

# SAMB for “MoS2”

Generated on 2023-05-24 23:01 by MultiPie 1.1.1

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- Group: No. 187  $D_{3h}^1$   $P-6m2$  [ hexagonal ]
  - Associated point group: No. 26  $D_{3h}$   $-6m2$  (-6m2 setting) [ hexagonal ]
  - Generation condition
    - model type: **tight\_binding**
    - time-reversal type: **electric**
    - irrep: [A1']
    - **spinless**
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- Unit cell:
  - $a = 3.1661$ ,  $b = 3.1661$ ,  $c = 20.0$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 120.0$
- Lattice vectors:
  - $\mathbf{a}_1 = (3.1661 \ 0 \ 0)$
  - $\mathbf{a}_2 = (-1.58305 \ 2.74192303092191 \ 0)$
  - $\mathbf{a}_3 = (0 \ 0 \ 20.0)$

Table 1: High-symmetry line:  $\Gamma$ -M-K- $\Gamma$ -K'.

symbol	position	symbol	position	symbol	position
$\Gamma$	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	M	$\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	K	$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & 0 \end{pmatrix}$
K'	$\begin{pmatrix} -\frac{1}{3} & -\frac{1}{3} & 0 \end{pmatrix}$				

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- Kets: dimension = 11

Table 2: Hilbert space for full matrix.

No.	ket	No.	ket	No.	ket	No.	ket	No.	ket
1	$d_u@Mo_1$	2	$d_v@Mo_1$	3	$d_{yz}@Mo_1$	4	$d_{zx}@Mo_1$	5	$d_{xy}@Mo_1$
6	$p_x@S_1$	7	$p_y@S_1$	8	$p_z@S_1$	9	$p_x@S_2$	10	$p_y@S_2$
11	$p_z@S_2$								

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

site		position	mapping
S <sub>1</sub>	Mo <sub>1</sub>	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,2,3,4,5,6,7,8,9,10,11,12]
S <sub>2</sub>	S <sub>1</sub>	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0.12425 \end{pmatrix}$	[1,5,6,7,8,9]
	S <sub>2</sub>	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0.87575 \end{pmatrix}$	[2,3,4,10,11,12]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

bond	tail	head	$n$	#	$\mathbf{b@c}$	mapping	
B <sub>1</sub>	b <sub>1</sub>	Mo <sub>1</sub>	Mo <sub>1</sub>	1	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[1,-3,-8,10]
	b <sub>2</sub>	Mo <sub>1</sub>	Mo <sub>1</sub>	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 <sub>3</sub>	Mo <sub>1</sub>	Mo <sub>1</sub>	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[-4,6,-9,11]
B <sub>2</sub>	b <sub>4</sub>	Mo <sub>1</sub>	S <sub>1</sub>	1	1	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0.12425 \end{pmatrix} @ \begin{pmatrix} \frac{1}{3} & \frac{1}{6} & 0.062125 \end{pmatrix}$	[1,8]
	b <sub>5</sub>	Mo <sub>1</sub>	S <sub>2</sub>	1	1	$\begin{pmatrix} -\frac{1}{3} & \frac{1}{3} & -0.12425 \end{pmatrix} @ \begin{pmatrix} \frac{5}{6} & \frac{1}{6} & 0.937875 \end{pmatrix}$	[2,12]
	b <sub>6</sub>	Mo <sub>1</sub>	S <sub>2</sub>	1	1	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & -0.12425 \end{pmatrix} @ \begin{pmatrix} \frac{1}{3} & \frac{1}{6} & 0.937875 \end{pmatrix}$	[3,10]
	b <sub>7</sub>	Mo <sub>1</sub>	S <sub>2</sub>	1	1	$\begin{pmatrix} -\frac{1}{3} & -\frac{2}{3} & -0.12425 \end{pmatrix} @ \begin{pmatrix} \frac{5}{6} & \frac{2}{3} & 0.937875 \end{pmatrix}$	[4,11]

continued ...

Table 4

bond	tail	head	$n$	#	$\mathbf{b@c}$	mapping	
b <sub>8</sub>	Mo <sub>1</sub>	S <sub>1</sub>	1	1	$\left(\begin{smallmatrix} -\frac{1}{3} & \frac{1}{3} & 0.12425 \end{smallmatrix}\right) @ \left(\begin{smallmatrix} \frac{5}{6} & \frac{1}{6} & 0.062125 \end{smallmatrix}\right)$	[5,7]	
b <sub>9</sub>	Mo <sub>1</sub>	S <sub>1</sub>	1	1	$\left(\begin{smallmatrix} -\frac{1}{3} & -\frac{2}{3} & 0.12425 \end{smallmatrix}\right) @ \left(\begin{smallmatrix} \frac{5}{6} & \frac{2}{3} & 0.062125 \end{smallmatrix}\right)$	[6,9]	
B <sub>3</sub>	b <sub>10</sub>	S <sub>1</sub>	S <sub>1</sub>	1	1	$\left(\begin{smallmatrix} 1 & 0 & 0 \end{smallmatrix}\right) @ \left(\begin{smallmatrix} \frac{1}{6} & \frac{1}{3} & 0.12425 \end{smallmatrix}\right)$	[1,-7]
	b <sub>11</sub>	S <sub>2</sub>	S <sub>2</sub>	1	1	$\left(\begin{smallmatrix} 1 & 0 & 0 \end{smallmatrix}\right) @ \left(\begin{smallmatrix} \frac{1}{6} & \frac{1}{3} & 0.87575 \end{smallmatrix}\right)$	[-2,10]
	b <sub>12</sub>	S <sub>2</sub>	S <sub>2</sub>	1	1	$\left(\begin{smallmatrix} 1 & 1 & 0 \end{smallmatrix}\right) @ \left(\begin{smallmatrix} \frac{1}{6} & \frac{5}{6} & 0.87575 \end{smallmatrix}\right)$	[3,-11]
	b <sub>13</sub>	S <sub>2</sub>	S <sub>2</sub>	1	1	$\left(\begin{smallmatrix} 0 & 1 & 0 \end{smallmatrix}\right) @ \left(\begin{smallmatrix} \frac{2}{3} & \frac{5}{6} & 0.87575 \end{smallmatrix}\right)$	[-4,12]
	b <sub>14</sub>	S <sub>1</sub>	S <sub>1</sub>	1	1	$\left(\begin{smallmatrix} 0 & 1 & 0 \end{smallmatrix}\right) @ \left(\begin{smallmatrix} \frac{2}{3} & \frac{5}{6} & 0.12425 \end{smallmatrix}\right)$	[5,-9]
	b <sub>15</sub>	S <sub>1</sub>	S <sub>1</sub>	1	1	$\left(\begin{smallmatrix} 1 & 1 & 0 \end{smallmatrix}\right) @ \left(\begin{smallmatrix} \frac{1}{6} & \frac{5}{6} & 0.12425 \end{smallmatrix}\right)$	[-6,8]

- SAMB:

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

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

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

$$\boxed{\text{No. 2}} \quad \hat{\mathbb{Q}}_2^{(A'_1)} [\mathbf{M}_1, \mathbf{S}_1]$$

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

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

$$\boxed{\text{No. 3}} \quad \hat{\mathbb{Q}}_4^{(A'_1)} [\mathbf{M}_1, \mathbf{S}_1]$$

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

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

$$\boxed{\text{No. 4}} \quad \hat{\mathbb{Q}}_0^{(A'_1)} [\mathbb{M}_2, \mathbb{S}_2]$$

$$\hat{\mathbb{Z}}_4 = \mathbb{X}_{14}[\mathbb{Q}_0^{(a, A'_1)}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s, A'_1)}]$$

$$\hat{\mathbb{Z}}_4(\mathbf{k}) = \mathbb{X}_{14}[\mathbb{Q}_0^{(a, A'_1)}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s, A'_1)}]$$

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

$$\hat{\mathbb{Z}}_5 = \mathbb{X}_{15}[\mathbb{Q}_2^{(a, A'_1)}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s, A'_1)}]$$

$$\hat{\mathbb{Z}}_5(\mathbf{k}) = \mathbb{X}_{15}[\mathbb{Q}_2^{(a, A'_1)}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s, A'_1)}]$$

$$\boxed{\text{No. 6}} \quad \hat{\mathbb{Q}}_0^{(A'_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

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

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

$$\boxed{\text{No. 7}} \quad \hat{\mathbb{Q}}_2^{(A'_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbb{Z}}_7 = \mathbb{X}_2[\mathbb{Q}_2^{(a, A'_1)}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b, A'_1)}]$$

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

$$\boxed{\text{No. 8}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

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

$$\hat{\mathbb{Z}}_8(\mathbf{k}) = -\frac{\sqrt{2}\mathbb{X}_4[\mathbb{Q}_{2,0}^{(a, E')}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A'_1)}] \otimes \mathbb{F}_2[\mathbb{Q}_{1,0}^{(k, E')}] }{2} - \frac{\sqrt{2}\mathbb{X}_5[\mathbb{Q}_{2,1}^{(a, E')}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A'_1)}] \otimes \mathbb{F}_3[\mathbb{Q}_{1,1}^{(k, E')}] }{2}$$

$$\boxed{\text{No. 9}} \quad \hat{\mathbb{Q}}_4^{(A'_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbb{Z}}_9 = \mathbb{X}_3[\mathbb{Q}_4^{(a, A'_1)}] \otimes \mathbb{Y}_3[\mathbb{Q}_0^{(b, A'_1)}]$$

