SAMB for "MoS2"

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- Generation condition
 - model type: tight_binding
 - time-reversal type: electric
 - irrep: [A1']
 - spinless
- Unit cell:

$$a=3.1661,\ b=3.1661,\ c=20.0,\ \alpha=90.0,\ \beta=90.0,\ \gamma=120.0$$

• Lattice vectors:

$$a_1 = \begin{pmatrix} 3.1661 & 0 & 0 \end{pmatrix}$$

$$a_2 = \begin{pmatrix} -1.58305 & 2.74192303092191 & 0 \end{pmatrix}$$

$$\boldsymbol{a}_3 = \begin{pmatrix} 0 & 0 & 20.0 \end{pmatrix}$$

Table 1: High-symmetry line: Γ -M-K- Γ -K'.

symbol	position	symbol	position	symbol	position
Г К'	$ \begin{pmatrix} 0 & 0 & 0 \\ -\frac{1}{3} & -\frac{1}{3} & 0 \end{pmatrix} $	М	$\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	K	$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & 0 \end{pmatrix}$

• Kets: dimension = 11

Table 2: Hilbert space for full matrix.

No.	ket	No.	ket	No.	ket	No.	ket	No.	ket
1	$d_u@\mathrm{Mo}_1$	2	$d_v@\mathrm{Mo}_1$	3	$d_{yz}@\mathrm{Mo}_1$	4	$d_{zx}@\mathrm{Mo}_1$	5	$d_{xy}@\mathrm{Mo}_1$
6	$p_x@S_1$	7	$p_y@S_1$	8	$p_z@S_1$	9	$p_x@S_2$	10	$p_y@\mathrm{S}_2$
 11	$p_z@S_2$								

• Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S_1	Mo_1	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,2,3,4,5,6,7,8,9,10,11,12]
S_2	S_1	$\left(\frac{2}{3} \frac{1}{3} 0.12425\right)$	[1,5,6,7,8,9]
	S_2	$\left(\begin{array}{ccc} \frac{2}{3} & \frac{1}{3} & 0.87575 \end{array}\right)$	[2,3,4,10,11,12]

• Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	b@c	mapping
B_1	b_1	Mo_1	Mo_1	1	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[1,-3,-8,10]
	b_2	Mo_1	Mo_1	1	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[2,-5,7,-12]
	b_3	Mo_1	Mo_1	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[-4,6,-9,11]
B_2	b_4	S_1	Mo_1	1	1	$\left(\begin{array}{cccc} \frac{2}{3} & \frac{1}{3} & 0.12425 \end{array}\right) @ \left(\begin{array}{cccc} \frac{1}{3} & \frac{1}{6} & 0.062125 \end{array}\right)$	[1,8]
	b_5	S_2	Mo_1	1	1	$\left(-\frac{1}{3} \frac{1}{3} -0.12425\right) @ \left(\frac{5}{6} \frac{1}{6} 0.937875\right)$	[2,12]
	b_6	S_2	Mo_1	1	1	$\left(\begin{array}{cccccccccccccccccccccccccccccccccccc$	[3,10]
	b ₇	S_2	Mo_1	1	1	$\left(-\frac{1}{3} -\frac{2}{3} -0.12425\right)$ @ $\left(\frac{5}{6} \frac{2}{3} 0.937875\right)$	[4,11]

Table 4

	bond	tail	head	n	#	b@c	mapping
	b_8	S_1	Mo_1	1	1	$\left(-\frac{1}{3} \frac{1}{3} 0.12425\right) @ \left(\frac{5}{6} \frac{1}{6} 0.062125\right)$	[5,7]
	b_9	S_1	Mo_1	1	1	$\left(-\frac{1}{3} - \frac{2}{3} 0.12425\right)$ @ $\left(\frac{5}{6} \frac{2}{3} 0.062125\right)$	[6,9]
B_3	b ₁₀	S_1	S_1	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & \frac{1}{3} & 0.12425 \end{pmatrix}$	[1,-7]
	b_{11}	S_2	S_2	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & \frac{1}{3} & 0.87575 \end{pmatrix}$	[-2,10]
	b_{12}	S_2	S_2	1	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & \frac{5}{6} & 0.87575 \end{pmatrix}$	[3,-11]
	b_{13}	S_2	S_2	1	1	$(0 1 0) @ (\frac{2}{3} \frac{5}{6} 0.87575)$	[-4,12]
	b_{14}	S_1	S_1	1	1	$(0 1 0) @ (\frac{2}{3} \frac{5}{6} 0.12425)$	[5,-9]
	b_{15}	S_1	S_1	1	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & \frac{5}{6} & 0.12425 \end{pmatrix}$	[-6,8]

• SAMB:

No. 1
$$\hat{\mathbb{Q}}_0^{(A_1')}$$
 [M₁, S₁]

$$\hat{\mathbb{Z}}_1 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1')}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A_1')}]$$

$$\hat{\mathbb{Z}}_1(\boldsymbol{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1')}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_1')}]$$

No. 2
$$\hat{\mathbb{Q}}_2^{(A_1')}$$
 [M₁, S₁]

$$\hat{\mathbb{Z}}_2 = \mathbb{X}_2[\mathbb{Q}_2^{(a,A_1')}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A_1')}]$$

$$\hat{\mathbb{Z}}_2(\boldsymbol{k}) = \mathbb{X}_2[\mathbb{Q}_2^{(a,A_1')}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_1')}]$$

No. 3
$$\hat{\mathbb{Q}}_{4}^{(A_{1}')}$$
 [M₁, S₁]

$$\hat{\mathbb{Z}}_3 = \mathbb{X}_3[\mathbb{Q}_4^{(a,A_1')}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A_1')}]$$

$$\hat{\mathbb{Z}}_3(\boldsymbol{k}) = \mathbb{X}_3[\mathbb{Q}_4^{(a,A_1')}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_1')}]$$

No. 4
$$\hat{\mathbb{Q}}_0^{(A_1')}$$
 [M₂, S₂]

$$\hat{\mathbb{Z}}_4 = \mathbb{X}_{14}[\mathbb{Q}_0^{(a,A_1')}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s,A_1')}]$$

$$\hat{\mathbb{Z}}_4(\boldsymbol{k}) = \mathbb{X}_{14}[\mathbb{Q}_0^{(a,A_1')}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A_1')}]$$

No. 5
$$\hat{\mathbb{Q}}_{2}^{(A_{1}')}$$
 [M₂, S₂]

$$\hat{\mathbb{Z}}_5 = \mathbb{X}_{15}[\mathbb{Q}_2^{(a,A_1')}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s,A_1')}]$$

$$\hat{\mathbb{Z}}_5(\boldsymbol{k}) = \mathbb{X}_{15}[\mathbb{Q}_2^{(a,A_1')}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A_1')}]$$

No. 6
$$\hat{\mathbb{Q}}_0^{(A_1')}$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_6 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1')}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A_1')}]$$

$$\hat{\mathbb{Z}}_6(\boldsymbol{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1')}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_1')}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_1')}]$$

No. 7
$$\hat{\mathbb{Q}}_2^{(A_1')}$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_7 = \mathbb{X}_2[\mathbb{Q}_2^{(a,A_1')}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A_1')}]$$

$$\hat{\mathbb{Z}}_7(\boldsymbol{k}) = \mathbb{X}_2[\mathbb{Q}_2^{(a,A_1')}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_1')}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_1')}]$$

No. 8
$$\hat{\mathbb{Q}}_3^{(A_1')}$$
 [M₁, B₁]

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

$$\hat{\mathbb{Z}}_{8}(\boldsymbol{k}) = -\frac{\sqrt{2}\mathbb{X}_{4}[\mathbb{Q}_{2,0}^{(a,E')}] \otimes \mathbb{U}_{1}[\mathbb{Q}_{0}^{(s,A'_{1})}] \otimes \mathbb{F}_{2}[\mathbb{Q}_{1,0}^{(k,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{5}[\mathbb{Q}_{2,1}^{(a,E')}] \otimes \mathbb{U}_{1}[\mathbb{Q}_{0}^{(s,A'_{1})}] \otimes \mathbb{F}_{3}[\mathbb{Q}_{1,1}^{(k,E')}]}{2}$$

No. 9
$$\hat{\mathbb{Q}}_4^{(A_1')}$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_9 = \mathbb{X}_3[\mathbb{Q}_4^{(a,A_1')}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b,A_1')}]$$

$$\hat{\mathbb{Z}}_9(\mathbf{k}) = \mathbb{X}_3[\mathbb{Q}_4^{(a,A_1')}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_1')}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_1')}]$$

No. 10
$$\hat{\mathbb{Q}}_{3}^{(A_{1}')}$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{10} = \frac{\sqrt{406}\mathbb{X}_{6}[\mathbb{Q}_{4,0}^{(a,E',1)}] \otimes \mathbb{Y}_{4}[\mathbb{Q}_{1,0}^{(b,E')}]}{29} + \frac{\sqrt{406}\mathbb{X}_{7}[\mathbb{Q}_{4,1}^{(a,E',1)}] \otimes \mathbb{Y}_{5}[\mathbb{Q}_{1,1}^{(b,E')}]}{29} + \frac{\sqrt{58}\mathbb{X}_{8}[\mathbb{Q}_{4,0}^{(a,E',2)}] \otimes \mathbb{Y}_{4}[\mathbb{Q}_{1,0}^{(b,E')}]}{58} + \frac{\sqrt{58}\mathbb{X}_{9}[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{Y}_{5}[\mathbb{Q}_{1,1}^{(b,E')}]}{58} + \frac{\sqrt{58}\mathbb{X}_{9}[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{Y}_{4}[\mathbb{Q}_{1,0}^{(a,E',2)}]}{58} + \frac{\sqrt{58}\mathbb{X}_{9}[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{Y}_{5}[\mathbb{Q}_{1,1}^{(b,E')}]}{58} + \frac{\sqrt{58}\mathbb{X}_{9}[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{Y}_{4}[\mathbb{Q}_{1,0}^{(a,E',2)}]}{58} + \frac{\sqrt{58}\mathbb{X}_{9}[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{Y}_{4}[\mathbb{Q}_{1,0}^{(a,E',2)}]}{58} + \frac{\sqrt{58}\mathbb{X}_{9}[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{Y}_{4}[\mathbb{Q}_{1,0}^{(a,E',2)}]}{58} + \frac{\sqrt{58}\mathbb{X}_{9}[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{Y}_{5}[\mathbb{Q}_{4,1}^{(a,E',2)}]}{58} + \frac{\sqrt{58}\mathbb{X}_{9}[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{Y}_{9}[\mathbb{Q}_{4,1}^{(a,E',2)}]}{58} + \frac{\sqrt{58}\mathbb{X}_{9}[\mathbb{Q}_{4,1}^{(a,E',2)}$$

