

SAMB for “UPt2Si2”

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- Group: No. 129 D_{4h}^7 $P4/nmm$ [tetragonal]
 - Associated point group: No. 15 D_{4h} $4/mmm$ [tetragonal]
 - Generation condition
 - model type: **tight_binding**
 - time-reversal type: **electric**
 - irrep: **[A1g]**
 - **spinless**
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- Unit cell:
 $a = 4.1972$, $b = 4.1972$, $c = 9.6906$, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 90.0$
- Lattice vectors:
 $\mathbf{a}_1 = (4.1972 \ 0 \ 0)$
 $\mathbf{a}_2 = (0 \ 4.1972 \ 0)$
 $\mathbf{a}_3 = (0 \ 0 \ 9.6906)$

Table 1: High-symmetry line: Γ -X.

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

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- Kets: dimension = 46

Table 2: Hilbert space for full matrix.

No.	ket	No.	ket	No.	ket	No.	ket	No.	ket
1	$f_{xyz}@U_1$	2	$f_{ax}@U_1$	3	$f_{ay}@U_1$	4	$f_{az}@U_1$	5	$f_{bx}@U_1$
6	$f_{by}@U_1$	7	$f_{bz}@U_1$	8	$f_{xyz}@U_2$	9	$f_{ax}@U_2$	10	$f_{ay}@U_2$
11	$f_{az}@U_2$	12	$f_{bx}@U_2$	13	$f_{by}@U_2$	14	$f_{bz}@U_2$	15	$d_u@Pt1_1$
16	$d_v@Pt1_1$	17	$d_{yz}@Pt1_1$	18	$d_{zx}@Pt1_1$	19	$d_{xy}@Pt1_1$	20	$d_u@Pt1_2$
21	$d_v@Pt1_2$	22	$d_{yz}@Pt1_2$	23	$d_{zx}@Pt1_2$	24	$d_{xy}@Pt1_2$	25	$d_u@Pt2_1$
26	$d_v@Pt2_1$	27	$d_{yz}@Pt2_1$	28	$d_{zx}@Pt2_1$	29	$d_{xy}@Pt2_1$	30	$d_u@Pt2_2$
31	$d_v@Pt2_2$	32	$d_{yz}@Pt2_2$	33	$d_{zx}@Pt2_2$	34	$d_{xy}@Pt2_2$	35	$p_x@Si1_1$
36	$p_y@Si1_1$	37	$p_z@Si1_1$	38	$p_x@Si1_2$	39	$p_y@Si1_2$	40	$p_z@Si1_2$
41	$p_x@Si2_1$	42	$p_y@Si2_1$	43	$p_z@Si2_1$	44	$p_x@Si2_2$	45	$p_y@Si2_2$
46	$p_z@Si2_2$								

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

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

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	$\mathbf{b@c}$	mapping
B ₁	b ₁	Pt1 ₁	Si2 ₁	1	1	$\begin{pmatrix} \frac{1}{2} & 0 & 0.133 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{4} & 0.0665 \end{pmatrix}$	[1,12]
	b ₂	Pt1 ₁	Si2 ₁	1	1	$\begin{pmatrix} -\frac{1}{2} & 0 & 0.133 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{4} & 0.0665 \end{pmatrix}$	[2,11]
	b ₃	Pt1 ₂	Si2 ₂	1	1	$\begin{pmatrix} \frac{1}{2} & 0 & -0.133 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{3}{4} & 0.9335 \end{pmatrix}$	[3,10]
	b ₄	Pt1 ₂	Si2 ₂	1	1	$\begin{pmatrix} -\frac{1}{2} & 0 & -0.133 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{3}{4} & 0.9335 \end{pmatrix}$	[4,9]
	b ₅	Pt1 ₁	Si2 ₂	1	1	$\begin{pmatrix} 0 & \frac{1}{2} & -0.133 \end{pmatrix} @ \begin{pmatrix} \frac{3}{4} & \frac{1}{2} & 0.9335 \end{pmatrix}$	[5,16]
	b ₆	Pt1 ₁	Si2 ₂	1	1	$\begin{pmatrix} 0 & -\frac{1}{2} & -0.133 \end{pmatrix} @ \begin{pmatrix} \frac{3}{4} & 0 & 0.9335 \end{pmatrix}$	[6,15]
	b ₇	Pt1 ₂	Si2 ₁	1	1	$\begin{pmatrix} 0 & \frac{1}{2} & 0.133 \end{pmatrix} @ \begin{pmatrix} \frac{1}{4} & 0 & 0.0665 \end{pmatrix}$	[7,14]
	b ₈	Pt1 ₂	Si2 ₁	1	1	$\begin{pmatrix} 0 & -\frac{1}{2} & 0.133 \end{pmatrix} @ \begin{pmatrix} \frac{1}{4} & \frac{1}{2} & 0.0665 \end{pmatrix}$	[8,13]
B ₂	b ₉	Pt2 ₁	Si1 ₁	1	1	$\begin{pmatrix} -\frac{1}{2} & 0 & 0.1215 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{4} & 0.43925 \end{pmatrix}$	[1,12]
	b ₁₀	Pt2 ₁	Si1 ₁	1	1	$\begin{pmatrix} \frac{1}{2} & 0 & 0.1215 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{4} & 0.43925 \end{pmatrix}$	[2,11]
	b ₁₁	Pt2 ₂	Si1 ₂	1	1	$\begin{pmatrix} -\frac{1}{2} & 0 & -0.1215 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{3}{4} & 0.56075 \end{pmatrix}$	[3,10]
	b ₁₂	Pt2 ₂	Si1 ₂	1	1	$\begin{pmatrix} \frac{1}{2} & 0 & -0.1215 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{3}{4} & 0.56075 \end{pmatrix}$	[4,9]
	b ₁₃	Pt2 ₂	Si1 ₁	1	1	$\begin{pmatrix} 0 & -\frac{1}{2} & -0.1215 \end{pmatrix} @ \begin{pmatrix} \frac{3}{4} & \frac{1}{2} & 0.56075 \end{pmatrix}$	[5,16]
	b ₁₄	Pt2 ₂	Si1 ₁	1	1	$\begin{pmatrix} 0 & \frac{1}{2} & -0.1215 \end{pmatrix} @ \begin{pmatrix} \frac{3}{4} & 0 & 0.56075 \end{pmatrix}$	[6,15]
	b ₁₅	Pt2 ₁	Si1 ₂	1	1	$\begin{pmatrix} 0 & -\frac{1}{2} & 0.1215 \end{pmatrix} @ \begin{pmatrix} \frac{1}{4} & 0 & 0.43925 \end{pmatrix}$	[7,14]
	b ₁₆	Pt2 ₁	Si1 ₂	1	1	$\begin{pmatrix} 0 & \frac{1}{2} & 0.1215 \end{pmatrix} @ \begin{pmatrix} \frac{1}{4} & \frac{1}{2} & 0.43925 \end{pmatrix}$	[8,13]