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

$$\boxed{\text{No. 10}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbf{Z}}_{10} = \frac{\sqrt{406}\mathbb{X}_6[\mathbb{Q}_{4,0}^{(a,E',1)}] \otimes \mathbb{Y}_4[\mathbb{Q}_{1,0}^{(b,E')}] }{29} + \frac{\sqrt{406}\mathbb{X}_7[\mathbb{Q}_{4,1}^{(a,E',1)}] \otimes \mathbb{Y}_5[\mathbb{Q}_{1,1}^{(b,E')}] }{29} + \frac{\sqrt{58}\mathbb{X}_8[\mathbb{Q}_{4,0}^{(a,E',2)}] \otimes \mathbb{Y}_4[\mathbb{Q}_{1,0}^{(b,E')}] }{58} + \frac{\sqrt{58}\mathbb{X}_9[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{Y}_5[\mathbb{Q}_{1,1}^{(b,E')}] }{58}$$

$$\begin{aligned} \hat{\mathbf{Z}}_{10}(\mathbf{k}) &= \frac{\sqrt{406}\mathbb{X}_6[\mathbb{Q}_{4,0}^{(a,E',1)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A'_1)}] \otimes \mathbb{F}_2[\mathbb{Q}_{1,0}^{(k,E')}] }{29} + \frac{\sqrt{406}\mathbb{X}_7[\mathbb{Q}_{4,1}^{(a,E',1)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A'_1)}] \otimes \mathbb{F}_3[\mathbb{Q}_{1,1}^{(k,E')}] }{29} \\ &+ \frac{\sqrt{58}\mathbb{X}_8[\mathbb{Q}_{4,0}^{(a,E',2)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A'_1)}] \otimes \mathbb{F}_2[\mathbb{Q}_{1,0}^{(k,E')}] }{58} + \frac{\sqrt{58}\mathbb{X}_9[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A'_1)}] \otimes \mathbb{F}_3[\mathbb{Q}_{1,1}^{(k,E')}] }{58} \end{aligned}$$

$$\boxed{\text{No. 11}} \quad \hat{\mathbb{G}}_4^{(A'_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbf{Z}}_{11} = -\frac{\sqrt{58}\mathbb{X}_6[\mathbb{Q}_{4,0}^{(a,E',1)}] \otimes \mathbb{Y}_4[\mathbb{Q}_{1,0}^{(b,E')}] }{58} - \frac{\sqrt{58}\mathbb{X}_7[\mathbb{Q}_{4,1}^{(a,E',1)}] \otimes \mathbb{Y}_5[\mathbb{Q}_{1,1}^{(b,E')}] }{58} + \frac{\sqrt{406}\mathbb{X}_8[\mathbb{Q}_{4,0}^{(a,E',2)}] \otimes \mathbb{Y}_4[\mathbb{Q}_{1,0}^{(b,E')}] }{29} + \frac{\sqrt{406}\mathbb{X}_9[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{Y}_5[\mathbb{Q}_{1,1}^{(b,E')}] }{29}$$

$$\begin{aligned} \hat{\mathbf{Z}}_{11}(\mathbf{k}) &= -\frac{\sqrt{58}\mathbb{X}_6[\mathbb{Q}_{4,0}^{(a,E',1)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A'_1)}] \otimes \mathbb{F}_2[\mathbb{Q}_{1,0}^{(k,E')}] }{58} - \frac{\sqrt{58}\mathbb{X}_7[\mathbb{Q}_{4,1}^{(a,E',1)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A'_1)}] \otimes \mathbb{F}_3[\mathbb{Q}_{1,1}^{(k,E')}] }{58} \\ &+ \frac{\sqrt{406}\mathbb{X}_8[\mathbb{Q}_{4,0}^{(a,E',2)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A'_1)}] \otimes \mathbb{F}_2[\mathbb{Q}_{1,0}^{(k,E')}] }{29} + \frac{\sqrt{406}\mathbb{X}_9[\mathbb{Q}_{4,1}^{(a,E',2)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A'_1)}] \otimes \mathbb{F}_3[\mathbb{Q}_{1,1}^{(k,E')}] }{29} \end{aligned}$$

$$\boxed{\text{No. 12}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbf{Z}}_{12} = \mathbb{X}_{10}[\mathbb{M}_1^{(a,A'_2)}] \otimes \mathbb{Y}_8[\mathbb{T}_3^{(b,A'_2)}]$$

$$\hat{\mathbf{Z}}_{12}(\mathbf{k}) = \mathbb{X}_{10}[\mathbb{M}_1^{(a,A'_2)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A'_1)}] \otimes \mathbb{F}_6[\mathbb{T}_3^{(k,A'_2)}]$$

$$\boxed{\text{No. 13}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbf{Z}}_{13} = \frac{\sqrt{2}\mathbb{X}_{12}[\mathbb{M}_{3,0}^{(a,E')}] \otimes \mathbb{Y}_6[\mathbb{T}_{1,0}^{(b,E')}] }{2} + \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{M}_{3,1}^{(a,E')}] \otimes \mathbb{Y}_7[\mathbb{T}_{1,1}^{(b,E')}] }{2}$$

$$\hat{\mathbf{Z}}_{13}(\mathbf{k}) = \frac{\sqrt{2}\mathbb{X}_{12}[\mathbb{M}_{3,0}^{(a,E')}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A'_1)}] \otimes \mathbb{F}_4[\mathbb{T}_{1,0}^{(k,E')}] }{2} + \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{M}_{3,1}^{(a,E')}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A'_1)}] \otimes \mathbb{F}_5[\mathbb{T}_{1,1}^{(k,E')}] }{2}$$

$$\boxed{\text{No. 14}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\mathbf{M}_1, \mathbf{B}_1]$$

$$\hat{\mathbb{Z}}_{14} = -\mathbb{X}_{11}[\mathbf{M}_3^{(a, A'_2)}] \otimes \mathbb{Y}_8[\mathbf{T}_3^{(b, A'_2)}]$$

$$\hat{\mathbb{Z}}_{14}(\mathbf{k}) = -\mathbb{X}_{11}[\mathbf{M}_3^{(a, A'_2)}] \otimes \mathbb{U}_1[\mathbf{Q}_0^{(s, A'_1)}] \otimes \mathbb{F}_6[\mathbf{T}_3^{(k, A'_2)}]$$

$$\boxed{\text{No. 15}} \quad \hat{\mathbb{Q}}_0^{(A'_1)} [\mathbf{M}_3, \mathbf{B}_2]$$

$$\hat{\mathbb{Z}}_{15} = \frac{\sqrt{3}\mathbb{X}_{23}[\mathbf{Q}_1^{(a, A'_2)}] \otimes \mathbb{Y}_{10}[\mathbf{Q}_1^{(b, A'_2)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{25}[\mathbf{Q}_{1,0}^{(a, E')}] \otimes \mathbb{Y}_{11}[\mathbf{Q}_{1,0}^{(b, E')}] }{3} + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbf{Q}_{1,1}^{(a, E')}] \otimes \mathbb{Y}_{12}[\mathbf{Q}_{1,1}^{(b, E')}] }{3}$$