$$\begin{split} \hat{\mathbb{Z}}_{10}(\boldsymbol{k}) &= \frac{\sqrt{406}\mathbb{X}_{6}[\mathbb{Q}_{4,0}^{(a,E',1)}] \otimes \mathbb{U}_{1}[\mathbb{Q}_{0}^{(s,A'_{1})}] \otimes \mathbb{F}_{2}[\mathbb{Q}_{1,0}^{(k,E')}]}{29} + \frac{\sqrt{406}\mathbb{X}_{7}[\mathbb{Q}_{4,1}^{(a,E',1)}] \otimes \mathbb{U}_{1}[\mathbb{Q}_{0}^{(s,A'_{1})}] \otimes \mathbb{F}_{3}[\mathbb{Q}_{1,1}^{(k,E')}]}{29} \\ &+ \frac{\sqrt{58}\mathbb{X}_{8}[\mathbb{Q}_{4,0}^{(a,E',2)}] \otimes \mathbb{U}_{1}[\mathbb{Q}_{0}^{(s,A'_{1})}] \otimes \mathbb{F}_{2}[\mathbb{Q}_{1,0}^{(k,E')}]}{58} + \frac{\sqrt{58}\mathbb{X}_{9}[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{U}_{1}[\mathbb{Q}_{0}^{(s,A'_{1})}] \otimes \mathbb{F}_{3}[\mathbb{Q}_{1,1}^{(k,E')}]}{58} \end{split}$$

No. 11
$$\hat{\mathbb{G}}_{4}^{(A_{1}')}$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{11} = -\frac{\sqrt{58}\mathbb{X}_{6}[\mathbb{Q}_{4,0}^{(a,E',1)}] \otimes \mathbb{Y}_{4}[\mathbb{Q}_{1,0}^{(b,E')}]}{58} - \frac{\sqrt{58}\mathbb{X}_{7}[\mathbb{Q}_{4,1}^{(a,E',1)}] \otimes \mathbb{Y}_{5}[\mathbb{Q}_{1,1}^{(b,E')}]}{58} + \frac{\sqrt{406}\mathbb{X}_{8}[\mathbb{Q}_{4,0}^{(a,E',2)}] \otimes \mathbb{Y}_{4}[\mathbb{Q}_{1,0}^{(b,E')}]}{29} + \frac{\sqrt{406}\mathbb{X}_{9}[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{Y}_{5}[\mathbb{Q}_{1,1}^{(b,E')}]}{29} + \frac{\sqrt{406}\mathbb{X}_{9}[\mathbb{Q}_{1,0}^{(a,E',2)}] \otimes \mathbb{Y}_{1}[\mathbb{Q}_{1,0}^{(a,E',2)}] \otimes \mathbb{Y}_{2}[\mathbb{Q}_{1,1}^{(a,E',2)}]}{29} + \frac{\sqrt{406}\mathbb{X}_{9}[\mathbb{Q}_{1,0}^{(a,E',2)}] \otimes \mathbb{Y}_{1}[\mathbb{Q}_{1,0}^{(a,E',2)}]}{29} + \frac{\sqrt{406}\mathbb{X}_{9}[\mathbb{Q}_{1,0}^{(a,E',2)}] \otimes \mathbb{Y}_{1}[\mathbb{Q}_{1,0}^{(a,E',2)}]}{29} + \frac{\sqrt{406}\mathbb{X}_{9}[\mathbb{Q}_{1,0}^{(a,E',2)}] \otimes \mathbb{Y}_{1}[\mathbb{Q}_{1,0}^{(a,E',2)}]}{29} + \frac{\sqrt{406}\mathbb{X}_{9}[\mathbb{Q}_{1,0}^{(a,E',2)}] \otimes \mathbb{Y}_{1}[\mathbb{Q}_{1,0}^{(a,E',2)}]}{29} + \frac{\sqrt{406}\mathbb{X}_{9}[\mathbb{Q}_{1,0}^{(a,E',2)}]}{29} + \frac{\sqrt{40$$

$$\begin{split} \hat{\mathbb{Z}}_{11}(\textbf{\textit{k}}) &= -\frac{\sqrt{58}\mathbb{X}_{6}[\mathbb{Q}_{4,0}^{(a,E',1)}] \otimes \mathbb{U}_{1}[\mathbb{Q}_{0}^{(s,A'_{1})}] \otimes \mathbb{F}_{2}[\mathbb{Q}_{1,0}^{(k,E')}]}{58} - \frac{\sqrt{58}\mathbb{X}_{7}[\mathbb{Q}_{4,1}^{(a,E',1)}] \otimes \mathbb{U}_{1}[\mathbb{Q}_{0}^{(s,A'_{1})}] \otimes \mathbb{F}_{3}[\mathbb{Q}_{1,1}^{(k,E')}]}{58} \\ &+ \frac{\sqrt{406}\mathbb{X}_{8}[\mathbb{Q}_{4,0}^{(a,E',2)}] \otimes \mathbb{U}_{1}[\mathbb{Q}_{0}^{(s,A'_{1})}] \otimes \mathbb{F}_{2}[\mathbb{Q}_{1,0}^{(k,E')}]}{29} + \frac{\sqrt{406}\mathbb{X}_{9}[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{U}_{1}[\mathbb{Q}_{0}^{(s,A'_{1})}] \otimes \mathbb{F}_{3}[\mathbb{Q}_{1,1}^{(k,E')}]}{29} \end{split}$$

No. 12
$$\hat{\mathbb{Q}}_3^{(A_1')}$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{12} = \mathbb{X}_{10}[\mathbb{M}_1^{(a,A_2')}] \otimes \mathbb{Y}_{8}[\mathbb{T}_3^{(b,A_2')}]$$

$$\hat{\mathbb{Z}}_{12}(\textbf{\textit{k}}) = \mathbb{X}_{10}[\mathbb{M}_{1}^{(a,A'_{2})}] \otimes \mathbb{U}_{1}[\mathbb{Q}_{0}^{(s,A'_{1})}] \otimes \mathbb{F}_{6}[\mathbb{T}_{3}^{(k,A'_{2})}]$$

No. 13
$$\hat{\mathbb{Q}}_{3}^{(A_{1}')}$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{13} = \frac{\sqrt{2}\mathbb{X}_{12}[\mathbb{M}_{3,0}^{(a,E')}] \otimes \mathbb{Y}_{6}[\mathbb{T}_{1,0}^{(b,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{M}_{3,1}^{(a,E')}] \otimes \mathbb{Y}_{7}[\mathbb{T}_{1,1}^{(b,E')}]}{2}$$

$$\hat{\mathbb{Z}}_{13}(\boldsymbol{k}) = \frac{\sqrt{2}\mathbb{X}_{12}[\mathbb{M}_{3,0}^{(a,E')}] \otimes \mathbb{U}_{1}[\mathbb{Q}_{0}^{(s,A'_{1})}] \otimes \mathbb{F}_{4}[\mathbb{T}_{1,0}^{(k,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{M}_{3,1}^{(a,E')}] \otimes \mathbb{U}_{1}[\mathbb{Q}_{0}^{(s,A'_{1})}] \otimes \mathbb{F}_{5}[\mathbb{T}_{1,1}^{(k,E')}]}{2}$$

No. 14
$$\hat{\mathbb{Q}}_{3}^{(A_{1}')}$$
 [M₁, B₁]

$$\hat{\mathbb{Z}}_{14} = -\mathbb{X}_{11}[\mathbb{M}_3^{(a,A_2')}] \otimes \mathbb{Y}_8[\mathbb{T}_3^{(b,A_2')}]$$

$$\hat{\mathbb{Z}}_{14}(\pmb{k}) = -\mathbb{X}_{11}[\mathbb{M}_3^{(a,A_2')}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_1')}] \otimes \mathbb{F}_6[\mathbb{T}_3^{(k,A_2')}]$$

No. 15 $\hat{\mathbb{Q}}_0^{(A_1')}$ [M₃, B₂]

$$\hat{\mathbb{Z}}_{15} = \frac{\sqrt{3}\mathbb{X}_{23}[\mathbb{Q}_{1}^{(a,A_{2}^{\prime\prime})}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{1}^{(b,A_{2}^{\prime\prime})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{25}[\mathbb{Q}_{1,0}^{(a,E^{\prime})}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E^{\prime})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,E^{\prime})}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E^{\prime})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(b,E^{\prime})}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E^{\prime})}]}{3} + \frac{\sqrt{3}\mathbb{Z}_{26}[\mathbb{Q}_{1,1}^{(b,E^{\prime})}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E^{\prime})}]}{3} + \frac{\sqrt{3}\mathbb{Z}_{26}[\mathbb{Q}_{1,1}^{(b,E^{\prime})}] \otimes \mathbb{Z}_{26}[\mathbb{Q}_{1,1}^{(b,E^{\prime})}]}{3} + \frac{\sqrt{3}\mathbb{Z}_{26}[\mathbb{Q}_{1,1}^{(b,E^{\prime})}]}{3} + \frac{\sqrt{3}\mathbb{Z$$