- SAMB:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned}
\hat{Z}_{19}(\mathbf{k}) = & -\frac{\sqrt{3}\mathbb{X}_{13}[\mathbb{Q}_1^{(a,A_{2u})}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{T}_1^{(k,A_{2u})}]}{6} - \frac{\sqrt{3}\mathbb{X}_{13}[\mathbb{Q}_1^{(a,A_{2u})}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_8[\mathbb{T}_3^{(k,B_{2u})}]}{6} + \frac{\sqrt{3}\mathbb{X}_{13}[\mathbb{Q}_1^{(a,A_{2u})}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_{1g})}]}{6} \\
& + \frac{\sqrt{3}\mathbb{X}_{13}[\mathbb{Q}_1^{(a,A_{2u})}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_2[\mathbb{Q}_2^{(k,B_{1g})}]}{6} - \frac{\sqrt{3}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a,E_u)}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{T}_{1,0}^{(k,E_u)}]}{6} - \frac{\sqrt{3}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a,E_u)}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_6[\mathbb{T}_{1,0}^{(k,E_u)}]}{6} \\
& + \frac{\sqrt{3}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a,E_u)}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_4[\mathbb{Q}_{2,1}^{(k,E_g)}]}{6} + \frac{\sqrt{3}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a,E_u)}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_4[\mathbb{Q}_{2,1}^{(k,E_g)}]}{6} - \frac{\sqrt{3}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a,E_u)}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{T}_{1,1}^{(k,E_u)}]}{6} \\
& + \frac{\sqrt{3}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a,E_u)}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_7[\mathbb{T}_{1,1}^{(k,E_u)}]}{6} + \frac{\sqrt{3}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a,E_u)}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,0}^{(k,E_g)}]}{6} - \frac{\sqrt{3}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a,E_u)}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,0}^{(k,E_g)}]}{6}
\end{aligned}$$

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

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

$$\begin{aligned}
\hat{Z}_{20}(\mathbf{k}) = & -\frac{\sqrt{6}\mathbb{X}_{13}[\mathbb{Q}_1^{(a,A_{2u})}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{T}_1^{(k,A_{2u})}]}{6} - \frac{\sqrt{6}\mathbb{X}_{13}[\mathbb{Q}_1^{(a,A_{2u})}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_8[\mathbb{T}_3^{(k,B_{2u})}]}{6} + \frac{\sqrt{6}\mathbb{X}_{13}[\mathbb{Q}_1^{(a,A_{2u})}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_{1g})}]}{6} \\
& + \frac{\sqrt{6}\mathbb{X}_{13}[\mathbb{Q}_1^{(a,A_{2u})}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_2[\mathbb{Q}_2^{(k,B_{1g})}]}{6} + \frac{\sqrt{6}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a,E_u)}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{T}_{1,0}^{(k,E_u)}]}{12} + \frac{\sqrt{6}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a,E_u)}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_6[\mathbb{T}_{1,0}^{(k,E_u)}]}{12} \\
& - \frac{\sqrt{6}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a,E_u)}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_4[\mathbb{Q}_{2,1}^{(k,E_g)}]}{12} - \frac{\sqrt{6}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a,E_u)}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_4[\mathbb{Q}_{2,1}^{(k,E_g)}]}{12} + \frac{\sqrt{6}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a,E_u)}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{T}_{1,1}^{(k,E_u)}]}{12} \\
& - \frac{\sqrt{6}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a,E_u)}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_7[\mathbb{T}_{1,1}^{(k,E_u)}]}{12} - \frac{\sqrt{6}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a,E_u)}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,0}^{(k,E_g)}]}{12} + \frac{\sqrt{6}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a,E_u)}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,0}^{(k,E_g)}]}{12}
\end{aligned}$$

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

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

$$\begin{aligned}
\hat{Z}_{21}(\mathbf{k}) = & -\frac{\sqrt{21}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{T}_1^{(k,A_{2u})}]}{14} - \frac{\sqrt{21}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_8[\mathbb{T}_3^{(k,B_{2u})}]}{14} \\
& + \frac{\sqrt{21}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_{1g})}]}{14} + \frac{\sqrt{21}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_2[\mathbb{Q}_2^{(k,B_{1g})}]}{14} + \frac{\sqrt{21}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{T}_{1,0}^{(k,E_u)}]}{28} \\
& + \frac{\sqrt{21}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_6[\mathbb{T}_{1,0}^{(k,E_u)}]}{28} - \frac{\sqrt{21}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_4[\mathbb{Q}_{2,1}^{(k,E_g)}]}{28} - \frac{\sqrt{21}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_4[\mathbb{Q}_{2,1}^{(k,E_g)}]}{28} \\
& + \frac{\sqrt{21}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{T}_{1,1}^{(k,E_u)}]}{28} - \frac{\sqrt{21}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_7[\mathbb{T}_{1,1}^{(k,E_u)}]}{28} - \frac{\sqrt{21}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,0}^{(k,E_g)}]}{28} \\
& + \frac{\sqrt{21}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,0}^{(k,E_g)}]}{28} + \frac{\sqrt{35}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{T}_{1,0}^{(k,E_u)}]}{28} + \frac{\sqrt{35}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_6[\mathbb{T}_{1,0}^{(k,E_u)}]}{28} \\
& - \frac{\sqrt{35}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_4[\mathbb{Q}_{2,1}^{(k,E_g)}]}{28} - \frac{\sqrt{35}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_4[\mathbb{Q}_{2,1}^{(k,E_g)}]}{28} + \frac{\sqrt{35}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{T}_{1,1}^{(k,E_u)}]}{28} \\
& - \frac{\sqrt{35}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_7[\mathbb{T}_{1,1}^{(k,E_u)}]}{28} - \frac{\sqrt{35}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,0}^{(k,E_g)}]}{28} + \frac{\sqrt{35}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,0}^{(k,E_g)}]}{28}
\end{aligned}$$

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

$$\begin{aligned}
\hat{Z}_{22} = & \frac{\sqrt{3}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{Y}_6[\mathbb{Q}_1^{(b,A_{2u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{1,0}^{(b,E_u)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{Y}_8[\mathbb{Q}_{1,1}^{(b,E_u)}]}{3} \\
\hat{Z}_{22}(\mathbf{k}) = & -\frac{\sqrt{3}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{T}_1^{(k,A_{2u})}]}{6} - \frac{\sqrt{3}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_8[\mathbb{T}_3^{(k,B_{2u})}]}{6} + \frac{\sqrt{3}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_{1g})}]}{6} \\
& + \frac{\sqrt{3}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_2[\mathbb{Q}_2^{(k,B_{1g})}]}{6} - \frac{\sqrt{3}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{T}_{1,0}^{(k,E_u)}]}{6} - \frac{\sqrt{3}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_6[\mathbb{T}_{1,0}^{(k,E_u)}]}{6} \\
& + \frac{\sqrt{3}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_4[\mathbb{Q}_{2,1}^{(k,E_g)}]}{6} + \frac{\sqrt{3}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_4[\mathbb{Q}_{2,1}^{(k,E_g)}]}{6} - \frac{\sqrt{3}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{T}_{1,1}^{(k,E_u)}]}{6} \\
& + \frac{\sqrt{3}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_7[\mathbb{T}_{1,1}^{(k,E_u)}]}{6} + \frac{\sqrt{3}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,0}^{(k,E_g)}]}{6} - \frac{\sqrt{3}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,0}^{(k,E_g)}]}{6}
\end{aligned}$$