$$\begin{aligned} \hat{\mathbb{Z}}_{15}(\mathbf{k}) = & \frac{\sqrt{3}\mathbb{X}_{23}[\mathbf{Q}_1^{(a, A'_2)}] \otimes \mathbb{U}_4[\mathbf{Q}_0^{(u, A'_1)}] \otimes \mathbb{F}_8[\mathbf{Q}_1^{(k, A'_2)}]}{6} + \frac{\sqrt{3}\mathbb{X}_{23}[\mathbf{Q}_1^{(a, A'_2)}] \otimes \mathbb{U}_5[\mathbf{Q}_1^{(u, A'_2)}] \otimes \mathbb{F}_7[\mathbf{Q}_0^{(k, A'_1)}]}{6} - \frac{\sqrt{3}\mathbb{X}_{23}[\mathbf{Q}_1^{(a, A'_2)}] \otimes \mathbb{U}_6[\mathbf{T}_0^{(u, A'_1)}] \otimes \mathbb{F}_{14}[\mathbf{T}_1^{(k, A'_2)}]}{6} \\ & - \frac{\sqrt{3}\mathbb{X}_{23}[\mathbf{Q}_1^{(a, A'_2)}] \otimes \mathbb{U}_7[\mathbf{T}_1^{(u, A'_2)}] \otimes \mathbb{F}_{13}[\mathbf{T}_0^{(k, A'_1)}]}{6} + \frac{\sqrt{3}\mathbb{X}_{25}[\mathbf{Q}_{1,0}^{(a, E')}] \otimes \mathbb{U}_4[\mathbf{Q}_0^{(u, A'_1)}] \otimes \mathbb{F}_9[\mathbf{Q}_{1,0}^{(k, E')}] }{6} + \frac{\sqrt{3}\mathbb{X}_{25}[\mathbf{Q}_{1,0}^{(a, E')}] \otimes \mathbb{U}_5[\mathbf{Q}_1^{(u, A'_2)}] \otimes \mathbb{F}_{11}[\mathbf{Q}_{2,0}^{(k, E'')}] }{6} \\ & - \frac{\sqrt{3}\mathbb{X}_{25}[\mathbf{Q}_{1,0}^{(a, E')}] \otimes \mathbb{U}_6[\mathbf{T}_0^{(u, A'_1)}] \otimes \mathbb{F}_{15}[\mathbf{T}_{1,0}^{(k, E')}] }{6} - \frac{\sqrt{3}\mathbb{X}_{25}[\mathbf{Q}_{1,0}^{(a, E')}] \otimes \mathbb{U}_7[\mathbf{T}_1^{(u, A'_2)}] \otimes \mathbb{F}_{17}[\mathbf{T}_{2,0}^{(k, E'')}] }{6} + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbf{Q}_{1,1}^{(a, E')}] \otimes \mathbb{U}_4[\mathbf{Q}_0^{(u, A'_1)}] \otimes \mathbb{F}_{10}[\mathbf{Q}_{1,1}^{(k, E')}] }{6} \\ & + \frac{\sqrt{3}\mathbb{X}_{26}[\mathbf{Q}_{1,1}^{(a, E')}] \otimes \mathbb{U}_5[\mathbf{Q}_1^{(u, A'_2)}] \otimes \mathbb{F}_{12}[\mathbf{Q}_{2,1}^{(k, E'')}] }{6} - \frac{\sqrt{3}\mathbb{X}_{26}[\mathbf{Q}_{1,1}^{(a, E')}] \otimes \mathbb{U}_6[\mathbf{T}_0^{(u, A'_1)}] \otimes \mathbb{F}_{16}[\mathbf{T}_{1,1}^{(k, E')}] }{6} - \frac{\sqrt{3}\mathbb{X}_{26}[\mathbf{Q}_{1,1}^{(a, E')}] \otimes \mathbb{U}_7[\mathbf{T}_1^{(u, A'_2)}] \otimes \mathbb{F}_{18}[\mathbf{T}_{2,1}^{(k, E'')}] }{6} \end{aligned}$$

$$\boxed{\text{No. 16}} \quad \hat{\mathbb{Q}}_2^{(A'_1)} [\mathbf{M}_3, \mathbf{B}_2]$$

$$\hat{\mathbb{Z}}_{16} = \frac{\sqrt{6}\mathbb{X}_{23}[\mathbf{Q}_1^{(a, A'_2)}] \otimes \mathbb{Y}_{10}[\mathbf{Q}_1^{(b, A'_2)}]}{3} - \frac{\sqrt{6}\mathbb{X}_{25}[\mathbf{Q}_{1,0}^{(a, E')}] \otimes \mathbb{Y}_{11}[\mathbf{Q}_{1,0}^{(b, E')}] }{6} - \frac{\sqrt{6}\mathbb{X}_{26}[\mathbf{Q}_{1,1}^{(a, E')}] \otimes \mathbb{Y}_{12}[\mathbf{Q}_{1,1}^{(b, E')}] }{6}$$

$$\begin{aligned} \hat{\mathbb{Z}}_{16}(\mathbf{k}) = & \frac{\sqrt{6}\mathbb{X}_{23}[\mathbf{Q}_1^{(a, A'_2)}] \otimes \mathbb{U}_4[\mathbf{Q}_0^{(u, A'_1)}] \otimes \mathbb{F}_8[\mathbf{Q}_1^{(k, A'_2)}]}{6} + \frac{\sqrt{6}\mathbb{X}_{23}[\mathbf{Q}_1^{(a, A'_2)}] \otimes \mathbb{U}_5[\mathbf{Q}_1^{(u, A'_2)}] \otimes \mathbb{F}_7[\mathbf{Q}_0^{(k, A'_1)}]}{6} - \frac{\sqrt{6}\mathbb{X}_{23}[\mathbf{Q}_1^{(a, A'_2)}] \otimes \mathbb{U}_6[\mathbf{T}_0^{(u, A'_1)}] \otimes \mathbb{F}_{14}[\mathbf{T}_1^{(k, A'_2)}]}{6} \\ & - \frac{\sqrt{6}\mathbb{X}_{23}[\mathbf{Q}_1^{(a, A'_2)}] \otimes \mathbb{U}_7[\mathbf{T}_1^{(u, A'_2)}] \otimes \mathbb{F}_{13}[\mathbf{T}_0^{(k, A'_1)}]}{6} - \frac{\sqrt{6}\mathbb{X}_{25}[\mathbf{Q}_{1,0}^{(a, E')}] \otimes \mathbb{U}_4[\mathbf{Q}_0^{(u, A'_1)}] \otimes \mathbb{F}_9[\mathbf{Q}_{1,0}^{(k, E')}] }{12} - \frac{\sqrt{6}\mathbb{X}_{25}[\mathbf{Q}_{1,0}^{(a, E')}] \otimes \mathbb{U}_5[\mathbf{Q}_1^{(u, A'_2)}] \otimes \mathbb{F}_{11}[\mathbf{Q}_{2,0}^{(k, E'')}] }{12} \\ & + \frac{\sqrt{6}\mathbb{X}_{25}[\mathbf{Q}_{1,0}^{(a, E')}] \otimes \mathbb{U}_6[\mathbf{T}_0^{(u, A'_1)}] \otimes \mathbb{F}_{15}[\mathbf{T}_{1,0}^{(k, E')}] }{12} + \frac{\sqrt{6}\mathbb{X}_{25}[\mathbf{Q}_{1,0}^{(a, E')}] \otimes \mathbb{U}_7[\mathbf{T}_1^{(u, A'_2)}] \otimes \mathbb{F}_{17}[\mathbf{T}_{2,0}^{(k, E'')}] }{12} - \frac{\sqrt{6}\mathbb{X}_{26}[\mathbf{Q}_{1,1}^{(a, E')}] \otimes \mathbb{U}_4[\mathbf{Q}_0^{(u, A'_1)}] \otimes \mathbb{F}_{10}[\mathbf{Q}_{1,1}^{(k, E')}] }{12} \\ & - \frac{\sqrt{6}\mathbb{X}_{26}[\mathbf{Q}_{1,1}^{(a, E')}] \otimes \mathbb{U}_5[\mathbf{Q}_1^{(u, A'_2)}] \otimes \mathbb{F}_{12}[\mathbf{Q}_{2,1}^{(k, E'')}] }{12} + \frac{\sqrt{6}\mathbb{X}_{26}[\mathbf{Q}_{1,1}^{(a, E')}] \otimes \mathbb{U}_6[\mathbf{T}_0^{(u, A'_1)}] \otimes \mathbb{F}_{16}[\mathbf{T}_{1,1}^{(k, E')}] }{12} + \frac{\sqrt{6}\mathbb{X}_{26}[\mathbf{Q}_{1,1}^{(a, E')}] \otimes \mathbb{U}_7[\mathbf{T}_1^{(u, A'_2)}] \otimes \mathbb{F}_{18}[\mathbf{T}_{2,1}^{(k, E'')}] }{12} \end{aligned}$$

$$\boxed{\text{No. 17}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\mathbf{M}_3, \mathbf{B}_2]$$

$$\hat{\mathbb{Z}}_{17} = \mathbb{X}_{31}[\mathbf{Q}_3^{(a, A'_1)}] \otimes \mathbb{Y}_9[\mathbf{Q}_0^{(b, A'_1)}]$$

$$\hat{\mathbb{Z}}_{17}(\mathbf{k}) = \frac{\mathbb{X}_{31}[\mathbb{Q}_3^{(a,A'_1)}] \otimes \mathbb{U}_4[\mathbb{Q}_0^{(u,A'_1)}] \otimes \mathbb{F}_7[\mathbb{Q}_0^{(k,A'_1)}]}{2} + \frac{\mathbb{X}_{31}[\mathbb{Q}_3^{(a,A'_1)}] \otimes \mathbb{U}_5[\mathbb{Q}_1^{(u,A'_2)}] \otimes \mathbb{F}_8[\mathbb{Q}_1^{(k,A'_2)}]}{2} \\ - \frac{\mathbb{X}_{31}[\mathbb{Q}_3^{(a,A'_1)}] \otimes \mathbb{U}_6[\mathbb{T}_0^{(u,A'_1)}] \otimes \mathbb{F}_{13}[\mathbb{T}_0^{(k,A'_1)}]}{2} - \frac{\mathbb{X}_{31}[\mathbb{Q}_3^{(a,A'_1)}] \otimes \mathbb{U}_7[\mathbb{T}_1^{(u,A'_2)}] \otimes \mathbb{F}_{14}[\mathbb{T}_1^{(k,A'_2)}]}{2}$$

