

SAMB for “0h1”

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- Group: No. 221 O_h^1 $Pm-3m$ [cubic]
 - Associated point group: No. 32 O_h $m-3m$ [cubic]
 - Generation condition
 - model type: **tight_binding**
 - time-reversal type: **electric**
 - irrep: [A1g]
 - spinful
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- Unit cell:
 - $a = 1.0$, $b = 1.0$, $c = 1.0$, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 90.0$
- Lattice vectors:
 - $\mathbf{a}_1 = (1.0 \ 0 \ 0)$
 - $\mathbf{a}_2 = (0 \ 1.0 \ 0)$
 - $\mathbf{a}_3 = (0 \ 0 \ 1.0)$

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 = 8

Table 2: Hilbert space for full matrix.

No.	ket	No.	ket	No.	ket	No.	ket	No.	ket
1	$(s, \uparrow)@A_1$	2	$(s, \downarrow)@A_1$	3	$(p_x, \uparrow)@A_1$	4	$(p_x, \downarrow)@A_1$	5	$(p_y, \uparrow)@A_1$
6	$(p_y, \downarrow)@A_1$	7	$(p_z, \uparrow)@A_1$	8	$(p_z, \downarrow)@A_1$				

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

site	position	mapping
S ₁ A ₁	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

bond	tail	head	n	#	$\mathbf{b@c}$	mapping	
B_1	b_1	A_1	A_1	1	1	$\begin{pmatrix} 0 & 0 & 1 \end{pmatrix} @ \begin{pmatrix} 0 & 0 & \frac{1}{2} \end{pmatrix}$	[1,2,-3,-4,-5,-8,19,22,-25,-26,27,28,29,32,-43,-46]
	b_2	A_1	A_1	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[6,-9,11,-12,13,-14,21,-24,-30,33,-35,36,-37,38,-45,48]
	b_3	A_1	A_1	1	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[7,-10,15,16,-17,-18,-20,23,-31,34,-39,-40,41,42,44,-47]
B_2	b_4	A_1	A_1	2	1	$\begin{pmatrix} 0 & 1 & 1 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$	[1,-3,7,-10,-25,27,-31,34]
	b_5	A_1	A_1	2	1	$\begin{pmatrix} 0 & 1 & -1 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$	[-2,4,-20,23,26,-28,44,-47]
	b_6	A_1	A_1	2	1	$\begin{pmatrix} 1 & 0 & -1 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$	[5,-12,13,-19,-29,36,-37,43]
	b_7	A_1	A_1	2	1	$\begin{pmatrix} 1 & -1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[6,-16,18,-24,-30,40,-42,48]
	b_8	A_1	A_1	2	1	$\begin{pmatrix} 1 & 0 & 1 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$	[-8,11,-14,22,32,-35,38,-46]
	b_9	A_1	A_1	2	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[-9,15,-17,21,33,-39,41,-45]

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- SAMB:

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

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

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

$$\boxed{\text{No. 2}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\mathbf{M}_3, \mathbf{S}_1]$$

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

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

$$\boxed{\text{No. 3}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, 1) [\mathbf{M}_3, \mathbf{S}_1]$$

$$\hat{\mathbb{Z}}_3 = \mathbb{X}_6[\mathbb{Q}_0^{(a, A_{1g})}(1, 1)] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_{1g})}]$$

$$\hat{\mathbb{Z}}_3(\mathbf{k}) = \mathbb{X}_6[\mathbb{Q}_0^{(a, A_{1g})}(1, 1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s, A_{1g})}]$$

$$\boxed{\text{No. 4}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\mathbf{M}_1, \mathbf{B}_1]$$

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

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

$$\boxed{\text{No. 5}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\mathbf{M}_3, \mathbf{B}_1]$$

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

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

$$\boxed{\text{No. 6}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, 1) [\mathbf{M}_3, \mathbf{B}_1]$$

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

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

$$\boxed{\text{No. 7}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_3, \text{B}_1]$$

$$\hat{\mathbb{Z}}_7 = \frac{\sqrt{2}\mathbb{X}_7[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{Y}_3[\mathbb{Q}_{2,0}^{(b,E_g)}]}{2} + \frac{\sqrt{2}\mathbb{X}_8[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{Y}_4[\mathbb{Q}_{2,1}^{(b,E_g)}]}{2}$$

$$\hat{\mathbb{Z}}_7(\mathbf{k}) = \frac{\sqrt{2}\mathbb{X}_7[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_2[\mathbb{Q}_{2,0}^{(k,E_g)}]}{2} + \frac{\sqrt{2}\mathbb{X}_8[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,1}^{(k,E_g)}]}{2}$$

