pmatrix} 0 & \frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0\\ -\frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0\\ 0 & -\frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{5} & -\frac{\sqrt{5}}{10} & 0\\ -\frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{5} & 0 & 0 & \frac{\sqrt{5}}{10}\\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & \frac{\sqrt{5}i}{10}\\ 0 & 0 & 0 & \frac{\sqrt{5}}{10} & -\frac{\sqrt{5}i}{10} & 0 \end{pmatrix} $ $ \begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} & 0\\ 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \end{pmatrix} $
\mathbb{X}_{23}	$\mathbb{M}_{3,0}^{(a,E_g,2)}(1,-1)$	M_1	$\begin{bmatrix} 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ -\frac{\sqrt{3}}{3} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{3} \end{bmatrix}$
\mathbb{X}_{24}	$\mathbb{M}_{3,1}^{(a,E_g,2)}(1,-1)$	M_1	$\begin{pmatrix} 6 & \sqrt{3} & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \\ 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \end{pmatrix}$ $\begin{pmatrix} 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}i}{6} & 0 \end{pmatrix}$
\mathbb{X}_{25}	$\mathbb{T}_{2,0}^{(a,E_g)}(1,0)$	M_1	$ \begin{pmatrix} 0 & 0 & -\frac{6}{6} & 0 & 0 & -\frac{6}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}i}{6} & 0 \end{pmatrix} $ $ \begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \end{pmatrix} $
\mathbb{X}_{26}	$\mathbb{T}_{2,1}^{(a,E_g)}(1,0)$	M_1	$\begin{pmatrix} 12 & 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}i}{6} & 0 \end{pmatrix}$