$$\hat{\mathbb{Z}}_{15}(\textbf{\textit{k}}) = \frac{\sqrt{3}\mathbb{X}_{23}[\mathbb{Q}_{1}^{(a,A_{2}^{\prime\prime})}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{0}^{(u,A_{1}^{\prime})}] \otimes \mathbb{F}_{8}[\mathbb{Q}_{1}^{(k,A_{2}^{\prime\prime})}]}{6} + \frac{\sqrt{3}\mathbb{X}_{23}[\mathbb{Q}_{1}^{(a,A_{2}^{\prime\prime})}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1}^{(u,A_{2}^{\prime\prime})}] \otimes \mathbb{F}_{7}[\mathbb{Q}_{0}^{(k,A_{1}^{\prime\prime})}]}{6} - \frac{\sqrt{3}\mathbb{X}_{23}[\mathbb{Q}_{1}^{(a,A_{2}^{\prime\prime})}] \otimes \mathbb{U}_{7}[\mathbb{T}_{1}^{(u,A_{2}^{\prime\prime})}] \otimes \mathbb{F}_{13}[\mathbb{T}_{0}^{(k,A_{1}^{\prime\prime})}]}{6} + \frac{\sqrt{3}\mathbb{X}_{25}[\mathbb{Q}_{1,0}^{(a,E^{\prime\prime})}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{0}^{(u,A_{1}^{\prime\prime})}] \otimes \mathbb{F}_{9}[\mathbb{Q}_{1,0}^{(k,E^{\prime\prime})}]}{6} + \frac{\sqrt{3}\mathbb{X}_{25}[\mathbb{Q}_{1,0}^{(a,E^{\prime\prime})}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1,0}^{(u,A_{1}^{\prime\prime})}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1,0}^{(u,A_{2}^{\prime\prime})}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k,E^{\prime\prime})}]}{6} \\ - \frac{\sqrt{3}\mathbb{X}_{25}[\mathbb{Q}_{1,0}^{(a,E^{\prime\prime})}] \otimes \mathbb{U}_{6}[\mathbb{T}_{0}^{(u,A_{1}^{\prime\prime})}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,0}^{(k,E^{\prime\prime})}]}{6} - \frac{\sqrt{3}\mathbb{X}_{25}[\mathbb{Q}_{1,0}^{(a,E^{\prime\prime})}] \otimes \mathbb{U}_{7}[\mathbb{T}_{1}^{(u,A_{2}^{\prime\prime})}] \otimes \mathbb{F}_{17}[\mathbb{T}_{2,0}^{(k,E^{\prime\prime})}]}{6} + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,A_{1}^{\prime\prime})}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{0}^{(u,A_{1}^{\prime\prime})}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(k,E^{\prime\prime})}]}{6} \\ + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,A_{2}^{\prime\prime})}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1}^{(u,A_{2}^{\prime\prime})}]} \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E^{\prime\prime})}]}{6} - \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,A_{2}^{\prime\prime})}] \otimes \mathbb{F}_{16}[\mathbb{T}_{1,1}^{(k,E^{\prime\prime})}]}{6} - \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,A_{2}^{\prime\prime})}] \otimes \mathbb{F}_{17}[\mathbb{Q}_{1,1}^{(k,E^{\prime\prime})}]}{6} \\ + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,A_{2}^{\prime\prime})}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1,1}^{(u,A_{2}^{\prime\prime})}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E^{\prime\prime})}]}{6} - \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,A_{2}^{\prime\prime})}] \otimes \mathbb{F}_{16}[\mathbb{T}_{1,1}^{(k,E^{\prime\prime})}]}{6} - \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,A_{2}^{\prime\prime})}] \otimes \mathbb{F}_{17}[\mathbb{Q}_{1,1}^{(k,E^{\prime\prime})}]}{6} \\ + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,A_{2}^{\prime\prime})}] \otimes \mathbb{F}_{18}[\mathbb{Q}_{1,1}^{(k,E^{\prime\prime})}]}{6} - \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,A_{2}^{\prime\prime})}] \otimes \mathbb{F}_{18}[\mathbb{Q}_{1,1}^{(k,E^{\prime\prime})}]}{6} \\ + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,A_{2}^{\prime\prime})}] \otimes \mathbb{P}_{18}[\mathbb{Q}_{1,1}^{(a,A_{2}^{\prime\prime})}]}{6} - \frac{\sqrt{3}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,A_{2}^{\prime\prime})}] \otimes \mathbb{P}_{18}[\mathbb{Q}_{1,1}^{(a,A_{2}^{\prime\prime})}]}{6} \\ + \frac{\sqrt{3}\mathbb{Q}$$

No. 16 $\hat{\mathbb{Q}}_{2}^{(A_{1}')}$ [M₃, B₂]

$$\hat{\mathbb{Z}}_{16} = \frac{\sqrt{6}\mathbb{X}_{23}[\mathbb{Q}_{1}^{(a,A_{2}'')}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{1}^{(b,A_{2}'')}]}{3} - \frac{\sqrt{6}\mathbb{X}_{25}[\mathbb{Q}_{1,0}^{(a,E')}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E')}]}{6} - \frac{\sqrt{6}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E')}]}{6}$$

$$\hat{\mathbb{Z}}_{16}(\textbf{\textit{k}}) = \frac{\sqrt{6}\mathbb{X}_{23}[\mathbb{Q}_{1}^{(a,A_{2}'')}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{8}[\mathbb{Q}_{1}^{(k,A_{2}'')}]}{6} + \frac{\sqrt{6}\mathbb{X}_{23}[\mathbb{Q}_{1}^{(a,A_{2}'')}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1}^{(u,A_{2}'')}] \otimes \mathbb{F}_{7}[\mathbb{Q}_{0}^{(k,A_{1}')}]}{6} - \frac{\sqrt{6}\mathbb{X}_{23}[\mathbb{Q}_{1}^{(a,A_{2}'')}] \otimes \mathbb{U}_{6}[\mathbb{T}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{14}[\mathbb{T}_{1}^{(k,A_{2}'')}]}{6} \otimes \mathbb{F}_{14}[\mathbb{T}_{1}^{(k,A_{2}'')}] \otimes \mathbb{F}_{15}[\mathbb{T}_{0}^{(k,A_{1}')}]}{6} - \frac{\sqrt{6}\mathbb{X}_{25}[\mathbb{Q}_{1,0}^{(a,E'')}] \otimes \mathbb{F}_{9}[\mathbb{Q}_{1,0}^{(k,E'')}]}{6} - \frac{\sqrt{6}\mathbb{X}_{25}[\mathbb{Q}_{1,0}^{(a,E'')}] \otimes \mathbb{F}_{15}[\mathbb{Q}_{2,0}^{(k,E'')}]}{12} + \frac{\sqrt{6}\mathbb{X}_{25}[\mathbb{Q}_{1,0}^{(a,E'')}] \otimes \mathbb{F}_{17}[\mathbb{T}_{2,0}^{(k,E'')}]}{12} + \frac{\sqrt{6}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,E'')}] \otimes \mathbb{F}_{17}[\mathbb{T}_{2,0}^{(k,E'')}]}{12} + \frac{\sqrt{6}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,E'')}] \otimes \mathbb{F}_{16}[\mathbb{T}_{1,1}^{(k,E'')}]}{12} + \frac{\sqrt{6}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,A_{2}'')}] \otimes \mathbb{F}_{16}[\mathbb{Q}_{1,1}^{(a,A_{2}'')}]}{12} + \frac{\sqrt{6}\mathbb{X}_{26}[\mathbb{Q}_{1,1}^{(a,A_{2}'')}] \otimes \mathbb{F}_{16}[\mathbb$$

No. 17
$$\hat{\mathbb{Q}}_{3}^{(A_{1}')}$$
 [M₃, B₂]

$$\hat{\mathbb{Z}}_{17} = \mathbb{X}_{31}[\mathbb{Q}_3^{(a,A_1')}] \otimes \mathbb{Y}_9[\mathbb{Q}_0^{(b,A_1')}]$$

$$\begin{split} \hat{\mathbb{Z}}_{17}(\textbf{\textit{k}}) &= \frac{\mathbb{X}_{31}[\mathbb{Q}_{3}^{(a,A_{1}')}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{7}[\mathbb{Q}_{0}^{(k,A_{1}')}]}{2} + \frac{\mathbb{X}_{31}[\mathbb{Q}_{3}^{(a,A_{1}')}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1}^{(u,A_{2}'')}] \otimes \mathbb{F}_{8}[\mathbb{Q}_{1}^{(k,A_{2}'')}]}{2} \\ &- \frac{\mathbb{X}_{31}[\mathbb{Q}_{3}^{(a,A_{1}')}] \otimes \mathbb{U}_{6}[\mathbb{T}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{13}[\mathbb{T}_{0}^{(k,A_{1}')}]}{2} - \frac{\mathbb{X}_{31}[\mathbb{Q}_{3}^{(a,A_{1}')}] \otimes \mathbb{U}_{7}[\mathbb{T}_{1}^{(u,A_{2}'')}] \otimes \mathbb{F}_{14}[\mathbb{T}_{1}^{(k,A_{2}'')}]}{2} \end{split}$$

No. 18 $\hat{\mathbb{Q}}_{2}^{(A_{1}')}$ [M₃, B₂]

$$\hat{\mathbb{Z}}_{18} = \frac{\sqrt{21}\mathbb{X}_{24}[\mathbb{Q}_{3}^{(a,A_{2}'')}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{1}^{(b,A_{2}'')}]}{7} + \frac{\sqrt{14}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E')}]}{7} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E')}]}{7} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(a,E')}]}{7} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(a,E')}]}{7} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(a,E')}]}{7} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{1,1}^{(a,E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(a,E')}]}{7} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{1,1}^{(a,E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(a,E')}]}{7} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{1,1}^{(a,E')}]}{7} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{1,1}^{(a,E')}]}{7} + \frac{\sqrt{14}\mathbb{X$$

$$\hat{\mathbb{Z}}_{18}(\boldsymbol{k}) = \frac{\sqrt{21}\mathbb{X}_{24}[\mathbb{Q}_{3}^{(a,A_{2}'')}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{8}[\mathbb{Q}_{1}^{(k,A_{2}'')}]}{14} + \frac{\sqrt{21}\mathbb{X}_{24}[\mathbb{Q}_{3}^{(a,A_{2}'')}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1}^{(u,A_{2}'')}] \otimes \mathbb{F}_{7}[\mathbb{Q}_{0}^{(k,A_{1}')}]}{14} - \frac{\sqrt{21}\mathbb{X}_{24}[\mathbb{Q}_{3}^{(a,A_{2}'')}] \otimes \mathbb{F}_{18}[\mathbb{T}_{0}^{(k,A_{1}')}]}{14} + \frac{\sqrt{14}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{9}[\mathbb{Q}_{1,0}^{(k,E'')}]}{14} + \frac{\sqrt{14}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{9}[\mathbb{Q}_{1,0}^{(k,E'')}]}{14} + \frac{\sqrt{14}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1,0}^{(u,A_{1}')}] \otimes \mathbb{F}_{18}[\mathbb{Q}_{1,0}^{(u,A_{1}')}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k,E'')}]}{14} + \frac{\sqrt{14}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{U}_{9}[\mathbb{T}_{1}^{(u,A_{2}'')}] \otimes \mathbb{F}_{17}[\mathbb{T}_{2,0}^{(k,E'')}]}{14} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{U}_{9}[\mathbb{Q}_{1,1}^{(k,E'')}]}{14} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(k,E'')}] \otimes \mathbb{U}_{9}[\mathbb{Q}_{1,1}^{(k,E'')}]}{14} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(k,E'')}] \otimes \mathbb{U}_{9}[\mathbb{Q}_{1,1}^{(k,E'')}]}{14} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{1,1}^{(k,E'')}] \otimes \mathbb{U}_{9}[\mathbb{Q}_{1,1}^{(k,E'')}]}{14} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{1,1}^{(k,E'')}]}{14$$