$$\boxed{\text{No. 8}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1,-1) [\text{M}_3, \text{B}_1]$$

$$\hat{\mathbb{Z}}_8 = \frac{\sqrt{2}\mathbb{X}_{12}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_3[\mathbb{Q}_{2,0}^{(b,E_g)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_4[\mathbb{Q}_{2,1}^{(b,E_g)}]}{2}$$

$$\hat{\mathbb{Z}}_8(\mathbf{k}) = \frac{\sqrt{2}\mathbb{X}_{12}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_2[\mathbb{Q}_{2,0}^{(k,E_g)}]}{2} + \frac{\sqrt{2}\mathbb{X}_{13}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_3[\mathbb{Q}_{2,1}^{(k,E_g)}]}{2}$$

$$\boxed{\text{No. 9}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\text{M}_1, \text{B}_2]$$

$$\hat{\mathbb{Z}}_9 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{\mathbb{Z}}_9(\mathbf{k}) = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_4[\mathbb{Q}_0^{(k,A_{1g})}]$$

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

$$\hat{\mathbb{Z}}_{10} = \frac{\sqrt{3}\mathbb{X}_2[\mathbb{M}_{2,0}^{(a,T_{2u})}(1,-1)] \otimes \mathbb{Y}_{11}[\mathbb{T}_{3,0}^{(b,T_{2u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_3[\mathbb{M}_{2,1}^{(a,T_{2u})}(1,-1)] \otimes \mathbb{Y}_{12}[\mathbb{T}_{3,1}^{(b,T_{2u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_4[\mathbb{M}_{2,2}^{(a,T_{2u})}(1,-1)] \otimes \mathbb{Y}_{13}[\mathbb{T}_{3,2}^{(b,T_{2u})}]}{3}$$

$$\begin{aligned} \hat{\mathbb{Z}}_{10}(\mathbf{k}) &= \frac{\sqrt{3}\mathbb{X}_2[\mathbb{M}_{2,0}^{(a,T_{2u})}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_{10}[\mathbb{T}_{3,0}^{(k,T_{2u})}]}{3} + \frac{\sqrt{3}\mathbb{X}_3[\mathbb{M}_{2,1}^{(a,T_{2u})}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_{11}[\mathbb{T}_{3,1}^{(k,T_{2u})}]}{3} \\ &+ \frac{\sqrt{3}\mathbb{X}_4[\mathbb{M}_{2,2}^{(a,T_{2u})}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_{12}[\mathbb{T}_{3,2}^{(k,T_{2u})}]}{3} \end{aligned}$$

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

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

$$\hat{\mathbb{Z}}_{11}(\mathbf{k}) = \mathbb{X}_5[\mathbb{Q}_0^{(a,A_{1g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_4[\mathbb{Q}_0^{(k,A_{1g})}]$$

$$\boxed{\text{No. 12}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, 1) \text{ } [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{12} = \mathbb{X}_6[\mathbb{Q}_0^{(a,A_{1g})}(1, 1)] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b,A_{1g})}]$$

$$\hat{\mathbb{Z}}_{12}(\mathbf{k}) = \mathbb{X}_6[\mathbb{Q}_0^{(a,A_{1g})}(1, 1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_4[\mathbb{Q}_0^{(k,A_{1g})}]$$

$$\boxed{\text{No. 13}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} \text{ } [\text{M}_3, \text{B}_2]$$

$$\hat{\mathbb{Z}}_{13} = \frac{\sqrt{5}\mathbb{X}_{10}[\mathbb{Q}_{2,1}^{(a,T_{2g})}] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,1}^{(b,T_{2g})}]}{5} + \frac{\sqrt{5}\mathbb{X}_{11}[\mathbb{Q}_{2,2}^{(a,T_{2g})}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,2}^{(b,T_{2g})}]}{5} + \frac{\sqrt{5}\mathbb{X}_7[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{Y}_6[\mathbb{Q}_{2,0}^{(b,E_g)}]}{5} + \frac{\sqrt{5}\mathbb{X}_8[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{2,1}^{(b,E_g)}]}{5} + \frac{\sqrt{5}\mathbb{X}_9[\mathbb{Q}_{2,0}^{(a,T_{2g})}] \otimes \mathbb{Y}_8[\mathbb{Q}_{2,0}^{(b,T_{2g})}]}{5}$$