Table 6

symbol	4		form
Symbol	type	group	
\mathbb{X}_{27}	$\mathbb{M}_{3}^{(a,B_{1g})}(1,-1)$	$ m M_1$	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & \frac{\sqrt{6}}{12} & 0 \end{pmatrix}$
\mathbb{X}_{28}	$\mathbb{T}_{2}^{(a,B_{1g})}(1,0)$	$ m M_1$	$ \left[\begin{array}{cccccccccccccccccccccccccccccccccccc$
\mathbb{X}_{29}	$\mathbb{M}_{3}^{(a,B_{2g})}(1,-1)$	$ m M_1$	$ \begin{bmatrix} 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{bmatrix} $
\mathbb{X}_{30}	$\mathbb{T}_{2}^{(a,B_{2g})}(1,0)$	M_1	$\begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}t}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ 0 & -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{bmatrix}$
\mathbb{X}_{31}	$\mathbb{T}_2^{(a,A_{1g})}(1,0)$	$ m M_1$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
$\frac{\mathbb{Y}_1}{\mathbb{Y}_1}$	$\mathbb{Q}_0^{(s,A_{1g})}$	S_1	$\begin{pmatrix} \sqrt{2} & \sqrt{2} \\ 2 & 2 \end{pmatrix}$
\mathbb{Y}_2	$\mathbb{Q}_0^{(s,A_{1g})}$	S_2	$\left(\frac{\sqrt{2}}{2} \frac{\sqrt{2}}{2}\right)$
\mathbb{Y}_3	\bigcirc (s, A_{1g})	S_3	$\left(\begin{array}{cc} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{array}\right)$
\mathbb{Y}_4	$\mathbb{Q}_0^{(b,A_{1g})}$	B_1	$ \begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} \end{pmatrix} $
\mathbb{Y}_5	$\mathbb{Q}_2^{(b,B_{1g})}$	B_1	$\left(\frac{\sqrt{2}}{4} \frac{\sqrt{2}}{4} \frac{\sqrt{2}}{4} \frac{\sqrt{2}}{4} -\frac{\sqrt{2}}{4} -\frac{\sqrt{2}}{4} -\frac{\sqrt{2}}{4} -\frac{\sqrt{2}}{4}\right)$
\mathbb{Y}_6	$\mathbb{Q}_{2,0}^{(b,E_g)}$	B_1	
\mathbb{Y}_7	\bigcap (b, E_g)	B_1	$\begin{pmatrix} 0 & 0 & 0 & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$
\mathbb{Y}_8	$\mathbb{T}_0^{(b,A_{1g})}$	B_1	$\left(\begin{array}{cccc} \sqrt{2}i & \sqrt{2}i \end{array}\right)$
\mathbb{Y}_9	$\mathbb{T}_2^{(b,B_{1g})}$	B_1	$\begin{pmatrix} 4 & 4 & 4 & 4 & 4 & 4 & 4 & 4 & 4 \\ \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} \end{pmatrix}$
\mathbb{Y}_{10}	$\mathbb{T}_{2,0}^{(b,E_g)}$	B_1	$\left(egin{array}{cccccccccccccccccccccccccccccccccccc$
\mathbb{Y}_{11}	$\mathbb{T}_{2,1}^{(b,E_g)}$	B_1	$\left(egin{matrix} 0 & 0 & 0 & -rac{i}{2} & rac{i}{2} & -rac{i}{2} & rac{i}{2} \end{matrix} ight)$
\mathbb{Y}_{12}	$\mathbb{Q}_0^{(b,A_{1g})}$	B_2	$ \begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} \end{pmatrix} $
\mathbb{Y}_{13}	$\mathbb{Q}_2^{(b,B_{2g})}$	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} & \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} & \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}_{14}	$\mathbb{Q}_{2,0}^{(b,E_g)}$	B_2	$\left(\frac{\sqrt{2}}{4} - \frac{\sqrt{2}}{4} \frac{\sqrt{2}}{4} - \frac{\sqrt{2}}{4} - \frac{\sqrt{2}}{4} \frac{\sqrt{2}}{4} \frac{\sqrt{2}}{4} - \frac{\sqrt{2}}{4} \right)$
\mathbb{Y}_{15}	$\mathbb{Q}_{2,1}^{(b,E_g)}$	B_2	$\left(egin{array}{cccccc} rac{\sqrt{2}}{4} & -rac{\sqrt{2}}{4} & -rac{\sqrt{2}}{4} & rac{\sqrt{2}}{4} & -rac{\sqrt{2}}{4} & rac{\sqrt{2}}{4} & -rac{\sqrt{2}}{4} \end{array} ight)$
\mathbb{Y}_{16}	$\mathbb{T}_0^{(b,A_{1g})}$	B_2	$\begin{pmatrix} \sqrt{2}i & \sqrt{2}i \end{pmatrix}$
\mathbb{Y}_{17}	$\mathbb{T}_2^{(b,B_{2g})}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} \end{pmatrix}$
\mathbb{Y}_{18}	$\mathbb{T}_{2,0}^{(b,E_g)}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} \end{pmatrix}$
\mathbb{Y}_{19}	$\mathbb{T}_{2,1}^{(b,E_g)}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} \\ \left(\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} \\ & & & & & & & & & & & & \\ \begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} \\ & & & & & & & & & & & \\ \end{pmatrix} & \begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} \\ & & & & & & & & & \\ \end{pmatrix}$
\mathbb{Y}_{20}	$\mathbb{Q}_0^{(b,A_{1g})}$	B_3	$ \begin{pmatrix} \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} \end{pmatrix} $ $ \begin{pmatrix} \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} \end{pmatrix} $ $ \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} \end{pmatrix} $
\mathbb{Y}_{21}	$\mathbb{Q}_2^{(b,B_{1g})}$	B_3	$\left(\begin{array}{cccccccccccccccccccccccccccccccccccc$
\mathbb{Y}_{22}	$\mathbb{Q}_{2,0}^{(b,E_g)}$	B_3	$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{Y}_{23}	$\mathbb{Q}_{2,1}^{(b,E_g)}$	B_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$
\mathbb{Y}_{24}	$\mathbb{T}_0^{(b,A_{1g})}$	B_3	$\begin{pmatrix} \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} \end{pmatrix}$
\mathbb{Y}_{25}	$\mathbb{T}_2^{(b,B_{1g})}$	B_3	$\left(\frac{\sqrt{2}i}{4} \frac{\sqrt{2}i}{4} \frac{\sqrt{2}i}{4} \frac{\sqrt{2}i}{4} -\frac{\sqrt{2}i}{4} -\frac{\sqrt{2}i}{4} -\frac{\sqrt{2}i}{4} -\frac{\sqrt{2}i}{4} \right)$
\mathbb{Y}_{26}	$\mathbb{T}_{2,0}^{(b,E_g)}$	B_3	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} & 0 & 0 & 0 & 0 \\ & \frac{i}{2} & \frac{i}{2} & \frac{i}{2} & -\frac{i}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{Y}_{27}	$\mathbb{T}_{2,1}^{(b,E_g)}$	B_3	$\begin{pmatrix} 0 & 0 & 0 & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} \end{pmatrix}$