No. 19 $\hat{\mathbb{Q}}_{4}^{(A_{1}')}$ [M₃, B₂]

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

$$\begin{split} \hat{\mathbb{Z}}_{19}(\textbf{\textit{k}}) &= \frac{\sqrt{7}\mathbb{X}_{24}[\mathbb{Q}_{3}^{(a,A_{2}'')}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{8}[\mathbb{Q}_{1}^{(k,A_{2}'')}]}{7} + \frac{\sqrt{7}\mathbb{X}_{24}[\mathbb{Q}_{3}^{(a,A_{2}'')}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1}^{(u,A_{2}'')}] \otimes \mathbb{F}_{7}[\mathbb{Q}_{0}^{(k,A_{1}')}]}{7} - \frac{\sqrt{7}\mathbb{X}_{24}[\mathbb{Q}_{3}^{(a,A_{2}'')}] \otimes \mathbb{U}_{6}[\mathbb{T}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{14}[\mathbb{T}_{1}^{(k,A_{2}'')}]}{7} \\ &- \frac{\sqrt{7}\mathbb{X}_{24}[\mathbb{Q}_{3}^{(a,A_{2}'')}] \otimes \mathbb{U}_{7}[\mathbb{T}_{1}^{(u,A_{2}'')}] \otimes \mathbb{F}_{13}[\mathbb{T}_{0}^{(k,A_{1}')}]}{7} - \frac{\sqrt{42}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{9}[\mathbb{Q}_{1,0}^{(k,E')}]}{28} - \frac{\sqrt{42}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1}^{(u,A_{1}')}] \otimes \mathbb{F}_{15}[\mathbb{Q}_{2,0}^{(k,E'')}]}{28} \\ &+ \frac{\sqrt{42}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{U}_{6}[\mathbb{T}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,0}^{(k,E'')}]}{28} + \frac{\sqrt{42}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{U}_{7}[\mathbb{T}_{1}^{(u,A_{2}'')}] \otimes \mathbb{F}_{17}[\mathbb{T}_{2,0}^{(k,E'')}]}{28} - \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{U}_{9}[\mathbb{Q}_{1,1}^{(k,E'')}]}{28} \\ &- \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1}^{(u,A_{2}'')}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E''')}]}{28} + \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{U}_{9}[\mathbb{T}_{1}^{(u,A_{1}')}]}{28} + \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{F}_{16}[\mathbb{T}_{1,1}^{(k,E'')}]}{28} \\ &- \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E''')}]}{28} + \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{F}_{16}[\mathbb{T}_{1,1}^{(k,E'')}]}{28} + \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{F}_{16}[\mathbb{T}_{1,1}^{(k,E'')}]}{28} \\ &- \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E''')}]}{28} + \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{F}_{16}[\mathbb{T}_{1,1}^{(k,E'')}]}{28} \\ &- \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{F}_{16}[\mathbb{Q}_{1,1}^{(k,E'')}]}{28} \\ &- \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{F}_{16}[\mathbb{Q}_{1,1}^{(k,E'')}]}{28} \\ &- \frac{\mathbb{E}_{1,1}}[\mathbb{Q}_{1,1}^{(k,E'')}] \otimes \mathbb{E}_{1,1}[\mathbb{Q}_{1,1}^{(k,E'')}]}{28} \\ &- \frac{\mathbb{E}_{1,1}}[\mathbb{Q}_{1,1}^{(k,E'')}] \otimes \mathbb{E}_{1,1}[\mathbb{Q}_{1,1}^{(k,E'')}]}{28} \\ &- \frac{$$

No. 20 $\hat{\mathbb{Q}}_3^{(A_1')}$ [M₃, B₂]

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

$$\begin{split} \hat{\mathbb{Z}}_{20}(\boldsymbol{k}) &= -\frac{\sqrt{2}\mathbb{X}_{32}[\mathbb{Q}_{3,0}^{(a,E'')}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k,E'')}]}{4} - \frac{\sqrt{2}\mathbb{X}_{32}[\mathbb{Q}_{3,0}^{(a,E'')}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1}^{(u,A_{2}'')}] \otimes \mathbb{F}_{9}[\mathbb{Q}_{1,0}^{(k,E')}]}{4} + \frac{\sqrt{2}\mathbb{X}_{32}[\mathbb{Q}_{3,0}^{(a,E'')}] \otimes \mathbb{U}_{7}[\mathbb{T}_{1}^{(u,A_{1}')}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,0}^{(k,E')}]}{4} - \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E'')}]}{4} \\ - \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1,1}^{(u,A_{2}')}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(k,E')}]}{4} + \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{U}_{6}[\mathbb{T}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{18}[\mathbb{T}_{2,1}^{(k,E'')}]}{4} + \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{U}_{7}[\mathbb{T}_{1}^{(u,A_{2}'')}] \otimes \mathbb{F}_{16}[\mathbb{T}_{1,1}^{(k,E')}]}{4} \\ - \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1}^{(u,A_{2}')}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(k,E')}]}{4} + \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{F}_{18}[\mathbb{T}_{2,1}^{(u,A_{1}')}]}{4} + \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{F}_{16}[\mathbb{T}_{1,1}^{(k,E')}]}{4} \\ - \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{V}_{5}[\mathbb{Q}_{1}^{(u,A_{2}')}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(u,A_{2}')}]}{4} + \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(u,A_{2}')}]}{4} \\ - \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(u,A_{2}')}]}{4} + \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(u,A_{2}')}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(u,A_{2}')}]}{4} \\ - \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(u,A_{2}')}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(u,A_{2}')}]}{4} + \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(u,A_{2}')}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(u,A_{2}')}]}{4} \\ - \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(u,A_{2}')}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(u,A_{2}')}]}{4} + \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(u,A_{2}')}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(u,A_{2}')}]}{4} \\ - \frac{\mathbb{Q}_{1,1}}{\mathbb{Q}_{1,1}} \otimes \mathbb{Q}_{1,1}^{(u,A_{2}')}] \otimes \mathbb{Q}_{1,1}^{(u,A_{2}')}}{4} + \frac{\mathbb{Q}_{1,1}}{\mathbb{Q}_{1,1}^{(u,A_{2}')}} \otimes \mathbb{Q}_{1,1}^{(u,A_{2}')}] \otimes \mathbb{Q}_{1,1}^{(u,A_{2}')} \otimes \mathbb{Q}_{1,1}^{(u,A_{2}')}}{4} \\ + \frac{\mathbb{Q}_{1,1}}{\mathbb{Q}_{1,1}} \otimes \mathbb{Q}_{1,1}^{(u,A_$$

No. 21 $\hat{\mathbb{Q}}_2^{(A_1')}$ [M₃, B₂]

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

$$\begin{split} \hat{\mathbb{Z}}_{21}(\textbf{\textit{k}}) &= \frac{\sqrt{2}\mathbb{X}_{29}[\mathbb{G}_{2,0}^{(a,E')}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{9}[\mathbb{Q}_{1,0}^{(k,E')}]}{4} + \frac{\sqrt{2}\mathbb{X}_{29}[\mathbb{G}_{2,0}^{(a,E')}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1}^{(u,A_{2}')}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k,E'')}]}{4} - \frac{\sqrt{2}\mathbb{X}_{29}[\mathbb{G}_{2,0}^{(a,E')}] \otimes \mathbb{U}_{7}[\mathbb{T}_{1}^{(u,A_{2}')}] \otimes \mathbb{F}_{17}[\mathbb{T}_{2,0}^{(k,E'')}]}{4} + \frac{\sqrt{2}\mathbb{X}_{30}[\mathbb{G}_{2,1}^{(a,E')}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(k,E'')}]}{4} \\ &+ \frac{\sqrt{2}\mathbb{X}_{30}[\mathbb{G}_{2,1}^{(a,E')}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1}^{(u,A_{2}'')}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E'')}]}{4} - \frac{\sqrt{2}\mathbb{X}_{30}[\mathbb{G}_{2,1}^{(a,E')}] \otimes \mathbb{U}_{6}[\mathbb{T}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{16}[\mathbb{T}_{1,1}^{(k,E')}]}{4} - \frac{\sqrt{2}\mathbb{X}_{30}[\mathbb{G}_{2,1}^{(a,E')}] \otimes \mathbb{F}_{18}[\mathbb{T}_{2,1}^{(k,E'')}]}{4} \\ \end{split}$$

No. 22 $\hat{\mathbb{Q}}_{3}^{(A_{1}')}$ [M₃, B₂]