$$\begin{aligned} \hat{\mathbb{Z}}_{13}(\mathbf{k}) = & \frac{\sqrt{5}\mathbb{X}_{10}[\mathbb{Q}_{2,1}^{(a,T_{2g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_8[\mathbb{Q}_{2,1}^{(k,T_{2g})}]}{5} + \frac{\sqrt{5}\mathbb{X}_{11}[\mathbb{Q}_{2,2}^{(a,T_{2g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_9[\mathbb{Q}_{2,2}^{(k,T_{2g})}]}{5} + \frac{\sqrt{5}\mathbb{X}_7[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{Q}_{2,0}^{(k,E_g)}]}{5} \\ & + \frac{\sqrt{5}\mathbb{X}_8[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{Q}_{2,1}^{(k,E_g)}]}{5} + \frac{\sqrt{5}\mathbb{X}_9[\mathbb{Q}_{2,0}^{(a,T_{2g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{Q}_{2,0}^{(k,T_{2g})}]}{5} \end{aligned}$$

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

$$\begin{aligned} \hat{\mathbb{Z}}_{14} = & -\frac{\sqrt{30}\mathbb{X}_{10}[\mathbb{Q}_{2,1}^{(a,T_{2g})}] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,1}^{(b,T_{2g})}]}{15} - \frac{\sqrt{30}\mathbb{X}_{11}[\mathbb{Q}_{2,2}^{(a,T_{2g})}] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,2}^{(b,T_{2g})}]}{15} + \frac{\sqrt{30}\mathbb{X}_7[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{Y}_6[\mathbb{Q}_{2,0}^{(b,E_g)}]}{10} \\ & + \frac{\sqrt{30}\mathbb{X}_8[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{Y}_7[\mathbb{Q}_{2,1}^{(b,E_g)}]}{10} - \frac{\sqrt{30}\mathbb{X}_9[\mathbb{Q}_{2,0}^{(a,T_{2g})}] \otimes \mathbb{Y}_8[\mathbb{Q}_{2,0}^{(b,T_{2g})}]}{15} \end{aligned}$$

$$\begin{aligned} \hat{\mathbb{Z}}_{14}(\mathbf{k}) = & -\frac{\sqrt{30}\mathbb{X}_{10}[\mathbb{Q}_{2,1}^{(a,T_{2g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_8[\mathbb{Q}_{2,1}^{(k,T_{2g})}]}{15} - \frac{\sqrt{30}\mathbb{X}_{11}[\mathbb{Q}_{2,2}^{(a,T_{2g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_9[\mathbb{Q}_{2,2}^{(k,T_{2g})}]}{15} \\ & + \frac{\sqrt{30}\mathbb{X}_7[\mathbb{Q}_{2,0}^{(a,E_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{Q}_{2,0}^{(k,E_g)}]}{10} + \frac{\sqrt{30}\mathbb{X}_8[\mathbb{Q}_{2,1}^{(a,E_g)}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{Q}_{2,1}^{(k,E_g)}]}{10} - \frac{\sqrt{30}\mathbb{X}_9[\mathbb{Q}_{2,0}^{(a,T_{2g})}] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{Q}_{2,0}^{(k,T_{2g})}]}{15} \end{aligned}$$

$$\boxed{\text{No. 15}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})}(1, -1) \text{ } [\text{M}_3, \text{B}_2]$$

$$\begin{aligned} \hat{\mathbb{Z}}_{15} = & \frac{\sqrt{5}\mathbb{X}_{12}[\mathbb{Q}_{2,0}^{(a,E_g)}(1, -1)] \otimes \mathbb{Y}_6[\mathbb{Q}_{2,0}^{(b,E_g)}]}{5} + \frac{\sqrt{5}\mathbb{X}_{13}[\mathbb{Q}_{2,1}^{(a,E_g)}(1, -1)] \otimes \mathbb{Y}_7[\mathbb{Q}_{2,1}^{(b,E_g)}]}{5} + \frac{\sqrt{5}\mathbb{X}_{14}[\mathbb{Q}_{2,0}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{Y}_8[\mathbb{Q}_{2,0}^{(b,T_{2g})}]}{5} \\ & + \frac{\sqrt{5}\mathbb{X}_{15}[\mathbb{Q}_{2,1}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,1}^{(b,T_{2g})}]}{5} + \frac{\sqrt{5}\mathbb{X}_{16}[\mathbb{Q}_{2,2}^{(a,T_{2g})}(1, -1)] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,2}^{(b,T_{2g})}]}{5} \end{aligned}$$

$$\hat{\mathbb{Z}}_{15}(\mathbf{k}) = \frac{\sqrt{5}\mathbb{X}_{12}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{Q}_{2,0}^{(k,E_g)}]}{5} + \frac{\sqrt{5}\mathbb{X}_{13}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{Q}_{2,1}^{(k,E_g)}]}{5} \\ + \frac{\sqrt{5}\mathbb{X}_{14}[\mathbb{Q}_{2,0}^{(a,T_{2g})}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{Q}_{2,0}^{(k,T_{2g})}]}{5} + \frac{\sqrt{5}\mathbb{X}_{15}[\mathbb{Q}_{2,1}^{(a,T_{2g})}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_8[\mathbb{Q}_{2,1}^{(k,T_{2g})}]}{5} \\ + \frac{\sqrt{5}\mathbb{X}_{16}[\mathbb{Q}_{2,2}^{(a,T_{2g})}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_9[\mathbb{Q}_{2,2}^{(k,T_{2g})}]}{5}$$