$$\boxed{\text{No. 18}} \quad \hat{\mathbb{Q}}_2^{(A'_1)} [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{18} = \frac{\sqrt{21}\mathbb{X}_{24}[\mathbb{Q}_3^{(a,A'_2)}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_1^{(b,A'_2)}]}{7} + \frac{\sqrt{14}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E')}] }{7} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E')}] }{7}$$

$$\hat{\mathbb{Z}}_{18}(\mathbf{k}) = \frac{\sqrt{21}\mathbb{X}_{24}[\mathbb{Q}_3^{(a,A'_2)}] \otimes \mathbb{U}_4[\mathbb{Q}_0^{(u,A'_1)}] \otimes \mathbb{F}_8[\mathbb{Q}_1^{(k,A'_2)}]}{14} + \frac{\sqrt{21}\mathbb{X}_{24}[\mathbb{Q}_3^{(a,A'_2)}] \otimes \mathbb{U}_5[\mathbb{Q}_1^{(u,A'_2)}] \otimes \mathbb{F}_7[\mathbb{Q}_0^{(k,A'_1)}]}{14} - \frac{\sqrt{21}\mathbb{X}_{24}[\mathbb{Q}_3^{(a,A'_2)}] \otimes \mathbb{U}_6[\mathbb{T}_0^{(u,A'_1)}] \otimes \mathbb{F}_{14}[\mathbb{T}_1^{(k,A'_2)}]}{14} \\ - \frac{\sqrt{21}\mathbb{X}_{24}[\mathbb{Q}_3^{(a,A'_2)}] \otimes \mathbb{U}_7[\mathbb{T}_1^{(u,A'_2)}] \otimes \mathbb{F}_{13}[\mathbb{T}_0^{(k,A'_1)}]}{14} + \frac{\sqrt{14}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{U}_4[\mathbb{Q}_0^{(u,A'_1)}] \otimes \mathbb{F}_9[\mathbb{Q}_{1,0}^{(k,E')}] }{14} + \frac{\sqrt{14}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{U}_5[\mathbb{Q}_1^{(u,A'_2)}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k,E'')}] }{14} \\ - \frac{\sqrt{14}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{U}_6[\mathbb{T}_0^{(u,A'_1)}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,0}^{(k,E')}] }{14} - \frac{\sqrt{14}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{U}_7[\mathbb{T}_1^{(u,A'_2)}] \otimes \mathbb{F}_{17}[\mathbb{T}_{2,0}^{(k,E'')}] }{14} + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{U}_4[\mathbb{Q}_0^{(u,A'_1)}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(k,E')}] }{14} \\ + \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{U}_5[\mathbb{Q}_1^{(u,A'_2)}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E'')}] }{14} - \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{U}_6[\mathbb{T}_0^{(u,A'_1)}] \otimes \mathbb{F}_{16}[\mathbb{T}_{1,1}^{(k,E')}] }{14} - \frac{\sqrt{14}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{U}_7[\mathbb{T}_1^{(u,A'_2)}] \otimes \mathbb{F}_{18}[\mathbb{T}_{2,1}^{(k,E'')}] }{14}$$

$$\boxed{\text{No. 19}} \quad \hat{\mathbb{Q}}_4^{(A'_1)} [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{19} = \frac{2\sqrt{7}\mathbb{X}_{24}[\mathbb{Q}_3^{(a,A'_2)}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_1^{(b,A'_2)}]}{7} - \frac{\sqrt{42}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{Y}_{11}[\mathbb{Q}_{1,0}^{(b,E')}] }{14} - \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{Y}_{12}[\mathbb{Q}_{1,1}^{(b,E')}] }{14}$$

$$\hat{\mathbb{Z}}_{19}(\mathbf{k}) = \frac{\sqrt{7}\mathbb{X}_{24}[\mathbb{Q}_3^{(a,A'_2)}] \otimes \mathbb{U}_4[\mathbb{Q}_0^{(u,A'_1)}] \otimes \mathbb{F}_8[\mathbb{Q}_1^{(k,A'_2)}]}{7} + \frac{\sqrt{7}\mathbb{X}_{24}[\mathbb{Q}_3^{(a,A'_2)}] \otimes \mathbb{U}_5[\mathbb{Q}_1^{(u,A'_2)}] \otimes \mathbb{F}_7[\mathbb{Q}_0^{(k,A'_1)}]}{7} - \frac{\sqrt{7}\mathbb{X}_{24}[\mathbb{Q}_3^{(a,A'_2)}] \otimes \mathbb{U}_6[\mathbb{T}_0^{(u,A'_1)}] \otimes \mathbb{F}_{14}[\mathbb{T}_1^{(k,A'_2)}]}{7} \\ - \frac{\sqrt{7}\mathbb{X}_{24}[\mathbb{Q}_3^{(a,A'_2)}] \otimes \mathbb{U}_7[\mathbb{T}_1^{(u,A'_2)}] \otimes \mathbb{F}_{13}[\mathbb{T}_0^{(k,A'_1)}]}{7} - \frac{\sqrt{42}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{U}_4[\mathbb{Q}_0^{(u,A'_1)}] \otimes \mathbb{F}_9[\mathbb{Q}_{1,0}^{(k,E')}] }{28} - \frac{\sqrt{42}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{U}_5[\mathbb{Q}_1^{(u,A'_2)}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k,E'')}] }{28} \\ + \frac{\sqrt{42}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{U}_6[\mathbb{T}_0^{(u,A'_1)}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,0}^{(k,E')}] }{28} + \frac{\sqrt{42}\mathbb{X}_{27}[\mathbb{Q}_{3,0}^{(a,E')}] \otimes \mathbb{U}_7[\mathbb{T}_1^{(u,A'_2)}] \otimes \mathbb{F}_{17}[\mathbb{T}_{2,0}^{(k,E'')}] }{28} - \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{U}_4[\mathbb{Q}_0^{(u,A'_1)}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(k,E')}] }{28} \\ - \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{U}_5[\mathbb{Q}_1^{(u,A'_2)}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E'')}] }{28} + \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{U}_6[\mathbb{T}_0^{(u,A'_1)}] \otimes \mathbb{F}_{16}[\mathbb{T}_{1,1}^{(k,E')}] }{28} + \frac{\sqrt{42}\mathbb{X}_{28}[\mathbb{Q}_{3,1}^{(a,E')}] \otimes \mathbb{U}_7[\mathbb{T}_1^{(u,A'_2)}] \otimes \mathbb{F}_{18}[\mathbb{T}_{2,1}^{(k,E'')}] }{28}$$

$$\boxed{\text{No. 20}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\text{M}_3, \text{B}_2]$$

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

$$\begin{aligned}\hat{Z}_{20}(\mathbf{k}) = & -\frac{\sqrt{2}\mathbb{X}_{32}[\mathbb{Q}_{3,0}^{(a,E'')}] \otimes \mathbb{U}_4[\mathbb{Q}_0^{(u,A'_1)}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k,E'')}] }{4} - \frac{\sqrt{2}\mathbb{X}_{32}[\mathbb{Q}_{3,0}^{(a,E'')}] \otimes \mathbb{U}_5[\mathbb{Q}_1^{(u,A'_2)}] \otimes \mathbb{F}_9[\mathbb{Q}_{1,0}^{(k,E')}] }{4} + \frac{\sqrt{2}\mathbb{X}_{32}[\mathbb{Q}_{3,0}^{(a,E'')}] \otimes \mathbb{U}_6[\mathbb{T}_0^{(u,A'_1)}] \otimes \mathbb{F}_{17}[\mathbb{T}_{2,0}^{(k,E'')}] }{4} \\ & + \frac{\sqrt{2}\mathbb{X}_{32}[\mathbb{Q}_{3,0}^{(a,E'')}] \otimes \mathbb{U}_7[\mathbb{T}_1^{(u,A'_2)}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,0}^{(k,E')}] }{4} - \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{U}_4[\mathbb{Q}_0^{(u,A'_1)}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E'')}] }{4} \\ & - \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{U}_5[\mathbb{Q}_1^{(u,A'_2)}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(k,E')}] }{4} + \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{U}_6[\mathbb{T}_0^{(u,A'_1)}] \otimes \mathbb{F}_{18}[\mathbb{T}_{2,1}^{(k,E'')}] }{4} + \frac{\sqrt{2}\mathbb{X}_{33}[\mathbb{Q}_{3,1}^{(a,E'')}] \otimes \mathbb{U}_7[\mathbb{T}_1^{(u,A'_2)}] \otimes \mathbb{F}_{16}[\mathbb{T}_{1,1}^{(k,E')}] }{4}\end{aligned}$$

$$\boxed{\text{No. 21}} \quad \hat{\mathbb{Q}}_2^{(A'_1)} [\mathbb{M}_3, \mathbb{B}_2]$$