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

$$\begin{split} \hat{\mathbb{Z}}_{22}(\textbf{\textit{k}}) &= -\frac{\sqrt{2}\mathbb{X}_{34}[\mathbb{G}_{2,0}^{(a,E'')}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k,E'')}]}{4} - \frac{\sqrt{2}\mathbb{X}_{34}[\mathbb{G}_{2,0}^{(a,E'')}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1}^{(u,A_{2}')}] \otimes \mathbb{F}_{9}[\mathbb{Q}_{1,0}^{(k,E')}]}{4} + \frac{\sqrt{2}\mathbb{X}_{34}[\mathbb{G}_{2,0}^{(a,E'')}] \otimes \mathbb{U}_{7}[\mathbb{T}_{1}^{(u,A_{1}')}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,0}^{(k,E')}]}{4} - \frac{\sqrt{2}\mathbb{X}_{35}[\mathbb{G}_{2,1}^{(a,E'')}] \otimes \mathbb{U}_{4}[\mathbb{Q}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E'')}]}{4} \\ - \frac{\sqrt{2}\mathbb{X}_{35}[\mathbb{G}_{2,1}^{(a,A_{2}'')}] \otimes \mathbb{U}_{5}[\mathbb{Q}_{1,1}^{(k,A_{2}')}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(k,E')}]}{4} + \frac{\sqrt{2}\mathbb{X}_{35}[\mathbb{G}_{2,1}^{(a,E'')}] \otimes \mathbb{U}_{6}[\mathbb{T}_{0}^{(u,A_{1}')}] \otimes \mathbb{F}_{18}[\mathbb{T}_{2,1}^{(k,E'')}]}{4} + \frac{\sqrt{2}\mathbb{X}_{35}[\mathbb{G}_{2,1}^{(a,E'')}] \otimes \mathbb{U}_{7}[\mathbb{T}_{1}^{(u,A_{2}'')}] \otimes \mathbb{F}_{16}[\mathbb{T}_{1,1}^{(k,E')}]}{4} \\ \end{pmatrix}$$

No. 23 $\hat{\mathbb{Q}}_0^{(A_1')}$ [M₂, B₃]

$$\hat{\mathbb{Z}}_{23} = \mathbb{X}_{14}[\mathbb{Q}_0^{(a,A_1')}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_0^{(b,A_1')}]$$

$$\hat{\mathbb{Z}}_{23}(\mathbf{k}) = \mathbb{X}_{14}[\mathbb{Q}_0^{(a,A_1')}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A_1')}] \otimes \mathbb{F}_{19}[\mathbb{Q}_0^{(k,A_1')}]$$

No. 24
$$\hat{\mathbb{Q}}_2^{(A_1')}$$
 [M₂, B₃]

$$\hat{\mathbb{Z}}_{24} = \mathbb{X}_{15}[\mathbb{Q}_2^{(a,A_1')}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_0^{(b,A_1')}]$$

$$\hat{\mathbb{Z}}_{24}(\mathbf{k}) = \mathbb{X}_{15}[\mathbb{Q}_2^{(a,A_1')}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A_1')}] \otimes \mathbb{F}_{19}[\mathbb{Q}_0^{(k,A_1')}]$$

No. 25
$$\hat{\mathbb{Q}}_{3}^{(A_{1}')}$$
 [M₂, B₃]

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

$$\hat{\mathbb{Z}}_{25}(\boldsymbol{k}) = -\frac{\sqrt{2}\mathbb{X}_{16}[\mathbb{Q}_{2,0}^{(a,E')}] \otimes \mathbb{U}_{2}[\mathbb{Q}_{0}^{(s,A'_{1})}] \otimes \mathbb{F}_{20}[\mathbb{Q}_{1,0}^{(k,E')}]}{2} - \frac{\sqrt{2}\mathbb{X}_{17}[\mathbb{Q}_{2,1}^{(a,E')}] \otimes \mathbb{U}_{2}[\mathbb{Q}_{0}^{(s,A'_{1})}] \otimes \mathbb{F}_{21}[\mathbb{Q}_{1,1}^{(k,E')}]}{2}$$

No. 26
$$\hat{\mathbb{Q}}_0^{(A_1')}$$
 [M₂, B₃]

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

$$\hat{\mathbb{Z}}_{26}(\textbf{\textit{k}}) = \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{Q}_{2,0}^{(a,E'')}] \otimes \mathbb{U}_{3}[\mathbb{Q}_{1}^{(s,A_{2}'')}] \otimes \mathbb{F}_{20}[\mathbb{Q}_{1,0}^{(k,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{19}[\mathbb{Q}_{2,1}^{(a,E'')}] \otimes \mathbb{U}_{3}[\mathbb{Q}_{1}^{(s,A_{2}'')}] \otimes \mathbb{F}_{21}[\mathbb{Q}_{1,1}^{(k,E')}]}{2}$$

No. 27
$$\hat{\mathbb{Q}}_{2}^{(A_{1}')}$$
 [M₂, B₃]

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

$$\hat{\mathbb{Z}}_{27}(\textbf{\textit{k}}) = \frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{M}_{1,0}^{(a,E'')}] \otimes \mathbb{U}_{3}[\mathbb{Q}_{1}^{(s,A_{2}'')}] \otimes \mathbb{F}_{22}[\mathbb{T}_{1,0}^{(k,E')}]}{2} + \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{M}_{1,1}^{(a,E'')}] \otimes \mathbb{U}_{3}[\mathbb{Q}_{1}^{(s,A_{2}'')}] \otimes \mathbb{F}_{23}[\mathbb{T}_{1,1}^{(k,E')}]}{2}$$

No. 28
$$\hat{\mathbb{Q}}_{3}^{(A_{1}')}$$
 [M₂, B₃]

$$\hat{\mathbb{Z}}_{28} = \mathbb{X}_{20}[\mathbb{M}_1^{(a,A_2')}] \otimes \mathbb{Y}_{22}[\mathbb{T}_3^{(b,A_2')}]$$

$$\hat{\mathbb{Z}}_{28}(\pmb{k}) = \mathbb{X}_{20}[\mathbb{M}_1^{(a,A_2')}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A_1')}] \otimes \mathbb{F}_{24}[\mathbb{T}_3^{(k,A_2')}]$$

Table 5: Atomic SAMB group.

group	bra	ket
M_1	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$
M_2	p_x, p_y, p_z	p_x, p_y, p_z
M_3	p_x, p_y, p_z	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$

Table 6: Atomic SAMB.

symbol	type	group	form
\mathbb{X}_1	$\mathbb{Q}_0^{(a,A_1')}$	M_1	$\begin{pmatrix} \frac{\sqrt{5}}{5} & 0 & 0 & 0 & 0\\ 0 & \frac{\sqrt{5}}{5} & 0 & 0 & 0\\ 0 & 0 & \frac{\sqrt{5}}{5} & 0 & 0\\ 0 & 0 & 0 & \frac{\sqrt{5}}{5} & 0\\ 0 & 0 & 0 & 0 & \frac{\sqrt{5}}{5} \end{pmatrix}$
\mathbb{X}_2	$\mathbb{Q}_2^{(a,A_1')}$	$ m M_1$	$ \begin{pmatrix} \frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{7} \end{pmatrix} $
\mathbb{X}_3	$\mathbb{Q}_4^{(a,A_1')}$	$ m M_1$	$ \begin{pmatrix} \frac{3\sqrt{70}}{35} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{70}}{70} & 0 & 0 & 0 \\ 0 & 0 & -\frac{2\sqrt{70}}{35} & 0 & 0 \\ 0 & 0 & 0 & -\frac{2\sqrt{70}}{35} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{70}}{70} \end{pmatrix} $
\mathbb{X}_4	$\mathbb{Q}_{2,0}^{(a,E')}$	$ m M_1$	$ \begin{pmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{7} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \\ -\frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \end{pmatrix} $

Table 6

symbol	type	group	form
\mathbb{X}_5	$\mathbb{Q}_{2,1}^{(a,E')}$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{14}}{7} & 0 & 0 & 0\\ \frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0\\ 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0\\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0\\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_6	$\mathbb{Q}_{4,0}^{(a,E',1)}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0$
\mathbb{X}_7	$\mathbb{Q}_{4,1}^{(a,E',1)}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 &$
\mathbb{X}_8	$\mathbb{Q}_{4,0}^{(a,E',2)}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0 \\ 0 & 0 & -\frac{\sqrt{14}}{7} & 0 & 0 \\ \frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_9	$\mathbb{Q}_{4,1}^{(a,E',2)}$	M_1	$\begin{pmatrix} 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0\\ -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0\\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0\\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0\\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{10}	$\mathbb{M}_1^{(a,A_2')}$	M_1	$ \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{10}i}{5} \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 & 0 \end{pmatrix} $

Table 6

symbol	type	group	form
\mathbb{X}_{11}	$\mathbb{M}_3^{(a,A_2')}$	M ₁	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{5} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{10} & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{12}	$\mathbb{M}_{3,0}^{(a,E')}$	$ m M_1$	$\begin{pmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0$
\mathbb{X}_{13}	$\mathbb{M}_{3,1}^{(a,E')}$	M_1	$\begin{pmatrix} 0 & \frac{\sqrt{2}i}{2} & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 &$
\mathbb{X}_{14}	$\mathbb{Q}_0^{(a,A_1')}$	M_2	$\begin{pmatrix} \frac{\sqrt{3}}{3} & 0 & 0\\ 0 & \frac{\sqrt{3}}{3} & 0\\ 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{X}_{15}	$\mathbb{Q}_2^{(a,A_1')}$	M_2	$\begin{pmatrix} -\frac{\sqrt{6}}{6} & 0 & 0\\ 0 & -\frac{\sqrt{6}}{6} & 0\\ 0 & 0 & \frac{\sqrt{6}}{3} \end{pmatrix}$
\mathbb{X}_{16}	$\mathbb{Q}_{2,0}^{(a,E')}$	M_2	$\begin{pmatrix} 0 & -\frac{\sqrt{2}}{2} & 0 \\ -\frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{17}	$\mathbb{Q}_{2,1}^{(a,E')}$	M_2	$\begin{pmatrix} -\frac{\sqrt{2}}{2} & 0 & 0\\ 0 & \frac{\sqrt{2}}{2} & 0\\ 0 & 0 & 0 \end{pmatrix}$
X ₁₈	$\mathbb{Q}_{2,0}^{(a,E^{\prime\prime})}$	M_2	$ \begin{pmatrix} 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \end{pmatrix} $