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

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

$$\begin{aligned}
\hat{Z}_{23}(\mathbf{k}) = & -\frac{\sqrt{105}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{T}_1^{(k,A_{2u})}]}{42} - \frac{\sqrt{105}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_8[\mathbb{T}_3^{(k,B_{2u})}]}{42} \\
& + \frac{\sqrt{105}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_{1g})}]}{42} + \frac{\sqrt{105}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_2[\mathbb{Q}_2^{(k,B_{1g})}]}{42} + \frac{\sqrt{105}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{T}_{1,0}^{(k,E_u)}]}{84} \\
& + \frac{\sqrt{105}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_6[\mathbb{T}_{1,0}^{(k,E_u)}]}{84} - \frac{\sqrt{105}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_4[\mathbb{Q}_{2,1}^{(k,E_g)}]}{84} - \frac{\sqrt{105}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_4[\mathbb{Q}_{2,1}^{(k,E_g)}]}{84} \\
& + \frac{\sqrt{105}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{T}_{1,1}^{(k,E_u)}]}{84} - \frac{\sqrt{105}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_7[\mathbb{T}_{1,1}^{(k,E_u)}]}{84} - \frac{\sqrt{105}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,0}^{(k,E_g)}]}{84} \\
& + \frac{\sqrt{105}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,0}^{(k,E_g)}]}{84} - \frac{3\sqrt{7}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{T}_{1,0}^{(k,E_u)}]}{28} - \frac{3\sqrt{7}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_6[\mathbb{T}_{1,0}^{(k,E_u)}]}{28} \\
& + \frac{3\sqrt{7}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_4[\mathbb{Q}_{2,1}^{(k,E_g)}]}{28} + \frac{3\sqrt{7}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_4[\mathbb{Q}_{2,1}^{(k,E_g)}]}{28} - \frac{3\sqrt{7}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{T}_{1,1}^{(k,E_u)}]}{28} \\
& + \frac{3\sqrt{7}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_7[\mathbb{T}_{1,1}^{(k,E_u)}]}{28} + \frac{3\sqrt{7}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,0}^{(k,E_g)}]}{28} - \frac{3\sqrt{7}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,0}^{(k,E_g)}]}{28}
\end{aligned}$$

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

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

$$\begin{aligned}
\hat{Z}_{24}(\mathbf{k}) = & -\frac{\mathbb{X}_{23}[\mathbb{Q}_3^{(a,B_{2u})}] \otimes \mathbb{U}_{10}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_8[\mathbb{T}_3^{(k,B_{2u})}]}{2} - \frac{\mathbb{X}_{23}[\mathbb{Q}_3^{(a,B_{2u})}] \otimes \mathbb{U}_{12}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_5[\mathbb{T}_1^{(k,A_{2u})}]}{2} \\
& + \frac{\mathbb{X}_{23}[\mathbb{Q}_3^{(a,B_{2u})}] \otimes \mathbb{U}_7[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_2[\mathbb{Q}_2^{(k,B_{1g})}]}{2} + \frac{\mathbb{X}_{23}[\mathbb{Q}_3^{(a,B_{2u})}] \otimes \mathbb{U}_9[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_{1g})}]}{2}
\end{aligned}$$

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

$$\hat{Z}_{25} = -\frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{M}_{2,0}^{(a,E_u)}] \otimes \mathbb{Y}_{10}[\mathbb{T}_{1,0}^{(b,E_u)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{M}_{2,1}^{(a,E_u)}] \otimes \mathbb{Y}_{11}[\mathbb{T}_{1,1}^{(b,E_u)}]}{2}$$

$$\begin{aligned}
\hat{Z}_{25}(\mathbf{k}) = & -\frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{M}_{2,0}^{(a,E_u)}] \otimes \mathbb{U}_{11}[\mathbb{T}_1^{(u,A_{2u})}] \otimes \mathbb{F}_4[\mathbb{Q}_{2,1}^{(k,E_g)}]}{4} - \frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{M}_{2,0}^{(a,E_u)}] \otimes \mathbb{U}_{13}[\mathbb{T}_3^{(u,B_{2u})}] \otimes \mathbb{F}_4[\mathbb{Q}_{2,1}^{(k,E_g)}]}{4} \\
& - \frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{M}_{2,0}^{(a,E_u)}] \otimes \mathbb{U}_6[\mathbb{Q}_0^{(u,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{T}_{1,0}^{(k,E_u)}]}{4} - \frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{M}_{2,0}^{(a,E_u)}] \otimes \mathbb{U}_8[\mathbb{Q}_2^{(u,B_{1g})}] \otimes \mathbb{F}_6[\mathbb{T}_{1,0}^{(k,E_u)}]}{4} + \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{M}_{2,1}^{(a,E_u)}] \otimes \mathbb{U}_{11}[\mathbb{T}_1^{(u,A_{2u})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,0}^{(k,E_g)}]}{4} \\
& - \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{M}_{2,1}^{(a,E_u)}] \otimes \mathbb{U}_{13}[\mathbb{T}_3^{(u,B_{2u})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,0}^{(k,E_g)}]}{4} + \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{M}_{2,1}^{(a,E_u)}] \otimes \mathbb{U}_6[\mathbb{Q}_0^{(u,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{T}_{1,1}^{(k,E_u)}]}{4} - \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{M}_{2,1}^{(a,E_u)}] \otimes \mathbb{U}_8[\mathbb{Q}_2^{(u,B_{1g})}] \otimes \mathbb{F}_7[\mathbb{T}_{1,1}^{(k,E_u)}]}{4}
\end{aligned}$$

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

$$\hat{\mathbb{Z}}_{26} = -\mathbb{X}_{24}[\text{M}_2^{(a, B_{2u})}] \otimes \mathbb{Y}_{12}[\mathbb{T}_3^{(b, B_{2u})}]$$

$$\begin{aligned} \hat{\mathbb{Z}}_{26}(\mathbf{k}) = & -\frac{\mathbb{X}_{24}[\text{M}_2^{(a, B_{2u})}] \otimes \mathbb{U}_{11}[\mathbb{T}_1^{(u, A_{2u})}] \otimes \mathbb{F}_2[\mathbb{Q}_2^{(k, B_{1g})}]}{2} - \frac{\mathbb{X}_{24}[\text{M}_2^{(a, B_{2u})}] \otimes \mathbb{U}_{13}[\mathbb{T}_3^{(u, B_{2u})}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k, A_{1g})}]}{2} \\ & - \frac{\mathbb{X}_{24}[\text{M}_2^{(a, B_{2u})}] \otimes \mathbb{U}_6[\mathbb{Q}_0^{(u, A_{1g})}] \otimes \mathbb{F}_8[\mathbb{T}_3^{(k, B_{2u})}]}{2} - \frac{\mathbb{X}_{24}[\text{M}_2^{(a, B_{2u})}] \otimes \mathbb{U}_8[\mathbb{Q}_2^{(u, B_{1g})}] \otimes \mathbb{F}_5[\mathbb{T}_1^{(k, A_{2u})}]}{2} \end{aligned}$$