$$\begin{aligned}\hat{Z}_{21} = & \frac{\sqrt{2}\mathbb{X}_{29}[\mathbb{M}_{2,0}^{(a,E')}] \otimes \mathbb{Y}_{15}[\mathbb{T}_{1,0}^{(b,E')}] }{2} + \frac{\sqrt{2}\mathbb{X}_{30}[\mathbb{M}_{2,1}^{(a,E')}] \otimes \mathbb{Y}_{16}[\mathbb{T}_{1,1}^{(b,E')}] }{2} \\ \hat{Z}_{21}(\mathbf{k}) = & \frac{\sqrt{2}\mathbb{X}_{29}[\mathbb{M}_{2,0}^{(a,E')}] \otimes \mathbb{U}_4[\mathbb{Q}_0^{(u,A'_1)}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,0}^{(k,E')}] }{4} + \frac{\sqrt{2}\mathbb{X}_{29}[\mathbb{M}_{2,0}^{(a,E')}] \otimes \mathbb{U}_5[\mathbb{Q}_1^{(u,A'_2)}] \otimes \mathbb{F}_{17}[\mathbb{T}_{2,0}^{(k,E'')}] }{4} + \frac{\sqrt{2}\mathbb{X}_{29}[\mathbb{M}_{2,0}^{(a,E')}] \otimes \mathbb{U}_6[\mathbb{T}_0^{(u,A'_1)}] \otimes \mathbb{F}_9[\mathbb{Q}_{1,0}^{(k,E')}] }{4} \\ & + \frac{\sqrt{2}\mathbb{X}_{29}[\mathbb{M}_{2,0}^{(a,E')}] \otimes \mathbb{U}_7[\mathbb{T}_1^{(u,A'_2)}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k,E'')}] }{4} + \frac{\sqrt{2}\mathbb{X}_{30}[\mathbb{M}_{2,1}^{(a,E')}] \otimes \mathbb{U}_4[\mathbb{Q}_0^{(u,A'_1)}] \otimes \mathbb{F}_{16}[\mathbb{T}_{1,1}^{(k,E')}] }{4} + \frac{\sqrt{2}\mathbb{X}_{30}[\mathbb{M}_{2,1}^{(a,E')}] \otimes \mathbb{U}_5[\mathbb{Q}_1^{(u,A'_2)}] \otimes \mathbb{F}_{18}[\mathbb{T}_{2,1}^{(k,E'')}] }{4} \\ & + \frac{\sqrt{2}\mathbb{X}_{30}[\mathbb{M}_{2,1}^{(a,E')}] \otimes \mathbb{U}_6[\mathbb{T}_0^{(u,A'_1)}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(k,E')}] }{4} + \frac{\sqrt{2}\mathbb{X}_{30}[\mathbb{M}_{2,1}^{(a,E')}] \otimes \mathbb{U}_7[\mathbb{T}_1^{(u,A'_2)}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E'')}] }{4}\end{aligned}$$

$$\boxed{\text{No. 22}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\mathbb{M}_3, \mathbb{B}_2]$$

$$\begin{aligned}\hat{Z}_{22} = & -\frac{\sqrt{2}\mathbb{X}_{34}[\mathbb{M}_{2,0}^{(a,E'')}] \otimes \mathbb{Y}_{17}[\mathbb{T}_{2,0}^{(b,E'')}] }{2} - \frac{\sqrt{2}\mathbb{X}_{35}[\mathbb{M}_{2,1}^{(a,E'')}] \otimes \mathbb{Y}_{18}[\mathbb{T}_{2,1}^{(b,E'')}] }{2} \\ \hat{Z}_{22}(\mathbf{k}) = & -\frac{\sqrt{2}\mathbb{X}_{34}[\mathbb{M}_{2,0}^{(a,E'')}] \otimes \mathbb{U}_4[\mathbb{Q}_0^{(u,A'_1)}] \otimes \mathbb{F}_{17}[\mathbb{T}_{2,0}^{(k,E'')}] }{4} - \frac{\sqrt{2}\mathbb{X}_{34}[\mathbb{M}_{2,0}^{(a,E'')}] \otimes \mathbb{U}_5[\mathbb{Q}_1^{(u,A'_2)}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,0}^{(k,E')}] }{4} - \frac{\sqrt{2}\mathbb{X}_{34}[\mathbb{M}_{2,0}^{(a,E'')}] \otimes \mathbb{U}_6[\mathbb{T}_0^{(u,A'_1)}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k,E'')}] }{4} \\ & - \frac{\sqrt{2}\mathbb{X}_{34}[\mathbb{M}_{2,0}^{(a,E'')}] \otimes \mathbb{U}_7[\mathbb{T}_1^{(u,A'_2)}] \otimes \mathbb{F}_9[\mathbb{Q}_{1,0}^{(k,E')}] }{4} - \frac{\sqrt{2}\mathbb{X}_{35}[\mathbb{M}_{2,1}^{(a,E'')}] \otimes \mathbb{U}_4[\mathbb{Q}_0^{(u,A'_1)}] \otimes \mathbb{F}_{18}[\mathbb{T}_{2,1}^{(k,E'')}] }{4} - \frac{\sqrt{2}\mathbb{X}_{35}[\mathbb{M}_{2,1}^{(a,E'')}] \otimes \mathbb{U}_5[\mathbb{Q}_1^{(u,A'_2)}] \otimes \mathbb{F}_{16}[\mathbb{T}_{1,1}^{(k,E')}] }{4} \\ & - \frac{\sqrt{2}\mathbb{X}_{35}[\mathbb{M}_{2,1}^{(a,E'')}] \otimes \mathbb{U}_6[\mathbb{T}_0^{(u,A'_1)}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E'')}] }{4} - \frac{\sqrt{2}\mathbb{X}_{35}[\mathbb{M}_{2,1}^{(a,E'')}] \otimes \mathbb{U}_7[\mathbb{T}_1^{(u,A'_2)}] \otimes \mathbb{F}_{10}[\mathbb{Q}_{1,1}^{(k,E')}] }{4}\end{aligned}$$

$$\boxed{\text{No. 23}} \quad \hat{\mathbb{Q}}_0^{(A'_1)} [\mathbb{M}_2, \mathbb{B}_3]$$

$$\hat{Z}_{23} = \mathbb{X}_{14}[\mathbb{Q}_0^{(a,A'_1)}] \otimes \mathbb{Y}_{19}[\mathbb{Q}_0^{(b,A'_1)}]$$

$$\hat{Z}_{23}(\mathbf{k}) = \mathbb{X}_{14}[\mathbb{Q}_0^{(a,A'_1)}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A'_1)}] \otimes \mathbb{F}_{19}[\mathbb{Q}_0^{(k,A'_1)}]$$



$$\boxed{\text{No. 24}} \quad \hat{\mathbb{Q}}_2^{(A'_1)} [\text{M}_2, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{24} = \mathbb{X}_{15}[\mathbb{Q}_2^{(a,A'_1)}] \otimes \mathbb{Y}_{19}[\mathbb{Q}_0^{(b,A'_1)}]$$

$$\hat{\mathbb{Z}}_{24}(\mathbf{k}) = \mathbb{X}_{15}[\mathbb{Q}_2^{(a,A'_1)}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A'_1)}] \otimes \mathbb{F}_{19}[\mathbb{Q}_0^{(k,A'_1)}]$$

$$\boxed{\text{No. 25}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\text{M}_2, \text{B}_3]$$

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

$$\hat{\mathbb{Z}}_{25}(\mathbf{k}) = -\frac{\sqrt{2}\mathbb{X}_{16}[\mathbb{Q}_{2,0}^{(a,E')}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A'_1)}] \otimes \mathbb{F}_{20}[\mathbb{Q}_{1,0}^{(k,E')}] }{2} - \frac{\sqrt{2}\mathbb{X}_{17}[\mathbb{Q}_{2,1}^{(a,E')}] \otimes \mathbb{U}_2[\mathbb{Q}_0^{(s,A'_1)}] \otimes \mathbb{F}_{21}[\mathbb{Q}_{1,1}^{(k,E')}] }{2}$$

$$\boxed{\text{No. 26}} \quad \hat{\mathbb{Q}}_0^{(A'_1)} [\text{M}_2, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{26} = \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{Q}_{2,0}^{(a,E'')}] \otimes \mathbb{Y}_{22}[\mathbb{Q}_{2,0}^{(b,E'')}] }{2} + \frac{\sqrt{2}\mathbb{X}_{19}[\mathbb{Q}_{2,1}^{(a,E'')}] \otimes \mathbb{Y}_{23}[\mathbb{Q}_{2,1}^{(b,E'')}] }{2}$$

$$\hat{\mathbb{Z}}_{26}(\mathbf{k}) = \frac{\sqrt{2}\mathbb{X}_{18}[\mathbb{Q}_{2,0}^{(a,E'')}] \otimes \mathbb{U}_3[\mathbb{Q}_1^{(s,A'_2)}] \otimes \mathbb{F}_{20}[\mathbb{Q}_{1,0}^{(k,E')}] }{2} + \frac{\sqrt{2}\mathbb{X}_{19}[\mathbb{Q}_{2,1}^{(a,E'')}] \otimes \mathbb{U}_3[\mathbb{Q}_1^{(s,A'_2)}] \otimes \mathbb{F}_{21}[\mathbb{Q}_{1,1}^{(k,E')}] }{2}$$