Table 6

Table 6			
symbol	type	group	form
\mathbb{X}_{19}	$\mathbb{Q}_{2,1}^{(a,E^{\prime\prime})}$	M_2	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
\mathbb{X}_{20}	$\mathbb{M}_1^{(a,A_2')}$	M_2	$\begin{pmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0\\ \frac{\sqrt{2}i}{2} & 0 & 0\\ 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{21}	$\mathbb{M}_{1,0}^{(a,E'')}$	M_2	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \end{pmatrix}$
\mathbb{X}_{22}	$\mathbb{M}_{1,1}^{(a,E'')}$	M_2	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & \frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$
\mathbb{X}_{23}	$\mathbb{Q}_1^{(a,A_2^{\prime\prime})}$	M_3	$\begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{30}}{10} & 0 \\ 0 & 0 & \frac{\sqrt{30}}{10} & 0 & 0 \\ \frac{\sqrt{10}}{5} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{24}	$\mathbb{Q}_3^{(a,A_2^{\prime\prime})}$	M_3	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{5}}{5} & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{5} & 0 & 0 \\ \frac{\sqrt{15}}{5} & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} -\frac{\sqrt{10}}{10} & \frac{\sqrt{30}}{10} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{30} \end{pmatrix}$
\mathbb{X}_{25}	$\mathbb{Q}_{1,0}^{(a,E')}$	M_3	$\begin{pmatrix} -\frac{\sqrt{10}}{10} & \frac{\sqrt{30}}{10} & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & -\frac{\sqrt{30}}{10}\\ 0 & 0 & 0 & \frac{\sqrt{30}}{10} & 0 \end{pmatrix}$
\mathbb{X}_{26}	$\mathbb{Q}_{1,1}^{(a,E')}$	M_3	$ \begin{pmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{30}}{10} \\ -\frac{\sqrt{10}}{10} & -\frac{\sqrt{30}}{10} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{30}}{10} & 0 & 0 \end{pmatrix} $
\mathbb{X}_{27}	$\mathbb{Q}_{3,0}^{(a,E')}$	M_3	$\begin{pmatrix} \frac{\sqrt{10}}{5} & -\frac{\sqrt{30}}{30} & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{30}\\ 0 & 0 & 0 & \frac{2\sqrt{30}}{15} & 0 \end{pmatrix}$
X ₂₈	$\mathbb{Q}_{3,1}^{(a,E')}$	M_3	$ \begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{30} \\ \frac{\sqrt{10}}{5} & \frac{\sqrt{30}}{30} & 0 & 0 & 0 \\ 0 & 0 & \frac{2\sqrt{30}}{15} & 0 & 0 \end{pmatrix} $

Table 6

symbol	type	group	form
\mathbb{X}_{29}	$\mathbb{G}_{2,0}^{(a,E')}$	M_3	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{6}}{6} & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6}\\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \end{pmatrix}$
\mathbb{X}_{30}	$\mathbb{G}_{2,1}^{(a,E')}$	M_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ \frac{\sqrt{2}}{2} & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 \end{pmatrix}$
\mathbb{X}_{31}	$\mathbb{Q}_3^{(a,A_1')}$	M_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{32}	$\mathbb{Q}_{3,0}^{(a,E^{\prime\prime})}$	M_3	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{3}}{3} & 0 & 0\\ 0 & 0 & 0 & -\frac{\sqrt{3}}{3} & 0\\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{X}_{33}	$\mathbb{Q}_{3,1}^{(a,E^{\prime\prime})}$	M_3	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{3}}{3} & 0\\ 0 & 0 & \frac{\sqrt{3}}{3} & 0 & 0\\ 0 & -\frac{\sqrt{3}}{3} & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{34}	$\mathbb{G}_{2,0}^{(a,E^{\prime\prime})}$	M_3	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{3} \end{pmatrix}$
X ₃₅	$\mathbb{G}_{2,1}^{(a,E^{\prime\prime})}$	M_3	$ \begin{pmatrix} 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{3} & 0 & 0 & 0 \end{pmatrix} $

Table 7: Cluster SAMB.

symbol	type	cluster	form
\mathbb{Y}_1	$\mathbb{Q}_0^{(s,A_1')}$	S_1	(1)
\mathbb{Y}_2	$\mathbb{Q}_0^{(s,A_1')}$	S_2	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{Y}_3	$\mathbb{Q}_0^{(b,A_1')}$	B_1	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \end{pmatrix}$

Table 7

Table 1			
symbol	type	cluster	form
\mathbb{Y}_4	$\mathbb{Q}_{1,0}^{(b,E')}$	B_1	$\begin{pmatrix} -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
\mathbb{Y}_5	$\mathbb{Q}_{1,1}^{(b,E')}$	B_1	$\left(-\frac{\sqrt{6}}{6} -\frac{\sqrt{6}}{6} \frac{\sqrt{6}}{3}\right)$
\mathbb{Y}_6	$\mathbb{T}_{1,0}^{(b,E')}$	B_1	$\begin{pmatrix} \sqrt{6}i & -\frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{3} \end{pmatrix}$
\mathbb{Y}_7	$\mathbb{T}^{(b,E')}$	B_1	$\left(-\frac{\sqrt{2}i}{2} -\frac{\sqrt{2}i}{2} 0\right)$
\mathbb{Y}_8	$\mathbb{T}_3^{(b,A_2')}$	B_1	$\begin{pmatrix} \sqrt{3}i \\ 3 \end{pmatrix} - \frac{\sqrt{3}i}{3} & \frac{\sqrt{3}i}{3} \end{pmatrix}$
\mathbb{Y}_9	$\mathbb{Q}_0^{(b,A_1')}$	B_2	$\begin{pmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{Y}_{10}	$\mathbb{Q}_1^{(b,A_2'')}$	B_2	$\left(\frac{\sqrt{6}}{6} - \frac{\sqrt{6}}{6} - \frac{\sqrt{6}}{6} - \frac{\sqrt{6}}{6} - \frac{\sqrt{6}}{6} - \frac{\sqrt{6}}{6} \right)$
\mathbb{Y}_{11}	$\mathbb{Q}_{1,0}^{(b,E')}$	B_2	$\left(-\frac{1}{2} \frac{1}{2} -\frac{1}{2} 0 \frac{1}{2} 0\right)$
\mathbb{Y}_{12}	$\mathbb{Q}_{1,1}^{(b,E')}$	B_2	$\begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & \frac{1}{2} & 0 \\ -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{Y}_{13}	$\mathbb{Q}_{2,0}^{(b,E^{\prime\prime})}$	B_2	$\left(-\frac{1}{2} -\frac{1}{2} \frac{1}{2} 0 \frac{1}{2} 0 \right)$
\mathbb{Y}_{14}	$\mathbb{Q}_{2,1}^{(b,E^{\prime\prime})}$	B_2	$\left(-\frac{\sqrt{3}}{6} \frac{\sqrt{3}}{6} \frac{\sqrt{3}}{6} -\frac{\sqrt{3}}{3} -\frac{\sqrt{3}}{6} \frac{\sqrt{3}}{3}\right)$
\mathbb{Y}_{15}	$\mathbb{Q}_0^{(b,A_1')}$	B_3	$ \frac{\left(-\frac{\sqrt{3}}{6} \frac{\sqrt{3}}{6} \frac{\sqrt{3}}{6} -\frac{\sqrt{3}}{3} -\frac{\sqrt{3}}{6} \frac{\sqrt{3}}{3}\right)}{\left(\frac{\sqrt{6}}{6} \frac{\sqrt{6}}{6} \frac{\sqrt{6}}{6} \frac{\sqrt{6}}{6} \frac{\sqrt{6}}{6}\right)} $
\mathbb{Y}_{16}	$\mathbb{Q}_{1,0}^{(b,E')}$	B_3	$\begin{pmatrix} 0 & 0 & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$
\mathbb{Y}_{17}	$\mathbb{Q}_{1,1}^{(b,E')}$	B_3	$\left(-\frac{\sqrt{3}}{2} - \frac{\sqrt{3}}{2} - \frac{\sqrt{3}}{2} - \frac{\sqrt{3}}{2} - \frac{\sqrt{3}}{2} - \frac{\sqrt{3}}{2}\right)$
\mathbb{Y}_{18}	$\mathbb{Q}_{2,0}^{(b,E^{\prime\prime})}$	B_3	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$
\mathbb{Y}_{19}	$\mathbb{Q}_{2,1}^{(b,E^{\prime\prime})}$	B_3	$\left(-\frac{\sqrt{3}}{3} \frac{\sqrt{3}}{3} -\frac{\sqrt{3}}{6} -\frac{\sqrt{3}}{6} \frac{\sqrt{3}}{6} \frac{\sqrt{3}}{6}\right)$
\mathbb{Y}_{20}	$\mathbb{T}_{2,0}^{(b,E^{\prime\prime})}$	B_3	$\left(-\frac{\sqrt{3}i}{3} \frac{\sqrt{3}i}{3} \frac{\sqrt{3}i}{6} -\frac{\sqrt{3}i}{6} \frac{\sqrt{3}i}{6} -\frac{\sqrt{3}i}{6}\right)$
\mathbb{Y}_{21}	$\mathbb{T}_{2,1}^{(b,E^{\prime\prime})}$	B_3	$ \begin{pmatrix} 3 & 3 & 6 & 6 & 6 \\ 0 & 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix} $ $ \begin{pmatrix} -\frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} \end{pmatrix} $ $ \begin{pmatrix} -\frac{\sqrt{3}i}{3} & \frac{\sqrt{3}i}{3} & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} \end{pmatrix} $ $ \begin{pmatrix} 0 & 0 & \frac{i}{2} & \frac{i}{2} & -\frac{i}{2} & -\frac{i}{2} \end{pmatrix} $
\mathbb{Y}_{22}	$\mathbb{T}_3^{(b,A_2')}$	B_3	$ \frac{\left(\frac{\sqrt{6}i}{6} \frac{\sqrt{6}i}{6} -\frac{\sqrt{6}i}{6} \frac{\sqrt{6}i}{6} \frac{\sqrt{6}i}{6} -\frac{\sqrt{6}i}{6} \right) }{ } $

Table 8: Uniform SAMB.

symbol	type	cluster	form
\mathbb{U}_1	$\mathbb{Q}_0^{(s,A_1')}$	S_1	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
\mathbb{U}_2	$\mathbb{Q}_0^{(s,A_1')}$	S_2	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{U}_3	$\mathbb{Q}_1^{(s,A_2'')}$	S_2	$ \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & -\frac{\sqrt{2}}{2} \end{pmatrix} $
\mathbb{U}_4	$\mathbb{Q}_0^{(u,A_1')}$	B_2	$\begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 \end{pmatrix}$
\mathbb{U}_5	$\mathbb{Q}_1^{(u,A_2'')}$	B_2	$\begin{pmatrix} 0 & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 \end{pmatrix}$
\mathbb{U}_6	$\mathbb{T}_0^{(u,A_1')}$	$ m B_2$	$\begin{pmatrix} 0 & -\frac{i}{2} & -\frac{i}{2} \\ \frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 \end{pmatrix}$
\mathbb{U}_7	$\mathbb{T}_1^{(u,A_2'')}$	B_2	$ \begin{pmatrix} 0 & -\frac{i}{2} & \frac{i}{2} \\ \frac{i}{2} & 0 & 0 \\ -\frac{i}{2} & 0 & 0 \end{pmatrix} $