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

$$\hat{\mathbb{Z}}_{27} = \frac{\sqrt{3}\mathbb{X}_{13}[\mathbb{Q}_1^{(a, A_{2u})}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_1^{(b, A_{2u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a, Eu)}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{1,0}^{(b, Eu)}]}{3} + \frac{\sqrt{3}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a, Eu)}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{1,1}^{(b, Eu)}]}{3}$$

$$\begin{aligned} \hat{\mathbb{Z}}_{27}(\mathbf{k}) = & \frac{\sqrt{3}\mathbb{X}_{13}[\mathbb{Q}_1^{(a, A_{2u})}] \otimes \mathbb{U}_{15}[\mathbb{Q}_1^{(u, A_{2u})}] \otimes \mathbb{F}_9[\mathbb{Q}_0^{(k, A_{1g})}]}{6} + \frac{\sqrt{3}\mathbb{X}_{13}[\mathbb{Q}_1^{(a, A_{2u})}] \otimes \mathbb{U}_{17}[\mathbb{Q}_3^{(u, B_{2u})}] \otimes \mathbb{F}_{10}[\mathbb{Q}_2^{(k, B_{1g})}]}{6} - \frac{\sqrt{3}\mathbb{X}_{13}[\mathbb{Q}_1^{(a, A_{2u})}] \otimes \mathbb{U}_{18}[\mathbb{T}_0^{(u, A_{1g})}] \otimes \mathbb{F}_{13}[\mathbb{T}_1^{(k, A_{2u})}]}{6} \\ & - \frac{\sqrt{3}\mathbb{X}_{13}[\mathbb{Q}_1^{(a, A_{2u})}] \otimes \mathbb{U}_{20}[\mathbb{T}_2^{(u, B_{1g})}] \otimes \mathbb{F}_{16}[\mathbb{T}_3^{(k, B_{2u})}]}{6} + \frac{\sqrt{3}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a, Eu)}] \otimes \mathbb{U}_{15}[\mathbb{Q}_1^{(u, A_{2u})}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k, Eg)}]}{6} + \frac{\sqrt{3}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a, Eu)}] \otimes \mathbb{U}_{17}[\mathbb{Q}_3^{(u, B_{2u})}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k, Eg)}]}{6} \\ & - \frac{\sqrt{3}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a, Eu)}] \otimes \mathbb{U}_{18}[\mathbb{T}_0^{(u, A_{1g})}] \otimes \mathbb{F}_{14}[\mathbb{T}_{1,0}^{(k, Eu)}]}{6} - \frac{\sqrt{3}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a, Eu)}] \otimes \mathbb{U}_{20}[\mathbb{T}_2^{(u, B_{1g})}] \otimes \mathbb{F}_{14}[\mathbb{T}_{1,0}^{(k, Eu)}]}{6} + \frac{\sqrt{3}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a, Eu)}] \otimes \mathbb{U}_{15}[\mathbb{Q}_1^{(u, A_{2u})}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k, Eg)}]}{6} \\ & - \frac{\sqrt{3}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a, Eu)}] \otimes \mathbb{U}_{17}[\mathbb{Q}_3^{(u, B_{2u})}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k, Eg)}]}{6} - \frac{\sqrt{3}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a, Eu)}] \otimes \mathbb{U}_{18}[\mathbb{T}_0^{(u, A_{1g})}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,1}^{(k, Eu)}]}{6} + \frac{\sqrt{3}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a, Eu)}] \otimes \mathbb{U}_{20}[\mathbb{T}_2^{(u, B_{1g})}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,1}^{(k, Eu)}]}{6} \end{aligned}$$

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

$$\hat{\mathbb{Z}}_{28} = \frac{\sqrt{6}\mathbb{X}_{13}[\mathbb{Q}_1^{(a, A_{2u})}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_1^{(b, A_{2u})}]}{3} - \frac{\sqrt{6}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a, Eu)}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{1,0}^{(b, Eu)}]}{6} - \frac{\sqrt{6}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a, Eu)}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{1,1}^{(b, Eu)}]}{6}$$

$$\begin{aligned} \hat{\mathbb{Z}}_{28}(\mathbf{k}) = & \frac{\sqrt{6}\mathbb{X}_{13}[\mathbb{Q}_1^{(a, A_{2u})}] \otimes \mathbb{U}_{15}[\mathbb{Q}_1^{(u, A_{2u})}] \otimes \mathbb{F}_9[\mathbb{Q}_0^{(k, A_{1g})}]}{6} + \frac{\sqrt{6}\mathbb{X}_{13}[\mathbb{Q}_1^{(a, A_{2u})}] \otimes \mathbb{U}_{17}[\mathbb{Q}_3^{(u, B_{2u})}] \otimes \mathbb{F}_{10}[\mathbb{Q}_2^{(k, B_{1g})}]}{6} - \frac{\sqrt{6}\mathbb{X}_{13}[\mathbb{Q}_1^{(a, A_{2u})}] \otimes \mathbb{U}_{18}[\mathbb{T}_0^{(u, A_{1g})}] \otimes \mathbb{F}_{13}[\mathbb{T}_1^{(k, A_{2u})}]}{6} \\ & - \frac{\sqrt{6}\mathbb{X}_{13}[\mathbb{Q}_1^{(a, A_{2u})}] \otimes \mathbb{U}_{20}[\mathbb{T}_2^{(u, B_{1g})}] \otimes \mathbb{F}_{16}[\mathbb{T}_3^{(k, B_{2u})}]}{6} - \frac{\sqrt{6}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a, Eu)}] \otimes \mathbb{U}_{15}[\mathbb{Q}_1^{(u, A_{2u})}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k, Eg)}]}{12} - \frac{\sqrt{6}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a, Eu)}] \otimes \mathbb{U}_{17}[\mathbb{Q}_3^{(u, B_{2u})}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k, Eg)}]}{12} \\ & + \frac{\sqrt{6}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a, Eu)}] \otimes \mathbb{U}_{18}[\mathbb{T}_0^{(u, A_{1g})}] \otimes \mathbb{F}_{14}[\mathbb{T}_{1,0}^{(k, Eu)}]}{12} + \frac{\sqrt{6}\mathbb{X}_{15}[\mathbb{Q}_{1,0}^{(a, Eu)}] \otimes \mathbb{U}_{20}[\mathbb{T}_2^{(u, B_{1g})}] \otimes \mathbb{F}_{14}[\mathbb{T}_{1,0}^{(k, Eu)}]}{12} - \frac{\sqrt{6}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a, Eu)}] \otimes \mathbb{U}_{15}[\mathbb{Q}_1^{(u, A_{2u})}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k, Eg)}]}{12} \\ & + \frac{\sqrt{6}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a, Eu)}] \otimes \mathbb{U}_{17}[\mathbb{Q}_3^{(u, B_{2u})}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k, Eg)}]}{12} + \frac{\sqrt{6}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a, Eu)}] \otimes \mathbb{U}_{18}[\mathbb{T}_0^{(u, A_{1g})}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,1}^{(k, Eu)}]}{12} - \frac{\sqrt{6}\mathbb{X}_{16}[\mathbb{Q}_{1,1}^{(a, Eu)}] \otimes \mathbb{U}_{20}[\mathbb{T}_2^{(u, B_{1g})}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,1}^{(k, Eu)}]}{12} \end{aligned}$$