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

$$\hat{\mathbb{Z}}_{16} = \frac{\sqrt{30}\mathbb{X}_{12}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_6[\mathbb{Q}_{2,0}^{(b,E_g)}]}{10} + \frac{\sqrt{30}\mathbb{X}_{13}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{Y}_7[\mathbb{Q}_{2,1}^{(b,E_g)}]}{10} - \frac{\sqrt{30}\mathbb{X}_{14}[\mathbb{Q}_{2,0}^{(a,T_{2g})}(1,-1)] \otimes \mathbb{Y}_8[\mathbb{Q}_{2,0}^{(b,T_{2g})}]}{15} \\ - \frac{\sqrt{30}\mathbb{X}_{15}[\mathbb{Q}_{2,1}^{(a,T_{2g})}(1,-1)] \otimes \mathbb{Y}_9[\mathbb{Q}_{2,1}^{(b,T_{2g})}]}{15} - \frac{\sqrt{30}\mathbb{X}_{16}[\mathbb{Q}_{2,2}^{(a,T_{2g})}(1,-1)] \otimes \mathbb{Y}_{10}[\mathbb{Q}_{2,2}^{(b,T_{2g})}]}{15}$$

$$\hat{\mathbb{Z}}_{16}(\mathbf{k}) = \frac{\sqrt{30}\mathbb{X}_{12}[\mathbb{Q}_{2,0}^{(a,E_g)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_5[\mathbb{Q}_{2,0}^{(k,E_g)}]}{10} + \frac{\sqrt{30}\mathbb{X}_{13}[\mathbb{Q}_{2,1}^{(a,E_g)}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_6[\mathbb{Q}_{2,1}^{(k,E_g)}]}{10} \\ - \frac{\sqrt{30}\mathbb{X}_{14}[\mathbb{Q}_{2,0}^{(a,T_{2g})}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_7[\mathbb{Q}_{2,0}^{(k,T_{2g})}]}{15} - \frac{\sqrt{30}\mathbb{X}_{15}[\mathbb{Q}_{2,1}^{(a,T_{2g})}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_8[\mathbb{Q}_{2,1}^{(k,T_{2g})}]}{15} \\ - \frac{\sqrt{30}\mathbb{X}_{16}[\mathbb{Q}_{2,2}^{(a,T_{2g})}(1,-1)] \otimes \mathbb{U}_1[\mathbb{Q}_0^{(s,A_{1g})}] \otimes \mathbb{F}_9[\mathbb{Q}_{2,2}^{(k,T_{2g})}]}{15}$$

Table 5: Atomic SAMB group.

group	bra	ket
M ₁	$(s, \uparrow), (s, \downarrow)$	$(s, \uparrow), (s, \downarrow)$
M ₂	$(s, \uparrow), (s, \downarrow)$	$(p_x, \uparrow), (p_x, \downarrow), (p_y, \uparrow), (p_y, \downarrow), (p_z, \uparrow), (p_z, \downarrow)$
M ₃	$(p_x, \uparrow), (p_x, \downarrow), (p_y, \uparrow), (p_y, \downarrow), (p_z, \uparrow), (p_z, \downarrow)$	$(p_x, \uparrow), (p_x, \downarrow), (p_y, \uparrow), (p_y, \downarrow), (p_z, \uparrow), (p_z, \downarrow)$

Table 6: Atomic SAMB.