Table 9: Structure SAMB.

symbol	type	cluster	form
\mathbb{F}_1	$\mathbb{Q}_0^{(k,A_1')}$	B_1	$\frac{\sqrt{6}c_{001}}{3} + \frac{\sqrt{6}c_{002}}{3} + \frac{\sqrt{6}c_{003}}{3}$
\mathbb{F}_2	$\mathbb{Q}_{1,0}^{(k,E')}$	B_1	$-c_{001} + c_{002}$
\mathbb{F}_3	$\mathbb{Q}_{1,1}^{(k,E')}$	B_1	$-\frac{\sqrt{3}c_{001}}{3} - \frac{\sqrt{3}c_{002}}{3} + \frac{2\sqrt{3}c_{003}}{3}$

Table 9

symbol	type	cluster	form
\mathbb{F}_4	$\mathbb{T}_{1,0}^{(k,E')}$	B_1	$\frac{\sqrt{3}s_{001}}{3} - \frac{\sqrt{3}s_{002}}{3} - \frac{2\sqrt{3}s_{003}}{3}$
\mathbb{F}_5	$\mathbb{T}_{1,1}^{(k,E')}$	B_1	$-s_{001}-s_{002}$
\mathbb{F}_6	$\mathbb{T}_3^{(k,A_2')}$	B_1	$\frac{\sqrt{6}s_{001}}{3} - \frac{\sqrt{6}s_{002}}{3} + \frac{\sqrt{6}s_{003}}{3}$
\mathbb{F}_7	$\mathbb{O}_{0}^{(k,A_{1}^{\prime})}$	B_2	$\frac{\sqrt{3}c_{004}}{3} + \frac{\sqrt{3}c_{005}}{3} + \frac{\sqrt{3}c_{006}}{3} + \frac{\sqrt{3}c_{007}}{3} + \frac{\sqrt{3}c_{008}}{3} + \frac{\sqrt{3}c_{009}}{3}$
\mathbb{F}_8	$\mathbb{Q}_1^{(k,A_2'')}$	B_2	$\frac{\sqrt{3}c_{004}}{3} - \frac{\sqrt{3}c_{005}}{3} - \frac{\sqrt{3}c_{006}}{3} - \frac{\sqrt{3}c_{007}}{3} + \frac{\sqrt{3}c_{008}}{3} + \frac{\sqrt{3}c_{009}}{3}$
\mathbb{F}_9	$\mathbb{Q}_{1,0}^{(k,E')}$	B_2	$-\frac{\sqrt{2}c_{004}}{2} + \frac{\sqrt{2}c_{005}}{2} - \frac{\sqrt{2}c_{006}}{2} + \frac{\sqrt{2}c_{008}}{2}$
\mathbb{F}_{10}	$\mathbb{Q}_{1,1}^{(k,E')}$	B_2	$-\frac{\sqrt{6}c_{004}}{6} - \frac{\sqrt{6}c_{005}}{6} - \frac{\sqrt{6}c_{006}}{6} + \frac{\sqrt{6}c_{007}}{3} - \frac{\sqrt{6}c_{008}}{6} + \frac{\sqrt{6}c_{009}}{3}$
\mathbb{F}_{11}	$\mathbb{Q}_{2,0}^{(k,E'')}$	B_2	$-\frac{\sqrt{2}c_{004}}{2} - \frac{\sqrt{2}c_{005}}{2} + \frac{\sqrt{2}c_{006}}{2} + \frac{\sqrt{2}c_{008}}{2}$
\mathbb{F}_{12}	$\mathbb{Q}_{2,1}^{(k,E^{\prime\prime})}$	B_2	$-\frac{\sqrt{6}c_{004}}{6} + \frac{\sqrt{6}c_{005}}{6} + \frac{\sqrt{6}c_{006}}{6} - \frac{\sqrt{6}c_{007}}{3} - \frac{\sqrt{6}c_{008}}{6} + \frac{\sqrt{6}c_{009}}{3}$
\mathbb{F}_{13}	$\mathbb{T}_0^{(k,A_1')}$	B_2	$\frac{\sqrt{3}s_{004}}{3} + \frac{\sqrt{3}s_{005}}{3} + \frac{\sqrt{3}s_{006}}{3} + \frac{\sqrt{3}s_{007}}{3} + \frac{\sqrt{3}s_{008}}{3} + \frac{\sqrt{3}s_{009}}{3}$
\mathbb{F}_{14}	$\mathbb{T}_1^{(k,A_2'')}$	B_2	$\frac{\sqrt{3}s_{004}}{3} - \frac{\sqrt{3}s_{005}}{3} - \frac{\sqrt{3}s_{006}}{3} - \frac{\sqrt{3}s_{007}}{3} + \frac{\sqrt{3}s_{008}}{3} + \frac{\sqrt{3}s_{009}}{3}$
\mathbb{F}_{15}	$\mathbb{T}_{1,0}^{(k,E')}$	B_2	$-\frac{\sqrt{2}s_{004}}{2} + \frac{\sqrt{2}s_{005}}{2} - \frac{\sqrt{2}s_{006}}{2} + \frac{\sqrt{2}s_{008}}{2}$
\mathbb{F}_{16}	$\mathbb{T}_{1,1}^{(k,E')}$	B_2	$ -\frac{\sqrt{6}s_{004}}{6} - \frac{\sqrt{6}s_{005}}{6} - \frac{\sqrt{6}s_{006}}{6} + \frac{\sqrt{6}s_{007}}{3} - \frac{\sqrt{6}s_{008}}{6} + \frac{\sqrt{6}s_{009}}{3} $
\mathbb{F}_{17}	$\mathbb{T}_{2,0}^{(k,E^{\prime\prime})}$	B_2	$-\frac{\sqrt{2}s_{004}}{2} - \frac{\sqrt{2}s_{005}}{2} + \frac{\sqrt{2}s_{006}}{2} + \frac{\sqrt{2}s_{008}}{2}$
\mathbb{F}_{18}	$\mathbb{T}_{2,1}^{(k,E^{\prime\prime})}$	B_2	$-\frac{\sqrt{6}s_{004}}{6} + \frac{\sqrt{6}s_{005}}{6} + \frac{\sqrt{6}s_{006}}{6} - \frac{\sqrt{6}s_{007}}{3} - \frac{\sqrt{6}s_{008}}{6} + \frac{\sqrt{6}s_{009}}{3}$
\mathbb{F}_{19}	$\mathbb{Q}_0^{(k,A_1')}$	B_3	$\frac{\sqrt{6}c_{010}}{3} + \frac{\sqrt{6}c_{012}}{3} + \frac{\sqrt{6}c_{013}}{3}$
\mathbb{F}_{20}	$\mathbb{Q}_{1,0}^{(k,E')}$	B_3	$-c_{012} + c_{013}$
\mathbb{F}_{21}	$\mathbb{Q}_{1,1}^{(k,E')}$	B_3	$-\frac{2\sqrt{3}c_{010}}{3} + \frac{\sqrt{3}c_{012}}{3} + \frac{\sqrt{3}c_{013}}{3}$
\mathbb{F}_{22}	$\mathbb{T}_{1,0}^{(k,E')}$	B_3	$-\frac{2\sqrt{3}s_{010}}{3} - \frac{\sqrt{3}s_{012}}{3} + \frac{\sqrt{3}s_{013}}{3}$
\mathbb{F}_{23}	$\mathbb{T}^{(k,E')}$	B_3	$-s_{012} - s_{013}$
\mathbb{F}_{24}	$\mathbb{T}_3^{1,1}$	B_3	$\frac{\sqrt{6}s_{010}}{3} - \frac{\sqrt{6}s_{012}}{3} + \frac{\sqrt{6}s_{013}}{3}$

Table 10: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_1')}$	0	A'_1	_	_	1
2	$\mathbb{Q}_1^{(A_2^{\prime\prime})}$	1	$A_2^{\prime\prime}$	_	_	z
3	$\mathbb{Q}_{1,0}^{(E)}$	1	E'	_	0	x
4	$\mathbb{Q}_{1,1}^{(E')}$ $\mathbb{Q}_{2}^{(A'_{1})}$	1	E'	_	1	y
5	$\mathbb{Q}_2^{(A_1')}$	2	A_1'	_	_	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
6	$\mathbb{Q}_{2,0}^{(E^{\prime\prime})}$ $\mathbb{Q}_{2,1}^{(E^{\prime\prime})}$	2	$E^{\prime\prime}$	_	0	$\sqrt{3}xz$
7	$\mathbb{Q}_{2,1}^{(E^{\prime\prime})}$	2	$E^{\prime\prime}$	_	1	$\sqrt{3}yz$
8	$\mathbb{Q}_{2,0}^{(E')}$	2	E'	_	0	$-\sqrt{3}xy$
9	$\mathbb{Q}_{2,1}^{(E')}$	2	E'	_	1	$-\frac{\sqrt{3(x-y)(x+y)}}{2}$
10	$\mathbb{Q}_{2,0}^{(E')}$ $\mathbb{Q}_{2,1}^{(E')}$ $\mathbb{Q}_{3,1}^{(A'_{1})}$	3	A_1'	_	_	$-\frac{\sqrt{3}(x-y)(x+y)}{2}$ $-\frac{\sqrt{10}y(3x^2-y^2)}{4}$ $-\frac{z(3x^2+3y^2-2z^2)}{\sqrt{10}x(x^2-3y^2)}$
11	$\mathbb{Q}_2^{(A_2'')}$	3	$A_2^{\prime\prime}$	_	_	$-rac{z\left(3x^2+3y^2-2z^2 ight)}{2}$
12	$\mathbb{Q}_3^{(A_2')}$	3	A_2'	_	_	$\frac{\sqrt{10}x\left(x^2-3y^2\right)}{4}$
13	$\mathbb{Q}_{3.0}^{(E^{\prime\prime})}$	3	$E^{\prime\prime}$	_	0	, \(\frac{15}{15}\)
14	$\mathbb{Q}_{3,1}^{(E'')}$	3	$E^{\prime\prime}$	_	1	$-rac{\sqrt{15}z(x-y)(x+y)}{2}$
15	$\mathbb{Q}_{3,0}^{(E')}$	3	E'	_	0	$-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$
16	\bigcap (E')	3	E'	_	1	$-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$
17	$\mathbb{Q}_{4}^{(A_{1}^{\prime})}$	4	A'_1	_	_	$-\sqrt{15xyz} \\ -\frac{\sqrt{15z(x-y)(x+y)}}{\sqrt{6x(x^2+y^2-4z^2)}} \\ -\frac{\sqrt{6y(x^2+y^2-4z^2)}}{\sqrt{6y(x^2+y^2-4z^2)}} \\ -\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$
18	$\mathbb{Q}_{4,0}^{(E',1)}$	4	E'	1	0	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
19	$\mathbb{Q}_{4,1}^{(E',1)}$	4	E'	1	1	$-\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$
20	$\mathbb{Q}_{4,0}^{(E',2)}$	4	E'	2	0	$\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$
21	$\mathbb{Q}_{4,1}^{(E',2)}$	4	E'	2	1	$-\frac{\sqrt{35}xy(x-y)(x+y)}{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)} \\ -\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)} \\ -\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$