$$\boxed{\text{No. 31}} \quad \hat{\mathbb{Q}}_4^{(A_{1g},2)} [M_4, B_2]$$

$$\begin{aligned} \hat{\mathbb{Z}}_{31} = & \frac{\sqrt{105}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{Y}_{13}[\mathbb{Q}_1^{(b,A_{2u})}]}{21} - \frac{\sqrt{105}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{1,0}^{(b,E_u)}]}{42} \\ & - \frac{\sqrt{105}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{1,1}^{(b,E_u)}]}{42} + \frac{3\sqrt{7}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{Y}_{14}[\mathbb{Q}_{1,0}^{(b,E_u)}]}{14} + \frac{3\sqrt{7}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{Y}_{15}[\mathbb{Q}_{1,1}^{(b,E_u)}]}{14} \\ \hat{\mathbb{Z}}_{31}(\mathbf{k}) = & \frac{\sqrt{105}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{U}_{15}[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_9[\mathbb{T}_0^{(k,A_{1g})}]}{42} + \frac{\sqrt{105}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{U}_{17}[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_{10}[\mathbb{T}_2^{(k,B_{1g})}]}{42} \\ & - \frac{\sqrt{105}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{U}_{18}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_{13}[\mathbb{T}_1^{(k,A_{2u})}]}{42} - \frac{\sqrt{105}\mathbb{X}_{14}[\mathbb{Q}_3^{(a,A_{2u})}] \otimes \mathbb{U}_{20}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_{16}[\mathbb{T}_3^{(k,B_{2u})}]}{42} \\ & - \frac{\sqrt{105}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{U}_{15}[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E_g)}]}{84} - \frac{\sqrt{105}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{U}_{17}[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E_g)}]}{84} \\ & + \frac{\sqrt{105}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{U}_{18}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_{14}[\mathbb{T}_{1,0}^{(k,E_u)}]}{84} + \frac{\sqrt{105}\mathbb{X}_{17}[\mathbb{Q}_{3,0}^{(a,E_u,1)}] \otimes \mathbb{U}_{20}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_{14}[\mathbb{T}_{1,0}^{(k,E_u)}]}{84} \\ & - \frac{\sqrt{105}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{U}_{15}[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k,E_g)}]}{84} + \frac{\sqrt{105}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{U}_{17}[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k,E_g)}]}{84} \\ & + \frac{\sqrt{105}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{U}_{18}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,1}^{(k,E_u)}]}{84} - \frac{\sqrt{105}\mathbb{X}_{18}[\mathbb{Q}_{3,1}^{(a,E_u,1)}] \otimes \mathbb{U}_{20}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,1}^{(k,E_u)}]}{84} \\ & + \frac{3\sqrt{7}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{U}_{15}[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E_g)}]}{28} + \frac{3\sqrt{7}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{U}_{17}[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,E_g)}]}{28} \\ & - \frac{3\sqrt{7}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{U}_{18}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_{14}[\mathbb{T}_{1,0}^{(k,E_u)}]}{28} - \frac{3\sqrt{7}\mathbb{X}_{19}[\mathbb{Q}_{3,0}^{(a,E_u,2)}] \otimes \mathbb{U}_{20}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_{14}[\mathbb{T}_{1,0}^{(k,E_u)}]}{28} + \frac{3\sqrt{7}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{U}_{15}[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k,E_g)}]}{28} \\ & - \frac{3\sqrt{7}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{U}_{17}[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k,E_g)}]}{28} - \frac{3\sqrt{7}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{U}_{18}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,1}^{(k,E_u)}]}{28} + \frac{3\sqrt{7}\mathbb{X}_{20}[\mathbb{Q}_{3,1}^{(a,E_u,2)}] \otimes \mathbb{U}_{20}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,1}^{(k,E_u)}]}{28} \end{aligned}$$

$$\boxed{\text{No. 32}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [M_4, B_2]$$

$$\begin{aligned} \hat{\mathbb{Z}}_{32} = & \mathbb{X}_{23}[\mathbb{Q}_3^{(a,B_{2u})}] \otimes \mathbb{Y}_{16}[\mathbb{Q}_3^{(b,B_{2u})}] \\ \hat{\mathbb{Z}}_{32}(\mathbf{k}) = & \frac{\mathbb{X}_{23}[\mathbb{Q}_3^{(a,B_{2u})}] \otimes \mathbb{U}_{15}[\mathbb{Q}_1^{(u,A_{2u})}] \otimes \mathbb{F}_{10}[\mathbb{Q}_2^{(k,B_{1g})}]}{2} + \frac{\mathbb{X}_{23}[\mathbb{Q}_3^{(a,B_{2u})}] \otimes \mathbb{U}_{17}[\mathbb{Q}_3^{(u,B_{2u})}] \otimes \mathbb{F}_9[\mathbb{Q}_0^{(k,A_{1g})}]}{2} \\ & - \frac{\mathbb{X}_{23}[\mathbb{Q}_3^{(a,B_{2u})}] \otimes \mathbb{U}_{18}[\mathbb{T}_0^{(u,A_{1g})}] \otimes \mathbb{F}_{16}[\mathbb{T}_3^{(k,B_{2u})}]}{2} - \frac{\mathbb{X}_{23}[\mathbb{Q}_3^{(a,B_{2u})}] \otimes \mathbb{U}_{20}[\mathbb{T}_2^{(u,B_{1g})}] \otimes \mathbb{F}_{13}[\mathbb{T}_1^{(k,A_{2u})}]}{2} \end{aligned}$$

$$\boxed{\text{No. 33}} \quad \hat{\mathbb{Q}}_2^{(A_{1g})} [M_4, B_2]$$

$$\hat{\mathbb{Z}}_{33} = -\frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{M}_{2,0}^{(a,E_u)}] \otimes \mathbb{Y}_{17}[\mathbb{T}_{1,0}^{(b,E_u)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{M}_{2,1}^{(a,E_u)}] \otimes \mathbb{Y}_{18}[\mathbb{T}_{1,1}^{(b,E_u)}]}{2}$$