symbol	type	group	form
\mathbb{X}_1	$\mathbb{Q}_0^{(a, A_{1g})}$	M_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{X}_2	$\mathbb{M}_{2,0}^{(a, T_{2u})}(1, -1)$	M_2	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & 0 & -\frac{1}{2} & \frac{i}{2} & 0 \end{pmatrix}$
\mathbb{X}_3	$\mathbb{M}_{2,1}^{(a, T_{2u})}(1, -1)$	M_2	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & -\frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \end{pmatrix}$
\mathbb{X}_4	$\mathbb{M}_{2,2}^{(a, T_{2u})}(1, -1)$	M_2	$\begin{pmatrix} 0 & -\frac{i}{2} & 0 & \frac{1}{2} & 0 & 0 \\ \frac{i}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_5	$\mathbb{Q}_0^{(a, A_{1g})}$	M_3	$\begin{pmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{X}_6	$\mathbb{Q}_0^{(a, A_{1g})}(1, 1)$	M_3	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_7	$\mathbb{Q}_{2,0}^{(a, E_g)}$	M_3	$\begin{pmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{X}_8	$\mathbb{Q}_{2,1}^{(a, E_g)}$	M_3	$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
\mathbb{X}_9	$\mathbb{Q}_{2,0}^{(a,T_{2g})}$	M_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}$
\mathbb{X}_{10}	$\mathbb{Q}_{2,1}^{(a,T_{2g})}$	M_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{11}	$\mathbb{Q}_{2,2}^{(a,T_{2g})}$	M_3	$\begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{12}	$\mathbb{Q}_{2,0}^{(a,E_g)}(1, -1)$	M_3	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{13}	$\mathbb{Q}_{2,1}^{(a,E_g)}(1, -1)$	M_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{pmatrix}$

continued ...

Table 6

symbol	type	group	form
\mathbb{X}_{14}	$\mathbb{Q}_{2,0}^{(a,T_{2g})}(1,-1)$	M_3	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{X}_{15}	$\mathbb{Q}_{2,1}^{(a,T_{2g})}(1,-1)$	M_3	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{pmatrix}$
\mathbb{X}_{16}	$\mathbb{Q}_{2,2}^{(a,T_{2g})}(1,-1)$	M_3	$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
\mathbb{Y}_1	$\mathbb{Q}_0^{(s,A_{1g})}$	S_1	(1)
\mathbb{Y}_2	$\mathbb{Q}_0^{(b,A_{1g})}$	B_1	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{Y}_3	$\mathbb{Q}_{2,0}^{(b,E_g)}$	B_1	$\begin{pmatrix} -\frac{\sqrt{6}}{3} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{Y}_4	$\mathbb{Q}_{2,1}^{(b,E_g)}$	B_1	$\begin{pmatrix} 0 & -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{Y}_5	$\mathbb{Q}_0^{(b,A_{1g})}$	B_2	$\begin{pmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{Y}_6	$\mathbb{Q}_{2,0}^{(b,E_g)}$	B_2	$\begin{pmatrix} -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} \end{pmatrix}$

continued ...

Table 7

symbol	type	cluster	form
\mathbb{Y}_7	$\mathbb{Q}_{2,1}^{(b,E_g)}$	B_2	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & -\frac{1}{2} & 0 \end{pmatrix}$
\mathbb{Y}_8	$\mathbb{Q}_{2,0}^{(b,T_{2g})}$	B_2	$\begin{pmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \end{pmatrix}$
\mathbb{Y}_9	$\mathbb{Q}_{2,1}^{(b,T_{2g})}$	B_2	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
\mathbb{Y}_{10}	$\mathbb{Q}_{2,2}^{(b,T_{2g})}$	B_2	$\begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{Y}_{11}	$\mathbb{T}_{3,0}^{(b,T_{2u})}$	B_2	$\begin{pmatrix} 0 & 0 & \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & -\frac{i}{2} \end{pmatrix}$
\mathbb{Y}_{12}	$\mathbb{T}_{3,1}^{(b,T_{2u})}$	B_2	$\begin{pmatrix} -\frac{i}{2} & -\frac{i}{2} & 0 & -\frac{i}{2} & 0 & \frac{i}{2} \end{pmatrix}$
\mathbb{Y}_{13}	$\mathbb{T}_{3,2}^{(b,T_{2u})}$	B_2	$\begin{pmatrix} \frac{i}{2} & -\frac{i}{2} & \frac{i}{2} & 0 & -\frac{i}{2} & 0 \end{pmatrix}$

Table 8: Uniform SAMB.

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

Table 9: Structure SAMB.