$$\boxed{\text{No. 27}} \quad \hat{\mathbb{Q}}_2^{(A'_1)} [\text{M}_2, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{27} = \frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{M}_{1,0}^{(a,E'')}] \otimes \mathbb{Y}_{24}[\mathbb{T}_{2,0}^{(b,E'')}] }{2} + \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{M}_{1,1}^{(a,E'')}] \otimes \mathbb{Y}_{25}[\mathbb{T}_{2,1}^{(b,E'')}] }{2}$$

$$\hat{\mathbb{Z}}_{27}(\mathbf{k}) = \frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{M}_{1,0}^{(a,E'')}] \otimes \mathbb{U}_3[\mathbb{Q}_1^{(s,A'_2)}] \otimes \mathbb{F}_{22}[\mathbb{T}_{1,0}^{(k,E')}] }{2} + \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{M}_{1,1}^{(a,E'')}] \otimes \mathbb{U}_3[\mathbb{Q}_1^{(s,A'_2)}] \otimes \mathbb{F}_{23}[\mathbb{T}_{1,1}^{(k,E')}] }{2}$$

$$\boxed{\text{No. 28}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\text{M}_2, \text{B}_3]$$

$$\hat{\mathbb{Z}}_{28} = \mathbb{X}_{20}[\mathbb{M}_1^{(a,A'_2)}] \otimes \mathbb{Y}_{26}[\mathbb{T}_3^{(b,A'_2)}]$$

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

Table 5: Atomic SAMB group.

group	bra	ket
M <sub>1</sub>	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$
M <sub>2</sub>	$p_x, p_y, p_z$	$p_x, p_y, p_z$
M <sub>3</sub>	$d_u, d_v, d_{yz}, d_{zx}, d_{xy}$	$p_x, p_y, p_z$

Table 6: Atomic SAMB.

symbol	type	group	form
$\mathbb{X}_1$	$\mathbb{Q}_0^{(a, A'_1)}$	M <sub>1</sub>	$\begin{pmatrix} \frac{\sqrt{5}}{5} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{5}}{5} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{5}}{5} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{5}}{5} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{5}}{5} \end{pmatrix}$
$\mathbb{X}_2$	$\mathbb{Q}_2^{(a, A'_1)}$	M <sub>1</sub>	$\begin{pmatrix} \frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{7} \end{pmatrix}$
$\mathbb{X}_3$	$\mathbb{Q}_4^{(a, A'_1)}$	M <sub>1</sub>	$\begin{pmatrix} \frac{3\sqrt{70}}{35} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{70}}{70} & 0 & 0 & 0 \\ 0 & 0 & -\frac{2\sqrt{70}}{35} & 0 & 0 \\ 0 & 0 & 0 & -\frac{2\sqrt{70}}{35} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{70}}{70} \end{pmatrix}$
$\mathbb{X}_4$	$\mathbb{Q}_{2,0}^{(a, E')}$	M <sub>1</sub>	$\begin{pmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{7} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \\ -\frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \end{pmatrix}$

*continued ...*

Table 6

symbol	type	group	form
$\mathbb{X}_5$	$\mathbb{Q}_{2,1}^{(a,E')}$	$M_1$	$\begin{pmatrix} 0 & \frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ \frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_6$	$\mathbb{Q}_{4,0}^{(a,E',1)}$	$M_1$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_7$	$\mathbb{Q}_{4,1}^{(a,E',1)}$	$M_1$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{X}_8$	$\mathbb{Q}_{4,0}^{(a,E',2)}$	$M_1$	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0 \\ 0 & 0 & -\frac{\sqrt{14}}{7} & 0 & 0 \\ \frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_9$	$\mathbb{Q}_{4,1}^{(a,E',2)}$	$M_1$	$\begin{pmatrix} 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{10}$	$M_1^{(a,A'_2)}$	$M_1$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{10}i}{5} \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_{11}$	$\mathbb{M}_3^{(a, A'_2)}$	$M_1$	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{10}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{5} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{10} & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{12}$	$\mathbb{M}_{3,0}^{(a, E')}$	$M_1$	$\begin{pmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{13}$	$\mathbb{M}_{3,1}^{(a, E')}$	$M_1$	$\begin{pmatrix} 0 & \frac{\sqrt{2}i}{2} & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{14}$	$\mathbb{Q}_0^{(a, A'_1)}$	$M_2$	$\begin{pmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$
$\mathbb{X}_{15}$	$\mathbb{Q}_2^{(a, A'_1)}$	$M_2$	$\begin{pmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{pmatrix}$
$\mathbb{X}_{16}$	$\mathbb{Q}_{2,0}^{(a, E')}$	$M_2$	$\begin{pmatrix} 0 & -\frac{\sqrt{2}}{2} & 0 \\ -\frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{17}$	$\mathbb{Q}_{2,1}^{(a, E')}$	$M_2$	$\begin{pmatrix} -\frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{18}$	$\mathbb{Q}_{2,0}^{(a, E'')}$	$M_2$	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_{19}$	$\mathbb{Q}_{2,1}^{(a,E'')}$	$M_2$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
$\mathbb{X}_{20}$	$\mathbb{M}_1^{(a,A'_2)}$	$M_2$	$\begin{pmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{21}$	$\mathbb{M}_{1,0}^{(a,E'')}$	$M_2$	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{22}$	$\mathbb{M}_{1,1}^{(a,E'')}$	$M_2$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & \frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$
$\mathbb{X}_{23}$	$\mathbb{Q}_1^{(a,A'_2)}$	$M_3$	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{10}}{5} \\ 0 & 0 & 0 \\ 0 & \frac{\sqrt{30}}{10} & 0 \\ \frac{\sqrt{30}}{10} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{24}$	$\mathbb{Q}_3^{(a,A'_2)}$	$M_3$	$\begin{pmatrix} 0 & 0 & \frac{\sqrt{15}}{5} \\ 0 & 0 & 0 \\ 0 & -\frac{\sqrt{5}}{5} & 0 \\ -\frac{\sqrt{5}}{5} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{25}$	$\mathbb{Q}_{1,0}^{(a,E')}$	$M_3$	$\begin{pmatrix} -\frac{\sqrt{10}}{10} & 0 & 0 \\ \frac{\sqrt{30}}{10} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{30}}{10} \\ 0 & -\frac{\sqrt{30}}{10} & 0 \end{pmatrix}$
$\mathbb{X}_{26}$	$\mathbb{Q}_{1,1}^{(a,E')}$	$M_3$	$\begin{pmatrix} 0 & -\frac{\sqrt{10}}{10} & 0 \\ 0 & -\frac{\sqrt{30}}{10} & 0 \\ 0 & 0 & \frac{\sqrt{30}}{10} \\ 0 & 0 & 0 \\ -\frac{\sqrt{30}}{10} & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_{27}$	$\mathbb{Q}_{3,0}^{(a,E')}$	$M_3$	$\begin{pmatrix} \frac{\sqrt{10}}{5} & 0 & 0 \\ -\frac{\sqrt{30}}{30} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{2\sqrt{30}}{15} \\ 0 & \frac{\sqrt{30}}{30} & 0 \end{pmatrix}$
$\mathbb{X}_{28}$	$\mathbb{Q}_{3,1}^{(a,E')}$	$M_3$	$\begin{pmatrix} 0 & \frac{\sqrt{10}}{5} & 0 \\ 0 & \frac{\sqrt{30}}{30} & 0 \\ 0 & 0 & \frac{2\sqrt{30}}{15} \\ 0 & 0 & 0 \\ \frac{\sqrt{30}}{30} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{29}$	$\mathbb{M}_{2,0}^{(a,E')}$	$M_3$	$\begin{pmatrix} \frac{\sqrt{2i}}{2} & 0 & 0 \\ \frac{\sqrt{6i}}{6} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6i}}{6} \\ 0 & -\frac{\sqrt{6i}}{6} & 0 \end{pmatrix}$
$\mathbb{X}_{30}$	$\mathbb{M}_{2,1}^{(a,E')}$	$M_3$	$\begin{pmatrix} 0 & \frac{\sqrt{2i}}{2} & 0 \\ 0 & -\frac{\sqrt{6i}}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{6i}}{6} \\ 0 & 0 & 0 \\ -\frac{\sqrt{6i}}{6} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{31}$	$\mathbb{Q}_3^{(a,A'_1)}$	$M_3$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ -\frac{\sqrt{2}}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{32}$	$\mathbb{Q}_{3,0}^{(a,E'')}$	$M_3$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -\frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
$\mathbb{X}_{33}$	$\mathbb{Q}_{3,1}^{(a,E'')}$	$M_3$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{3} \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ -\frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_{34}$	$\mathbb{M}_{2,0}^{(a,E'')}$	$M_3$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & \frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{3} \end{pmatrix}$
$\mathbb{X}_{35}$	$\mathbb{M}_{2,1}^{(a,E'')}$	$M_3$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{3} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
$\mathbb{Y}_1$	$\mathbb{Q}_0^{(s,A'_1)}$	$S_1$	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{Y}_2$	$\mathbb{Q}_0^{(s,A'_1)}$	$S_2$	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_3$	$\mathbb{Q}_0^{(b,A'_1)}$	$B_1$	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \end{pmatrix}$
$\mathbb{Y}_4$	$\mathbb{Q}_{1,0}^{(b,E')}$	$B_1$	$\begin{pmatrix} -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
$\mathbb{Y}_5$	$\mathbb{Q}_{1,1}^{(b,E')}$	$B_1$	$\begin{pmatrix} -\frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{3} \end{pmatrix}$
$\mathbb{Y}_6$	$\mathbb{T}_{1,0}^{(b,E')}$	$B_1$	$\begin{pmatrix} \frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{3} \end{pmatrix}$
$\mathbb{Y}_7$	$\mathbb{T}_{1,1}^{(b,E')}$	$B_1$	$\begin{pmatrix} -\frac{\sqrt{2}i}{2} & -\frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$
$\mathbb{Y}_8$	$\mathbb{T}_3^{(b,A'_2)}$	$B_1$	$\begin{pmatrix} \frac{\sqrt{3}i}{3} & -\frac{\sqrt{3}i}{3} & \frac{\sqrt{3}i}{3} \end{pmatrix}$
$\mathbb{Y}_9$	$\mathbb{Q}_0^{(b,A'_1)}$	$B_2$	$\begin{pmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$