$$\begin{aligned}
\hat{Z}_{33}(\mathbf{k}) = & -\frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{M}_{2,0}^{(a,Eu)}] \otimes \mathbb{U}_{14}[\mathbb{Q}_0^{(u,A_{1g})}] \otimes \mathbb{F}_{14}[\mathbb{T}_{1,0}^{(k,Eu)}]}{4} - \frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{M}_{2,0}^{(a,Eu)}] \otimes \mathbb{U}_{16}[\mathbb{Q}_2^{(u,B_{1g})}] \otimes \mathbb{F}_{14}[\mathbb{T}_{1,0}^{(k,Eu)}]}{4} - \frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{M}_{2,0}^{(a,Eu)}] \otimes \mathbb{U}_{19}[\mathbb{T}_1^{(u,A_{2u})}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,Eg)}]}{4} \\
& - \frac{\sqrt{2}\mathbb{X}_{21}[\mathbb{M}_{2,0}^{(a,Eu)}] \otimes \mathbb{U}_{21}[\mathbb{T}_3^{(u,B_{2u})}] \otimes \mathbb{F}_{12}[\mathbb{Q}_{2,1}^{(k,Eg)}]}{4} + \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{M}_{2,1}^{(a,Eu)}] \otimes \mathbb{U}_{14}[\mathbb{Q}_0^{(u,A_{1g})}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,1}^{(k,Eu)}]}{4} - \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{M}_{2,1}^{(a,Eu)}] \otimes \mathbb{U}_{16}[\mathbb{Q}_2^{(u,B_{1g})}] \otimes \mathbb{F}_{15}[\mathbb{T}_{1,1}^{(k,Eu)}]}{4} \\
& + \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{M}_{2,1}^{(a,Eu)}] \otimes \mathbb{U}_{19}[\mathbb{T}_1^{(u,A_{2u})}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k,Eg)}]}{4} - \frac{\sqrt{2}\mathbb{X}_{22}[\mathbb{M}_{2,1}^{(a,Eu)}] \otimes \mathbb{U}_{21}[\mathbb{T}_3^{(u,B_{2u})}] \otimes \mathbb{F}_{11}[\mathbb{Q}_{2,0}^{(k,Eg)}]}{4}
\end{aligned}$$

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

$$\hat{Z}_{34} = -\mathbb{X}_{24}[\mathbb{M}_2^{(a,B_{2u})}] \otimes \mathbb{Y}_{19}[\mathbb{T}_3^{(b,B_{2u})}]$$

$$\begin{aligned}
\hat{Z}_{34}(\mathbf{k}) = & -\frac{\mathbb{X}_{24}[\mathbb{M}_2^{(a,B_{2u})}] \otimes \mathbb{U}_{14}[\mathbb{Q}_0^{(u,A_{1g})}] \otimes \mathbb{F}_{16}[\mathbb{T}_3^{(k,B_{2u})}]}{2} - \frac{\mathbb{X}_{24}[\mathbb{M}_2^{(a,B_{2u})}] \otimes \mathbb{U}_{16}[\mathbb{Q}_2^{(u,B_{1g})}] \otimes \mathbb{F}_{13}[\mathbb{T}_1^{(k,A_{2u})}]}{2} \\
& - \frac{\mathbb{X}_{24}[\mathbb{M}_2^{(a,B_{2u})}] \otimes \mathbb{U}_{19}[\mathbb{T}_1^{(u,A_{2u})}] \otimes \mathbb{F}_{10}[\mathbb{Q}_2^{(k,B_{1g})}]}{2} - \frac{\mathbb{X}_{24}[\mathbb{M}_2^{(a,B_{2u})}] \otimes \mathbb{U}_{21}[\mathbb{T}_3^{(u,B_{2u})}] \otimes \mathbb{F}_9[\mathbb{Q}_0^{(k,A_{1g})}]}{2}
\end{aligned}$$

Table 5: Atomic SAMB group.

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

Table 6: Atomic SAMB.

symbol	type	group	form
\mathbb{X}_1	$\mathbb{Q}_0^{(a,A_{1g})}$	M_1	$\begin{pmatrix} \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} \end{pmatrix}$
\mathbb{X}_2	$\mathbb{Q}_2^{(a,A_{1g})}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{21}}{21} & 0 & 0 & \frac{\sqrt{35}}{14} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{21}}{21} & 0 & 0 & -\frac{\sqrt{35}}{14} & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{21}}{21} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_3	$\mathbb{Q}_4^{(a,A_{1g},1)}$	M_1	$\begin{pmatrix} -\frac{\sqrt{66}}{11} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} \end{pmatrix}$
\mathbb{X}_4	$\mathbb{Q}_4^{(a,A_{1g},2)}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2310}}{308} & 0 & 0 & -\frac{3\sqrt{154}}{308} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2310}}{308} & 0 & 0 & \frac{3\sqrt{154}}{308} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2310}}{154} & 0 & 0 & 0 \\ 0 & -\frac{3\sqrt{154}}{308} & 0 & 0 & \frac{\sqrt{2310}}{132} & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{154}}{308} & 0 & 0 & \frac{\sqrt{2310}}{132} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2310}}{66} \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
\mathbb{X}_5	$\mathbb{Q}_6^{(a, A_{1g}, 1)}$	M_1	$\begin{pmatrix} \frac{2\sqrt{462}}{77} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{5\sqrt{462}}{462} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{5\sqrt{462}}{462} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{5\sqrt{462}}{462} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} \end{pmatrix}$
\mathbb{X}_6	$\mathbb{Q}_6^{(a, A_{1g}, 2)}$	M_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{5\sqrt{66}}{132} & 0 & 0 & -\frac{\sqrt{110}}{44} & 0 & 0 \\ 0 & 0 & -\frac{5\sqrt{66}}{132} & 0 & 0 & \frac{\sqrt{110}}{44} & 0 \\ 0 & 0 & 0 & \frac{5\sqrt{66}}{66} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{110}}{44} & 0 & 0 & -\frac{\sqrt{66}}{44} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{110}}{44} & 0 & 0 & -\frac{\sqrt{66}}{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{66}}{22} \end{pmatrix}$
\mathbb{X}_7	$\mathbb{Q}_0^{(a, A_{1g})}$	M_2	$\begin{pmatrix} \frac{\sqrt{5}}{5} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{5}}{5} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{5}}{5} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{5}}{5} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{5}}{5} \end{pmatrix}$
\mathbb{X}_8	$\mathbb{Q}_2^{(a, A_{1g})}$	M_2	$\begin{pmatrix} \frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{7} \end{pmatrix}$
\mathbb{X}_9	$\mathbb{Q}_4^{(a, A_{1g}, 1)}$	M_2	$\begin{pmatrix} \frac{\sqrt{30}}{10} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{30}}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{30}}{15} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{15} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{30}}{15} \end{pmatrix}$

continued ...