symbol	type	cluster	form
\mathbb{F}_1	$\mathbb{Q}_0^{(k,A_{1g})}$	B_1	$\frac{\sqrt{6}c_{001}}{3} + \frac{\sqrt{6}c_{002}}{3} + \frac{\sqrt{6}c_{003}}{3}$
\mathbb{F}_2	$\mathbb{Q}_{2,0}^{(k,E_g)}$	B_1	$-\frac{2\sqrt{3}c_{001}}{3} + \frac{\sqrt{3}c_{002}}{3} + \frac{\sqrt{3}c_{003}}{3}$
\mathbb{F}_3	$\mathbb{Q}_{2,1}^{(k,E_g)}$	B_1	$-c_{002} + c_{003}$
\mathbb{F}_4	$\mathbb{Q}_0^{(k,A_{1g})}$	B_2	$\frac{\sqrt{3}c_{004}}{3} + \frac{\sqrt{3}c_{005}}{3} + \frac{\sqrt{3}c_{006}}{3} + \frac{\sqrt{3}c_{007}}{3} + \frac{\sqrt{3}c_{008}}{3} + \frac{\sqrt{3}c_{009}}{3}$
\mathbb{F}_5	$\mathbb{Q}_{2,0}^{(k,E_g)}$	B_2	$-\frac{\sqrt{6}c_{004}}{6} - \frac{\sqrt{6}c_{005}}{6} - \frac{\sqrt{6}c_{006}}{6} + \frac{\sqrt{6}c_{007}}{3} - \frac{\sqrt{6}c_{008}}{6} + \frac{\sqrt{6}c_{009}}{3}$
\mathbb{F}_6	$\mathbb{Q}_{2,1}^{(k,E_g)}$	B_2	$\frac{\sqrt{2}c_{004}}{2} + \frac{\sqrt{2}c_{005}}{2} - \frac{\sqrt{2}c_{006}}{2} - \frac{\sqrt{2}c_{008}}{2}$
\mathbb{F}_7	$\mathbb{Q}_{2,0}^{(k,T_{2g})}$	B_2	$c_{004} - c_{005}$
\mathbb{F}_8	$\mathbb{Q}_{2,1}^{(k,T_{2g})}$	B_2	$-c_{006} + c_{008}$

continued ...

Table 9

symbol	type	cluster	form
\mathbb{F}_9	$\mathbb{Q}_{2,2}^{(k,T_{2g})}$	B_2	$-c_{007} + c_{009}$
\mathbb{F}_{10}	$\mathbb{T}_{3,0}^{(k,T_{2u})}$	B_2	$\frac{\sqrt{2}s_{006}}{2} - \frac{\sqrt{2}s_{007}}{2} + \frac{\sqrt{2}s_{008}}{2} - \frac{\sqrt{2}s_{009}}{2}$
\mathbb{F}_{11}	$\mathbb{T}_{3,1}^{(k,T_{2u})}$	B_2	$-\frac{\sqrt{2}s_{004}}{2} - \frac{\sqrt{2}s_{005}}{2} - \frac{\sqrt{2}s_{007}}{2} + \frac{\sqrt{2}s_{009}}{2}$
\mathbb{F}_{12}	$\mathbb{T}_{3,2}^{(k,T_{2u})}$	B_2	$\frac{\sqrt{2}s_{004}}{2} - \frac{\sqrt{2}s_{005}}{2} + \frac{\sqrt{2}s_{006}}{2} - \frac{\sqrt{2}s_{008}}{2}$

Table 10: Polar harmonics.

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

Table 11: Axial harmonics.

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

- Group info.: Generator = $\{2_{001}|0\}, \{2_{010}|0\}, \{3_{111}^+|0\}, \{2_{110}|0\}, \{-1|0\}$

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

rep. SO	symmetry operations
$\{1 0\}$	$\{1 0\}$
$\{2_{001} 0\}$	$\{2_{001} 0\}, \{2_{100} 0\}, \{2_{010} 0\}$
$\{2_{110} 0\}$	$\{2_{110} 0\}, \{2_{101} 0\}, \{2_{011} 0\}, \{2_{1-10} 0\}, \{2_{-101} 0\}, \{2_{01-1} 0\}$
$\{3_{111}^+ 0\}$	$\{3_{111}^+ 0\}, \{3_{1-1-1}^+ 0\}, \{3_{-11-1}^+ 0\}, \{3_{-1-11}^+ 0\}, \{3_{111}^- 0\}, \{3_{1-1-1}^- 0\}, \{3_{-11-1}^- 0\}, \{3_{-1-11}^- 0\}$
$\{4_{001}^+ 0\}$	$\{4_{001}^+ 0\}, \{4_{100}^+ 0\}, \{4_{010}^+ 0\}, \{4_{001}^- 0\}, \{4_{100}^- 0\}, \{4_{010}^- 0\}$
$\{-1 0\}$	$\{-1 0\}$
$\{m_{001} 0\}$	$\{m_{001} 0\}, \{m_{100} 0\}, \{m_{010} 0\}$
$\{m_{110} 0\}$	$\{m_{110} 0\}, \{m_{101} 0\}, \{m_{011} 0\}, \{m_{1-10} 0\}, \{m_{-101} 0\}, \{m_{01-1} 0\}$
$\{-3_{111}^+ 0\}$	$\{-3_{111}^+ 0\}, \{-3_{1-1-1}^+ 0\}, \{-3_{-11-1}^+ 0\}, \{-3_{-1-11}^+ 0\}, \{-3_{111}^- 0\}, \{-3_{1-1-1}^- 0\}, \{-3_{-11-1}^- 0\}, \{-3_{-1-11}^- 0\}$
$\{-4_{001}^+ 0\}$	$\{-4_{001}^+ 0\}, \{-4_{100}^+ 0\}, \{-4_{010}^+ 0\}, \{-4_{001}^- 0\}, \{-4_{100}^- 0\}, \{-4_{010}^- 0\}$