continued ...

Table 7

symbol	type	cluster	form
Y <sub>10</sub>	$\mathbb{Q}_1^{(b,A'_2)}$	B <sub>2</sub>	$\begin{pmatrix} \frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
Y <sub>11</sub>	$\mathbb{Q}_{1,0}^{(b,E')}$	B <sub>2</sub>	$\begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & \frac{1}{2} & 0 \end{pmatrix}$
Y <sub>12</sub>	$\mathbb{Q}_{1,1}^{(b,E')}$	B <sub>2</sub>	$\begin{pmatrix} -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} \end{pmatrix}$
Y <sub>13</sub>	$\mathbb{Q}_{2,0}^{(b,E'')}$	B <sub>2</sub>	$\begin{pmatrix} -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} & 0 \end{pmatrix}$
Y <sub>14</sub>	$\mathbb{Q}_{2,1}^{(b,E'')}$	B <sub>2</sub>	$\begin{pmatrix} -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} \end{pmatrix}$
Y <sub>15</sub>	$\mathbb{T}_{1,0}^{(b,E')}$	B <sub>2</sub>	$\begin{pmatrix} -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} & 0 & \frac{i}{2} & 0 \end{pmatrix}$
Y <sub>16</sub>	$\mathbb{T}_{1,1}^{(b,E')}$	B <sub>2</sub>	$\begin{pmatrix} -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} & \frac{\sqrt{3}i}{3} & -\frac{\sqrt{3}i}{6} & \frac{\sqrt{3}i}{3} \end{pmatrix}$
Y <sub>17</sub>	$\mathbb{T}_{2,0}^{(b,E'')}$	B <sub>2</sub>	$\begin{pmatrix} -\frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & 0 & \frac{i}{2} & 0 \end{pmatrix}$
Y <sub>18</sub>	$\mathbb{T}_{2,1}^{(b,E'')}$	B <sub>2</sub>	$\begin{pmatrix} -\frac{\sqrt{3}i}{6} & \frac{\sqrt{3}i}{6} & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{3} & -\frac{\sqrt{3}i}{6} & \frac{\sqrt{3}i}{3} \end{pmatrix}$
Y <sub>19</sub>	$\mathbb{Q}_0^{(b,A'_1)}$	B <sub>3</sub>	$\begin{pmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
Y <sub>20</sub>	$\mathbb{Q}_{1,0}^{(b,E')}$	B <sub>3</sub>	$\begin{pmatrix} 0 & 0 & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$
Y <sub>21</sub>	$\mathbb{Q}_{1,1}^{(b,E')}$	B <sub>3</sub>	$\begin{pmatrix} -\frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} \end{pmatrix}$
Y <sub>22</sub>	$\mathbb{Q}_{2,0}^{(b,E'')}$	B <sub>3</sub>	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$
Y <sub>23</sub>	$\mathbb{Q}_{2,1}^{(b,E'')}$	B <sub>3</sub>	$\begin{pmatrix} -\frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} \end{pmatrix}$
Y <sub>24</sub>	$\mathbb{T}_{2,0}^{(b,E'')}$	B <sub>3</sub>	$\begin{pmatrix} -\frac{\sqrt{3}i}{3} & \frac{\sqrt{3}i}{3} & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{6} \end{pmatrix}$
Y <sub>25</sub>	$\mathbb{T}_{2,1}^{(b,E'')}$	B <sub>3</sub>	$\begin{pmatrix} 0 & 0 & \frac{i}{2} & \frac{i}{2} & -\frac{i}{2} & -\frac{i}{2} \end{pmatrix}$
Y <sub>26</sub>	$\mathbb{T}_3^{(b,A'_2)}$	B <sub>3</sub>	$\begin{pmatrix} \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{6} \end{pmatrix}$

Table 8: Uniform SAMB.

symbol	type	cluster	form
U <sub>1</sub>	$\mathbb{Q}_0^{(s,A'_1)}$	S <sub>1</sub>	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

continued ...



Table 8

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

Table 9: Structure SAMB.

symbol	type	cluster	form
$\mathbb{F}_1$	$\mathbb{Q}_0^{(k,A'_1)}$	$B_1$	$\frac{\sqrt{6}c_{001}}{3} + \frac{\sqrt{6}c_{002}}{3} + \frac{\sqrt{6}c_{003}}{3}$
$\mathbb{F}_2$	$\mathbb{Q}_{1,0}^{(k,E')}$	$B_1$	$-c_{001} + c_{002}$
$\mathbb{F}_3$	$\mathbb{Q}_{1,1}^{(k,E')}$	$B_1$	$-\frac{\sqrt{3}c_{001}}{3} - \frac{\sqrt{3}c_{002}}{3} + \frac{2\sqrt{3}c_{003}}{3}$
$\mathbb{F}_4$	$\mathbb{T}_{1,0}^{(k,E')}$	$B_1$	$\frac{\sqrt{3}s_{001}}{3} - \frac{\sqrt{3}s_{002}}{3} - \frac{2\sqrt{3}s_{003}}{3}$
$\mathbb{F}_5$	$\mathbb{T}_{1,1}^{(k,E')}$	$B_1$	$-s_{001} - s_{002}$
$\mathbb{F}_6$	$\mathbb{T}_3^{(k,A'_2)}$	$B_1$	$\frac{\sqrt{6}s_{001}}{3} - \frac{\sqrt{6}s_{002}}{3} + \frac{\sqrt{6}s_{003}}{3}$
$\mathbb{F}_7$	$\mathbb{Q}_0^{(k,A'_1)}$	$B_2$	$\frac{\sqrt{3}c_{004}}{3} + \frac{\sqrt{3}c_{005}}{3} + \frac{\sqrt{3}c_{006}}{3} + \frac{\sqrt{3}c_{007}}{3} + \frac{\sqrt{3}c_{008}}{3} + \frac{\sqrt{3}c_{009}}{3}$

continued ...