Table 6

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

continued ...

Table 6

symbol	type	group	form
\mathbb{X}_{17}	$\mathbb{Q}_{3,0}^{(a,E_u,1)}$	M_4	$\begin{pmatrix} -\frac{\sqrt{15}}{10} & 0 & 0 \\ \frac{3\sqrt{5}}{10} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{5} \\ 0 & -\frac{\sqrt{5}}{5} & 0 \end{pmatrix}$
\mathbb{X}_{18}	$\mathbb{Q}_{3,1}^{(a,E_u,1)}$	M_4	$\begin{pmatrix} 0 & -\frac{\sqrt{15}}{10} & 0 \\ 0 & -\frac{3\sqrt{5}}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{5} \\ 0 & 0 & 0 \\ -\frac{\sqrt{5}}{5} & 0 & 0 \end{pmatrix}$
\mathbb{X}_{19}	$\mathbb{Q}_{3,0}^{(a,E_u,2)}$	M_4	$\begin{pmatrix} -\frac{1}{2} & 0 & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{3} \\ 0 & \frac{\sqrt{3}}{3} & 0 \end{pmatrix}$
\mathbb{X}_{20}	$\mathbb{Q}_{3,1}^{(a,E_u,2)}$	M_4	$\begin{pmatrix} 0 & -\frac{1}{2} & 0 \\ 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{3} \\ 0 & 0 & 0 \\ \frac{\sqrt{3}}{3} & 0 & 0 \end{pmatrix}$
\mathbb{X}_{21}	$\mathbb{M}_{2,0}^{(a,E_u)}$	M_4	$\begin{pmatrix} -\frac{\sqrt{2}i}{2} & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 \end{pmatrix}$
\mathbb{X}_{22}	$\mathbb{M}_{2,1}^{(a,E_u)}$	M_4	$\begin{pmatrix} 0 & \frac{\sqrt{2}i}{2} & 0 \\ 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
\mathbb{X}_{23}	$\mathbb{Q}_3^{(a, B_{2u})}$	M_4	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \\ 0 & -\frac{\sqrt{3}}{3} & 0 \\ \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{24}	$\mathbb{M}_2^{(a, B_{2u})}$	M_4	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{3} \\ 0 & \frac{\sqrt{6}i}{6} & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
\mathbb{Y}_1	$\mathbb{Q}_0^{(s, A_{1g})}$	S_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{Y}_2	$\mathbb{Q}_0^{(s, A_{1g})}$	S_2	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{Y}_3	$\mathbb{Q}_0^{(s, A_{1g})}$	S_3	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{Y}_4	$\mathbb{Q}_0^{(s, A_{1g})}$	S_4	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{Y}_5	$\mathbb{Q}_0^{(s, A_{1g})}$	S_5	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{Y}_6	$\mathbb{Q}_1^{(b, A_{2u})}$	B_1	$\begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} \end{pmatrix}$
\mathbb{Y}_7	$\mathbb{Q}_{1,0}^{(b, E_u)}$	B_1	$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{Y}_8	$\mathbb{Q}_{1,1}^{(b, E_u)}$	B_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$
\mathbb{Y}_9	$\mathbb{Q}_3^{(b, B_{2u})}$	B_1	$\begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} \end{pmatrix}$
\mathbb{Y}_{10}	$\mathbb{T}_{1,0}^{(b, E_u)}$	B_1	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{Y}_{11}	$\mathbb{T}_{1,1}^{(b, E_u)}$	B_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} \end{pmatrix}$
\mathbb{Y}_{12}	$\mathbb{T}_3^{(b, B_{2u})}$	B_1	$\begin{pmatrix} \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} \end{pmatrix}$
\mathbb{Y}_{13}	$\mathbb{Q}_1^{(b, A_{2u})}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} \end{pmatrix}$

continued ...

Table 7

symbol	type	cluster	form
\mathbb{Y}_{14}	$\mathbb{Q}_{1,0}^{(b,E_u)}$	B_2	$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{Y}_{15}	$\mathbb{Q}_{1,1}^{(b,E_u)}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$
\mathbb{Y}_{16}	$\mathbb{Q}_3^{(b,B_{2u})}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} \end{pmatrix}$
\mathbb{Y}_{17}	$\mathbb{T}_{1,0}^{(b,E_u)}$	B_2	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{Y}_{18}	$\mathbb{T}_{1,1}^{(b,E_u)}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} \end{pmatrix}$
\mathbb{Y}_{19}	$\mathbb{T}_3^{(b,B_{2u})}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} \end{pmatrix}$

Table 8: Uniform SAMB.

symbol	type	cluster	form
\mathbb{U}_1	$\mathbb{Q}_0^{(s,A_{1g})}$	S_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$

continued ...

[illegible]

continued ...

[illegible]

continued ...

Table 8

symbol	type	cluster	form
\mathbb{U}_8	$\mathbb{Q}_2^{(u, B_{1g})}$	B_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{U}_9	$\mathbb{Q}_3^{(u, B_{2u})}$	B_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{U}_{10}	$\mathbb{T}_0^{(u, A_{1g})}$	B_1	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$

continued ...

[illegible]

continued ...

[illegible]

continued ...

Table 8

symbol	type	cluster	form
\mathbb{U}_{17}	$\mathbb{Q}_3^{(u, B_{2u})}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{U}_{18}	$\mathbb{T}_0^{(u, A_{1g})}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{U}_{19}	$\mathbb{T}_1^{(u, A_{2u})}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 8

symbol	type	cluster	form
\mathbb{U}_{20}	$\mathbb{T}_2^{(u, B_{1g})}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{U}_{21}	$\mathbb{T}_3^{(u, B_{2u})}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$

Table 9: Structure SAMB.

symbol	type	cluster	form
\mathbb{F}_1	$\mathbb{Q}_0^{(k, A_{1g})}$	B_1	$\frac{\sqrt{2}c_{001}}{2} + \frac{\sqrt{2}c_{002}}{2} + \frac{\sqrt{2}c_{005}}{2} + \frac{\sqrt{2}c_{006}}{2}$
\mathbb{F}_2	$\mathbb{Q}_2^{(k, B_{1g})}$	B_1	$\frac{\sqrt{2}c_{001}}{2} + \frac{\sqrt{2}c_{002}}{2} - \frac{\sqrt{2}c_{005}}{2} - \frac{\sqrt{2}c_{006}}{2}$
\mathbb{F}_3	$\mathbb{Q}_{2,0}^{(k, E_g)}$	B_1	$-c_{005} + c_{006}$
\mathbb{F}_4	$\mathbb{Q}_{2,1}^{(k, E_g)}$	B_1	$c_{001} - c_{002}$
\mathbb{F}_5	$\mathbb{T}_1^{(k, A_{2u})}$	B_1	$\frac{\sqrt{2}s_{001}}{2} + \frac{\sqrt{2}s_{002}}{2} - \frac{\sqrt{2}s_{005}}{2} - \frac{\sqrt{2}s_{006}}{2}$

continued ...