Table 13: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1 0\}$	2	$\{2_{001} 0\}$	3	$\{2_{100} 0\}$	4	$\{2_{010} 0\}$	5	$\{2_{110} 0\}$
6	$\{2_{101} 0\}$	7	$\{2_{011} 0\}$	8	$\{2_{1-10} 0\}$	9	$\{2_{-101} 0\}$	10	$\{2_{01-1} 0\}$
11	$\{3_{111}^+ 0\}$	12	$\{3_{1-1-1}^+ 0\}$	13	$\{3_{-11-1}^+ 0\}$	14	$\{3_{-1-11}^+ 0\}$	15	$\{3_{111}^- 0\}$
16	$\{3_{1-1-1}^- 0\}$	17	$\{3_{-11-1}^- 0\}$	18	$\{3_{-1-11}^- 0\}$	19	$\{4_{001}^+ 0\}$	20	$\{4_{100}^+ 0\}$
21	$\{4_{010}^+ 0\}$	22	$\{4_{001}^- 0\}$	23	$\{4_{100}^- 0\}$	24	$\{4_{010}^- 0\}$	25	$\{-1 0\}$
26	$\{m_{001} 0\}$	27	$\{m_{100} 0\}$	28	$\{m_{010} 0\}$	29	$\{m_{110} 0\}$	30	$\{m_{101} 0\}$
31	$\{m_{011} 0\}$	32	$\{m_{1-10} 0\}$	33	$\{m_{-101} 0\}$	34	$\{m_{01-1} 0\}$	35	$\{-3_{111}^+ 0\}$
36	$\{-3_{1-1-1}^+ 0\}$	37	$\{-3_{-11-1}^+ 0\}$	38	$\{-3_{-1-11}^+ 0\}$	39	$\{-3_{111}^- 0\}$	40	$\{-3_{1-1-1}^- 0\}$
41	$\{-3_{-11-1}^- 0\}$	42	$\{-3_{-1-11}^- 0\}$	43	$\{-4_{001}^+ 0\}$	44	$\{-4_{100}^+ 0\}$	45	$\{-4_{010}^+ 0\}$

continued ...

Table 13

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
46	$\{-4_{001}^- 0\}$	47	$\{-4_{100}^- 0\}$	48	$\{-4_{010}^- 0\}$				

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

	1	2 ₀₀₁	2 ₁₁₀	3 ₁₁₁ ⁺	4 ₀₀₁ ⁺	-1	m ₀₀₁	m ₁₁₀	-3 ₁₁₁ ⁺	-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
E_g	2	2	0	-1	0	2	2	0	-1	0
T_{1g}	3	-1	-1	0	1	3	-1	-1	0	1
T_{2g}	3	-1	1	0	-1	3	-1	1	0	-1
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	-1	1	-1	-1	-1	1	-1	1
E_u	2	2	0	-1	0	-2	-2	0	1	0
T_{1u}	3	-1	-1	0	1	-3	1	1	0	-1
T_{2u}	3	-1	1	0	-1	-3	1	-1	0	1

Table 15: Parity conversion.

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

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

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

continued ...