Table 9

symbol	type	cluster	form
F <sub>8</sub>	$\mathbb{Q}_1^{(k,A_2'')}$	B <sub>2</sub>	$\frac{\sqrt{3}c_{004}}{3} - \frac{\sqrt{3}c_{005}}{3} - \frac{\sqrt{3}c_{006}}{3} - \frac{\sqrt{3}c_{007}}{3} + \frac{\sqrt{3}c_{008}}{3} + \frac{\sqrt{3}c_{009}}{3}$
F <sub>9</sub>	$\mathbb{Q}_{1,0}^{(k,E')}$	B <sub>2</sub>	$-\frac{\sqrt{2}c_{004}}{2} + \frac{\sqrt{2}c_{005}}{2} - \frac{\sqrt{2}c_{006}}{2} + \frac{\sqrt{2}c_{008}}{2}$
F <sub>10</sub>	$\mathbb{Q}_{1,1}^{(k,E')}$	B <sub>2</sub>	$-\frac{\sqrt{6}c_{004}}{6} - \frac{\sqrt{6}c_{005}}{6} - \frac{\sqrt{6}c_{006}}{6} + \frac{\sqrt{6}c_{007}}{3} - \frac{\sqrt{6}c_{008}}{6} + \frac{\sqrt{6}c_{009}}{3}$
F <sub>11</sub>	$\mathbb{Q}_{2,0}^{(k,E'')}$	B <sub>2</sub>	$-\frac{\sqrt{2}c_{004}}{2} - \frac{\sqrt{2}c_{005}}{2} + \frac{\sqrt{2}c_{006}}{2} + \frac{\sqrt{2}c_{008}}{2}$
F <sub>12</sub>	$\mathbb{Q}_{2,1}^{(k,E'')}$	B <sub>2</sub>	$-\frac{\sqrt{6}c_{004}}{6} + \frac{\sqrt{6}c_{005}}{6} + \frac{\sqrt{6}c_{006}}{6} - \frac{\sqrt{6}c_{007}}{3} - \frac{\sqrt{6}c_{008}}{6} + \frac{\sqrt{6}c_{009}}{3}$
F <sub>13</sub>	$\mathbb{T}_0^{(k,A_1')}$	B <sub>2</sub>	$\frac{\sqrt{3}s_{004}}{3} + \frac{\sqrt{3}s_{005}}{3} + \frac{\sqrt{3}s_{006}}{3} + \frac{\sqrt{3}s_{007}}{3} + \frac{\sqrt{3}s_{008}}{3} + \frac{\sqrt{3}s_{009}}{3}$
F <sub>14</sub>	$\mathbb{T}_1^{(k,A_2'')}$	B <sub>2</sub>	$\frac{\sqrt{3}s_{004}}{3} - \frac{\sqrt{3}s_{005}}{3} - \frac{\sqrt{3}s_{006}}{3} - \frac{\sqrt{3}s_{007}}{3} + \frac{\sqrt{3}s_{008}}{3} + \frac{\sqrt{3}s_{009}}{3}$
F <sub>15</sub>	$\mathbb{T}_{1,0}^{(k,E')}$	B <sub>2</sub>	$-\frac{\sqrt{2}s_{004}}{2} + \frac{\sqrt{2}s_{005}}{2} - \frac{\sqrt{2}s_{006}}{2} + \frac{\sqrt{2}s_{008}}{2}$
F <sub>16</sub>	$\mathbb{T}_{1,1}^{(k,E')}$	B <sub>2</sub>	$-\frac{\sqrt{6}s_{004}}{6} - \frac{\sqrt{6}s_{005}}{6} - \frac{\sqrt{6}s_{006}}{6} + \frac{\sqrt{6}s_{007}}{3} - \frac{\sqrt{6}s_{008}}{6} + \frac{\sqrt{6}s_{009}}{3}$
F <sub>17</sub>	$\mathbb{T}_{2,0}^{(k,E'')}$	B <sub>2</sub>	$-\frac{\sqrt{2}s_{004}}{2} - \frac{\sqrt{2}s_{005}}{2} + \frac{\sqrt{2}s_{006}}{2} + \frac{\sqrt{2}s_{008}}{2}$
F <sub>18</sub>	$\mathbb{T}_{2,1}^{(k,E'')}$	B <sub>2</sub>	$-\frac{\sqrt{6}s_{004}}{6} + \frac{\sqrt{6}s_{005}}{6} + \frac{\sqrt{6}s_{006}}{6} - \frac{\sqrt{6}s_{007}}{3} - \frac{\sqrt{6}s_{008}}{6} + \frac{\sqrt{6}s_{009}}{3}$
F <sub>19</sub>	$\mathbb{Q}_0^{(k,A_1')}$	B <sub>3</sub>	$\frac{\sqrt{6}c_{010}}{3} + \frac{\sqrt{6}c_{012}}{3} + \frac{\sqrt{6}c_{013}}{3}$
F <sub>20</sub>	$\mathbb{Q}_{1,0}^{(k,E')}$	B <sub>3</sub>	$-c_{012} + c_{013}$
F <sub>21</sub>	$\mathbb{Q}_{1,1}^{(k,E')}$	B <sub>3</sub>	$-\frac{2\sqrt{3}c_{010}}{3} + \frac{\sqrt{3}c_{012}}{3} + \frac{\sqrt{3}c_{013}}{3}$
F <sub>22</sub>	$\mathbb{T}_{1,0}^{(k,E')}$	B <sub>3</sub>	$-\frac{2\sqrt{3}s_{010}}{3} - \frac{\sqrt{3}s_{012}}{3} + \frac{\sqrt{3}s_{013}}{3}$
F <sub>23</sub>	$\mathbb{T}_{1,1}^{(k,E')}$	B <sub>3</sub>	$-s_{012} - s_{013}$
F <sub>24</sub>	$\mathbb{T}_3^{(k,A_2')}$	B <sub>3</sub>	$\frac{\sqrt{6}s_{010}}{3} - \frac{\sqrt{6}s_{012}}{3} + \frac{\sqrt{6}s_{013}}{3}$

Table 10: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_1')}$	0	$A_1'$	—	—	1
2	$\mathbb{Q}_1^{(A_2'')}$	1	$A_2''$	—	—	$z$
3	$\mathbb{Q}_{1,0}^{(E')}$	1	$E'$	—	0	$x$
4	$\mathbb{Q}_{1,1}^{(E')}$	1	$E'$	—	1	$y$
5	$\mathbb{Q}_2^{(A_1')}$	2	$A_1'$	—	—	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$

continued ...

Table 10

No.	symbol	rank	irrep.	mul.	comp.	form
6	$\mathbb{Q}_{2,0}^{(E'')}$	2	$E''$	—	0	$\sqrt{3}xz$
7	$\mathbb{Q}_{2,1}^{(E'')}$	2	$E''$	—	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	$\mathbb{Q}_3^{(A'_1)}$	3	$A'_1$	—	—	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$
11	$\mathbb{Q}_3^{(A''_2)}$	3	$A''_2$	—	—	$-\frac{z(3x^2+3y^2-2z^2)}{4}$
12	$\mathbb{Q}_3^{(A'_2)}$	3	$A'_2$	—	—	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$
13	$\mathbb{Q}_{3,0}^{(E'')}$	3	$E''$	—	0	$-\sqrt{15}xyz$
14	$\mathbb{Q}_{3,1}^{(E'')}$	3	$E''$	—	1	$-\frac{\sqrt{15}z(x-y)(x+y)}{2}$
15	$\mathbb{Q}_{3,0}^{(E')}$	3	$E'$	—	0	$-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$
16	$\mathbb{Q}_{3,1}^{(E')}$	3	$E'$	—	1	$-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$
17	$\mathbb{Q}_4^{(A'_1)}$	4	$A'_1$	—	—	$\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$
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	$\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$

Table 11: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_1^{(A'_2)}$	1	$A'_2$	—	—	$Z$
2	$\mathbb{G}_{1,0}^{(E'')}$	1	$E''$	—	0	$-Y$
3	$\mathbb{G}_{1,1}^{(E'')}$	1	$E''$	—	1	$X$
4	$\mathbb{G}_{2,0}^{(E'')}$	2	$E''$	—	0	$\frac{\sqrt{3}(X-Y)(X+Y)}{2}$
5	$\mathbb{G}_{2,1}^{(E'')}$	2	$E''$	—	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	$\sqrt{3}XZ$

continued ...

Table 11

No.	symbol	rank	irrep.	mul.	comp.	form
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	$-\sqrt{15}XYZ$

- 
- 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	2 <sub>120</sub>	3 <sup>+</sup> <sub>001</sub>	m <sub>100</sub>	m <sub>001</sub>	-6 <sup>+</sup> <sub>001</sub>
$A'_1$	1	1	1	1	1	1
$A'_2$	1	-1	1	-1	1	1
$A''_1$	1	1	1	-1	-1	-1
$A''_2$	1	-1	1	1	-1	-1
$E'$	2	0	-1	0	2	-1
$E''$	2	0	-1	0	-2	1

Table 15: Parity conversion.

$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$
$A'_1 (A''_1)$	$A'_2 (A''_2)$	$A''_1 (A'_1)$	$A''_2 (A'_2)$	$E'' (E')$
$E' (E'')$				

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

	$A'_1$	$A'_2$	$A''_1$	$A''_2$	$E'$	$E''$
$A'_1$	$A'_1$	$A'_2$	$A''_1$	$A''_2$	$E'$	$E''$
$A'_2$		$A'_1$	$A''_2$	$A''_1$	$E'$	$E''$
$A''_1$			$A'_1$	$A'_2$	$E''$	$E'$
$A''_2$				$A'_1$	$E''$	$E'$
$E'$					$A'_1 + E'$	$A'_1 + A'_2 + E''$
$E''$						$A'_1 + E'$

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

$A'_1$	$A'_2$	$A''_1$	$A''_2$	$E'$	$E''$
-	-	-	-	$A'_2$	$A'_2$

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
$\mathbb{Q}_0^{(A_1')}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$
$\mathbb{Q}_1^{(A_2'')}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$
$\mathbb{Q}_{1,0}^{(E')}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$
$\mathbb{Q}_{1,1}^{(E')}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$
$\mathbb{Q}_{2,0}^{(E')}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	0	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	0	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$
$\mathbb{Q}_{2,1}^{(E')}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
$\mathbb{Q}_{2,0}^{(E'')}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
$\mathbb{Q}_{2,1}^{(E'')}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	0	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
$\mathbb{Q}_3^{(A_2')}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$

*continued ...*

Table 19

symbol	1	2	3	4	5	6	7	8	9	10
	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$								
$\mathbb{Q}_{3,0}^{(E'')}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	0	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
	$-\frac{\sqrt{2}}{4}$	0								
$\mathbb{Q}_{3,1}^{(E'')}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$								
$\mathbb{Q}_4^{(A_1'')}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$
	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$								