Table 9

symbol	type	cluster	form
\mathbb{F}_6	$\mathbb{T}_{1,0}^{(k,E_u)}$	B_1	$s_{001} - s_{002}$
\mathbb{F}_7	$\mathbb{T}_{1,1}^{(k,E_u)}$	B_1	$s_{005} - s_{006}$
\mathbb{F}_8	$\mathbb{T}_3^{(k,B_{2u})}$	B_1	$\frac{\sqrt{2}s_{001}}{2} + \frac{\sqrt{2}s_{002}}{2} + \frac{\sqrt{2}s_{005}}{2} + \frac{\sqrt{2}s_{006}}{2}$
\mathbb{F}_9	$\mathbb{Q}_0^{(k,A_{1g})}$	B_2	$\frac{\sqrt{2}c_{009}}{2} + \frac{\sqrt{2}c_{010}}{2} + \frac{\sqrt{2}c_{013}}{2} + \frac{\sqrt{2}c_{014}}{2}$
\mathbb{F}_{10}	$\mathbb{Q}_2^{(k,B_{1g})}$	B_2	$\frac{\sqrt{2}c_{009}}{2} + \frac{\sqrt{2}c_{010}}{2} - \frac{\sqrt{2}c_{013}}{2} - \frac{\sqrt{2}c_{014}}{2}$
\mathbb{F}_{11}	$\mathbb{Q}_{2,0}^{(k,E_g)}$	B_2	$-c_{013} + c_{014}$
\mathbb{F}_{12}	$\mathbb{Q}_{2,1}^{(k,E_g)}$	B_2	$c_{009} - c_{010}$
\mathbb{F}_{13}	$\mathbb{T}_1^{(k,A_{2u})}$	B_2	$\frac{\sqrt{2}s_{009}}{2} + \frac{\sqrt{2}s_{010}}{2} - \frac{\sqrt{2}s_{013}}{2} - \frac{\sqrt{2}s_{014}}{2}$
\mathbb{F}_{14}	$\mathbb{T}_{1,0}^{(k,E_u)}$	B_2	$s_{009} - s_{010}$
\mathbb{F}_{15}	$\mathbb{T}_{1,1}^{(k,E_u)}$	B_2	$s_{013} - s_{014}$
\mathbb{F}_{16}	$\mathbb{T}_3^{(k,B_{2u})}$	B_2	$\frac{\sqrt{2}s_{009}}{2} + \frac{\sqrt{2}s_{010}}{2} + \frac{\sqrt{2}s_{013}}{2} + \frac{\sqrt{2}s_{014}}{2}$

Table 10: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_{1g})}$	0	A_{1g}	—	—	1
2	$\mathbb{Q}_1^{(A_{2u})}$	1	A_{2u}	—	—	z
3	$\mathbb{Q}_{1,0}^{(E_u)}$	1	E_u	—	0	x
4	$\mathbb{Q}_{1,1}^{(E_u)}$	1	E_u	—	1	y
5	$\mathbb{Q}_2^{(A_{1g})}$	2	A_{1g}	—	—	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
6	$\mathbb{Q}_2^{(B_{1g})}$	2	B_{1g}	—	—	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
7	$\mathbb{Q}_{2,0}^{(E_g)}$	2	E_g	—	0	$\sqrt{3}yz$
8	$\mathbb{Q}_{2,1}^{(E_g)}$	2	E_g	—	1	$\sqrt{3}xz$
9	$\mathbb{Q}_3^{(A_{2u})}$	3	A_{2u}	—	—	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
10	$\mathbb{Q}_3^{(B_{2u})}$	3	B_{2u}	—	—	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
11	$\mathbb{Q}_{3,0}^{(E_u,1)}$	3	E_u	1	0	$\frac{x(2x^2-3y^2-3z^2)}{2}$
12	$\mathbb{Q}_{3,1}^{(E_u,1)}$	3	E_u	1	1	$-\frac{y(3x^2-2y^2+3z^2)}{2}$

continued ...

Table 10

No.	symbol	rank	irrep.	mul.	comp.	form
13	$\mathbb{Q}_{3,0}^{(E_u,2)}$	3	E_u	2	0	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
14	$\mathbb{Q}_{3,1}^{(E_u,2)}$	3	E_u	2	1	$\frac{\sqrt{15}y(x-z)(x+z)}{2}$
15	$\mathbb{Q}_4^{(A_{1g},1)}$	4	A_{1g}	1	—	$\frac{\sqrt{21}(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4)}{2}$
16	$\mathbb{Q}_4^{(A_{1g},2)}$	4	A_{1g}	2	—	$-\frac{\sqrt{15}(x^4-12x^2y^2+6x^2z^2+y^4+6y^2z^2-2z^4)}{12}$
17	$\mathbb{Q}_6^{(A_{1g},1)}$	6	A_{1g}	1	—	$\frac{\sqrt{2} \cdot (2x^6-15x^4y^2-15x^4z^2-15x^2y^4+180x^2y^2z^2-15x^2z^4+2y^6-15y^4z^2-15y^2z^4+2z^6)}{12}$
18	$\mathbb{Q}_6^{(A_{1g},2)}$	6	A_{1g}	2	—	$-\frac{\sqrt{14}(x^6-15x^4z^2+15x^2z^4+y^6-15y^4z^2+15y^2z^4-2z^6)}{8}$

Table 11: Axial harmonics.

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

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

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

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

continued ...

Table 12

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

Table 13: Symmetry operations.

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

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

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

Table 15: Parity conversion.

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

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

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

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

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

Table 18: Virtual-cluster sites.

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

Table 19: Virtual-cluster basis.

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_0^{(A_{1g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$				
$\mathbb{Q}_1^{(A_{2u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$				
$\mathbb{Q}_{1,0}^{(E_u)}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$
	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$				
$\mathbb{Q}_{1,1}^{(E_u)}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$
	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$				
$\mathbb{Q}_2^{(B_{1g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$				
$\mathbb{Q}_2^{(B_{2g})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$				
$\mathbb{Q}_{2,0}^{(E_g)}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$
	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$				
$\mathbb{Q}_{2,1}^{(E_g)}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$
	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$				
$\mathbb{Q}_3^{(B_{1u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$				

continued ...

Table 19

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_3^{(B_{2u})}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
$\mathbb{Q}_{3,0}^{(E_u,1)}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$
$\mathbb{Q}_{3,1}^{(E_u,1)}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$
$\mathbb{Q}_4^{(A_{2g})}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$
$\mathbb{Q}_{4,0}^{(E_g,1)}$	$-\frac{\sqrt{10}}{10}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{20}$	$-\frac{\sqrt{10}}{20}$	$\frac{\sqrt{10}}{10}$	$-\frac{\sqrt{10}}{10}$
$\mathbb{Q}_{4,1}^{(E_g,1)}$	$-\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
$\mathbb{Q}_5^{(A_{1u})}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$