Table 11: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_1^{(A_2')}$	1	A_2'	_	_	Z

Table 11

No.	symbol	rank	irrep.	mul.	comp.	form
2	$\mathbb{G}_{1,0}^{(E'')}$	1	$E^{\prime\prime}$	_	0	-Y
3	$\mathbb{G}_{1,1}^{(E'')}$	1	$E^{\prime\prime}$	_	1	X
4	$\mathbb{G}_{2,0}^{(E'')}$	2	$E^{\prime\prime}$	_	0	$\frac{\sqrt{3}(X-Y)(X+Y)}{2}$
5	$\mathbb{G}_{2,1}^{(E'')}$	2	$E^{\prime\prime}$	_	1	$-\sqrt{3}XY$
6	$\mathbb{G}_{2,0}^{(E')}$	2	E'	_	0	$-\sqrt{3}YZ$
7	$\mathbb{G}_{2,1}^{(E'')}$	2	E'	_	1	$\sqrt{3}XZ$
8	$\mathbb{G}_3^{(A_2')}$	3	A_2'	_	_	$-\frac{Z(3X^2+3Y^2-2Z^2)}{2}$
9	$\mathbb{G}_{3,0}^{(E')}$	3	E'	_	0	$\frac{\sqrt{15}Z(X-Y)(X+Y)}{2}$
10	$\mathbb{G}_{3,1}^{(E')}$	3	E'	_	1	$-\sqrt{15}XYZ$

 \bullet Group info.: Generator = $\{3^{+}_{\ 001}|0\},\ \{m_{001}|0\},\ \{m_{110}|0\}$

Table 12: Conjugacy class (point-group part).

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

Table 13: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1 0\}$	2	$\{2_{120} 0\}$	3	$\{2_{210} 0\}$	4	$\{2_{1-10} 0\}$	5	$\{3^{+}_{001} 0\}$
6	$\{3^{-}_{001} 0\}$	7	$\{m_{100} 0\}$	8	$\{m_{010} 0\}$	9	$\{m_{110} 0\}$	10	$\{m_{001} 0\}$
 11	$\{-6^{+}_{001} 0\}$	12	$\{-6^{-}_{001} 0\}$						

Table 14: Character table (point-group part).

	1	2120	3 ⁺ ₀₀₁	m ₁₀₀	m ₀₀₁	-6^{+}_{001}
A'_1	1	1	1	1	1	1
$A_2^{\bar{\prime}}$	1	-1	1	-1	1	1
$A_1^{\prime\prime}$	1	1	1	-1	-1	-1
$A_2^{\dagger\prime}$	1	-1	1	1	-1	-1
$\tilde{E'}$	2	0	-1	0	2	-1
E''	2	0	-1	0	-2	1

Table 15: Parity conversion.

\leftrightarrow	\leftrightarrow	\leftrightarrow	\leftrightarrow	\leftrightarrow
$\begin{array}{c} A_1' \ (A_1'') \\ E' \ (E'') \end{array}$	A_2' (A_2'')	$A_1^{\prime\prime} \ (A_1^\prime)$	$A_2''(A_2')$	$E^{\prime\prime}$ (E^{\prime})

Table 16: Symmetric product, $[\Gamma \otimes \Gamma']_+$.

	A'_1	A_2'	$A_1^{\prime\prime}$	$A_2^{\prime\prime}$	E'	$E^{\prime\prime}$
A'_1	A_1^{\prime}	$A_2^{\overline{\prime}}$	$A_1^{\prime\prime\prime}$	$A_2^{\overline{\prime\prime}}$	E'	E''
A_2^{\prime}	_	$A_1^{\bar{\prime}}$	$A_2^{\prime\prime}$	$A_1^{\prime\prime}$	E'	$E^{\prime\prime}$
$A_1^{\tilde{\prime}\prime}$		•	$A_1^{\overline{\prime}}$	A_2^{\dagger}	$E^{\prime\prime}$	E'

Table 16

	A'_1	A_2'	$A_1^{\prime\prime}$	$A_2^{\prime\prime}$	E'	$E^{\prime\prime}$
$A_2^{\prime\prime}$				A'_1	$E^{\prime\prime}$	E'
E'					$A_1' + E'$	$A_1'' + A_2'' + E''$
$E^{\prime\prime}$						$A_1' + E'$

Table 17: Anti-symmetric product, $[\Gamma \otimes \Gamma]_-$.

A'_1	A_2'	$A_1^{\prime\prime}$	$A_2^{\prime\prime}$	E'	$E^{\prime\prime}$
_	_	_	_	A_2'	A_2'

Table 18: Virtual-cluster sites.

No.	position No		position	No.	position	No.	position
1	$\begin{pmatrix} -1 & -1 & 1 \end{pmatrix}$	2	$\begin{pmatrix} 0 & -1 & -1 \end{pmatrix}$	3	$\begin{pmatrix} -1 & 0 & -1 \end{pmatrix}$	4	$\begin{pmatrix} 1 & 1 & -1 \end{pmatrix}$
5	$\begin{pmatrix} 1 & 0 & 1 \end{pmatrix}$	6	$\begin{pmatrix} 0 & 1 & 1 \end{pmatrix}$	7	$\begin{pmatrix} 0 & -1 & 1 \end{pmatrix}$	8	$\begin{pmatrix} -1 & 0 & 1 \end{pmatrix}$
9	$\begin{pmatrix} 1 & 1 & 1 \end{pmatrix}$	10	$\begin{pmatrix} -1 & -1 & -1 \end{pmatrix}$	11	$\begin{pmatrix} 0 & 1 & -1 \end{pmatrix}$	12	$\begin{pmatrix} 1 & 0 & -1 \end{pmatrix}$

Table 19: Virtual-cluster basis.

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_0^{(A_1')}$	$\frac{\sqrt{3}}{6}$									
	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$								

Table 19

Table 19										
symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_1^{(A_2^{\prime\prime})}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$
	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$ $\frac{\sqrt{6}}{12}$								
$\mathbb{Q}_{1,0}^{(E')}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$ $-\frac{\sqrt{2}}{4}$	$\frac{\frac{\sqrt{6}}{6}}{-\frac{\sqrt{2}}{4}}$								
$\mathbb{Q}_{1,1}^{(E')}$	$-\frac{\sqrt{2}}{4}$		0	$\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$
(E/)	$\frac{\frac{\sqrt{2}}{4}}{-\frac{\sqrt{2}}{4}}$	0							<u></u>	
$\mathbb{Q}_{2,0}^{(E')}$		$\frac{\sqrt{2}}{4}$	0	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	0	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$
(E')	$\frac{\frac{\sqrt{2}}{4}}{\frac{\sqrt{6}}{12}}$	0	<u>/c</u>	<u> </u>	<u>/c</u>	<u></u>	<u> </u>	<u> </u>	<u> </u>	<u> </u>
$\mathbb{Q}_{2,1}^{(E')}$		$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
$\mathbb{Q}_{2,0}^{(E'')}$	$-\frac{\frac{\sqrt{6}}{12}}{-\frac{\sqrt{6}}{12}}$	$-\frac{\sqrt{6}}{6}$	<u>√6</u>	<u>√6</u>	<u>√6</u>	<u>√6</u>	-\sqrt{6}	./ <u>6</u>	<u>√6</u>	./ <u>6</u>
$\mathbb{Q}_{2,0}^{\leftarrow}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
$\mathbb{Q}_{2,1}^{(E^{\prime\prime})}$	$ \frac{\sqrt{6}}{12} $ $ -\frac{\sqrt{2}}{4} $	$-\frac{\sqrt{6}}{6}$ $\frac{\sqrt{2}}{4}$	0	$-\frac{\sqrt{2}}{4}$	0	$\sqrt{2}$	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
$\mathbb{Q}_{2,1}$	$-\frac{4}{4}$	0	U	4	U	4	4	U	4	4
$\mathbb{Q}_3^{(A_2')}$	$-\frac{\frac{\sqrt{2}}{4}}{\frac{\sqrt{3}}{6}}$		$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$
₹ 3	$\frac{6}{\sqrt{3}}$	$\frac{6}{\sqrt{3}}$	6	6	6	6	6	6	6	6
$\mathbb{Q}_{3,0}^{(E^{\prime\prime})}$	$\frac{\frac{\sqrt{3}}{6}}{-\frac{\sqrt{2}}{4}}$	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	0	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
-0,0		0		4		4	4		4	4
$\mathbb{Q}_{3,1}^{(E'')}$	$\frac{-\frac{\sqrt{2}}{4}}{\frac{\sqrt{6}}{12}}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$ $\frac{\sqrt{3}}{6}$								
$\mathbb{Q}_4^{(A_1'')}$	$-\frac{\sqrt{6}}{12}$ $\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$
	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$								