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	$\mathbb{Q}_2^{(B_{1g})}$	2	B_{1g}	_	_	$-\frac{2}{2} - \frac{2}{2} + 2$ $\frac{\sqrt{3}(x-y)(x+y)}{2}$
4	$\mathbb{Q}_2^{(B_{2g})}$	2	B_{2g}	_	_	$\sqrt{3}xy$
5	$\mathbb{Q}_{2,0}^{(E_g)}$	2	E_g	_	0	$\sqrt{3}yz$
6	$\mathbb{Q}_{2,1}^{(E_g)}$	2	E_g	_	1	$\sqrt{3}xz$

Table 9: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_{1,0}^{(E_g)}$	1	E_g	-	0	X
2	$\mathbb{G}_{1,1}^{(E_g)}$	1	E_g	_	1	Y
3	$\mathbb{G}_3^{(B_{1g})}$	3	B_{1g}	_	_	$\sqrt{15}XYZ$
4	$\mathbb{G}_3^{(B_{2g})}$	3	B_{2g}	_	_	$\frac{\sqrt{15}Z(X-Y)(X+Y)}{2}$
5	$\mathbb{G}_{3,0}^{(E_g,1)}$	3	E_g	1	0	$\frac{X(2X^2-3Y^2-3Z^2)}{2}$
6	$\mathbb{G}_{3,1}^{(E_g,1)}$	3	E_g	1	1	$-\frac{Y(3X^2-2Y^2+3Z^2)}{2}$
7	$\mathbb{C}^{(E_g,2)}$	3	E_g	2	0	$\frac{\sqrt{15}X(Y-Z)(Y+Z)}{2}$
- 8	$\mathbb{G}^{3,0}_{3,1}$	3	E_g	2	1	$\frac{\sqrt{15}Y(X-Z)(X+Z)}{2}$

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

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

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

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	2001	2100	2110	4 ⁺ ₀₀₁	-1	m ₀₀₁	m ₁₀₀	m ₁₁₀	-4^{+}_{001}
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2q}	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

Table 12

	1	2001	2100	2110	4 ⁺ ₀₀₁	-1	m ₀₀₁	m ₁₀₀	m ₁₁₀	-4^{+}_{001}
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}	$E_{m{g}}$
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
$\mathbb{Q}_0^{(A_{1g})}$	$\frac{1}{4}$	$\frac{1}{4}$								
	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$				
$\mathbb{Q}_1^{(A_{2u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$				
$\mathbb{Q}_{1,0}^{(E_u)}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$
	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$				
$\mathbb{Q}_{1,1}^{(E_u)}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$
	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$				
$\mathbb{Q}_2^{(B_{1g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$				

Table 17

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_2^{(B_{2g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$				
$\mathbb{Q}_{2,0}^{(E_g)}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$
	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$				
$\mathbb{Q}_{2,1}^{(E_g)}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$
	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$				
$\mathbb{Q}_3^{(B_{1u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$				
$\mathbb{Q}_3^{(B_{2u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$				
$\mathbb{Q}_{3,0}^{(E_u,1)}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$
	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$				
$\mathbb{Q}_{3,1}^{(E_u,1)}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$
	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$				
$\mathbb{Q}_4^{(A_{2g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$				
$\mathbb{Q}_{4,0}^{(E_g,1)}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$
	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$				
$\mathbb{Q}_{4,1}^{(E_g,1)}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$
	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$				
$\mathbb{Q}_{5}^{(A_{1u})}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$							
	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$				