Table 16

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

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

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

Table 18: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix} 3 & 2 & 1 \end{pmatrix}$	2	$\begin{pmatrix} -3 & -2 & 1 \end{pmatrix}$	3	$\begin{pmatrix} 3 & -2 & -1 \end{pmatrix}$	4	$\begin{pmatrix} -3 & 2 & -1 \end{pmatrix}$
5	$\begin{pmatrix} 2 & 3 & -1 \end{pmatrix}$	6	$\begin{pmatrix} 1 & -2 & 3 \end{pmatrix}$	7	$\begin{pmatrix} -3 & 1 & 2 \end{pmatrix}$	8	$\begin{pmatrix} -2 & -3 & -1 \end{pmatrix}$
9	$\begin{pmatrix} -1 & -2 & -3 \end{pmatrix}$	10	$\begin{pmatrix} -3 & -1 & -2 \end{pmatrix}$	11	$\begin{pmatrix} 1 & 3 & 2 \end{pmatrix}$	12	$\begin{pmatrix} -1 & -3 & 2 \end{pmatrix}$
13	$\begin{pmatrix} 1 & -3 & -2 \end{pmatrix}$	14	$\begin{pmatrix} -1 & 3 & -2 \end{pmatrix}$	15	$\begin{pmatrix} 2 & 1 & 3 \end{pmatrix}$	16	$\begin{pmatrix} -2 & 1 & -3 \end{pmatrix}$
17	$\begin{pmatrix} -2 & -1 & 3 \end{pmatrix}$	18	$\begin{pmatrix} 2 & -1 & -3 \end{pmatrix}$	19	$\begin{pmatrix} -2 & 3 & 1 \end{pmatrix}$	20	$\begin{pmatrix} 3 & -1 & 2 \end{pmatrix}$
21	$\begin{pmatrix} 1 & 2 & -3 \end{pmatrix}$	22	$\begin{pmatrix} 2 & -3 & 1 \end{pmatrix}$	23	$\begin{pmatrix} 3 & 1 & -2 \end{pmatrix}$	24	$\begin{pmatrix} -1 & 2 & 3 \end{pmatrix}$
25	$\begin{pmatrix} -3 & -2 & -1 \end{pmatrix}$	26	$\begin{pmatrix} 3 & 2 & -1 \end{pmatrix}$	27	$\begin{pmatrix} -3 & 2 & 1 \end{pmatrix}$	28	$\begin{pmatrix} 3 & -2 & 1 \end{pmatrix}$
29	$\begin{pmatrix} -2 & -3 & 1 \end{pmatrix}$	30	$\begin{pmatrix} -1 & 2 & -3 \end{pmatrix}$	31	$\begin{pmatrix} 3 & -1 & -2 \end{pmatrix}$	32	$\begin{pmatrix} 2 & 3 & 1 \end{pmatrix}$
33	$\begin{pmatrix} 1 & 2 & 3 \end{pmatrix}$	34	$\begin{pmatrix} 3 & 1 & 2 \end{pmatrix}$	35	$\begin{pmatrix} -1 & -3 & -2 \end{pmatrix}$	36	$\begin{pmatrix} 1 & 3 & -2 \end{pmatrix}$
37	$\begin{pmatrix} -1 & 3 & 2 \end{pmatrix}$	38	$\begin{pmatrix} 1 & -3 & 2 \end{pmatrix}$	39	$\begin{pmatrix} -2 & -1 & -3 \end{pmatrix}$	40	$\begin{pmatrix} 2 & -1 & 3 \end{pmatrix}$

continued ...

Table 18

No.	position	No.	position	No.	position	No.	position
41	$\begin{pmatrix} 2 & 1 & -3 \end{pmatrix}$	42	$\begin{pmatrix} -2 & 1 & 3 \end{pmatrix}$	43	$\begin{pmatrix} 2 & -3 & -1 \end{pmatrix}$	44	$\begin{pmatrix} -3 & 1 & -2 \end{pmatrix}$
45	$\begin{pmatrix} -1 & -2 & 3 \end{pmatrix}$	46	$\begin{pmatrix} -2 & 3 & -1 \end{pmatrix}$	47	$\begin{pmatrix} -3 & -1 & 2 \end{pmatrix}$	48	$\begin{pmatrix} 1 & -2 & -3 \end{pmatrix}$

Table 19: Virtual-cluster basis.

symbol	1	2	3	4	5	6	7	8	9	10
$Q_0^{(A_{1g})}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$
	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$
	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$
	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$
	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$
$Q_{1,0}^{(T_{1u})}$	$\frac{3\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$
	$\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$\frac{3\sqrt{14}}{56}$
	$\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{28}$	$\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{56}$
	$\frac{3\sqrt{14}}{56}$	$\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{28}$
	$\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{28}$	$-\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$	$-\frac{3\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$		
$Q_{1,1}^{(T_{1u})}$	$\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{28}$	$\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{56}$
	$\frac{3\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$
	$\frac{\sqrt{14}}{28}$	$-\frac{3\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$-\frac{3\sqrt{14}}{56}$	$\frac{\sqrt{14}}{28}$
	$-\frac{\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$
	$\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$	$\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$		
$Q_{1,2}^{(T_{1u})}$	$\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$
	$\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$\frac{3\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{28}$
	$-\frac{3\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$	$\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$
	$-\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{28}$	$-\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$
	$-\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{28}$	$-\frac{3\sqrt{14}}{56}$		
$Q_{2,0}^{(E_g)}$	$-\frac{11\sqrt{6}}{168}$	$-\frac{11\sqrt{6}}{168}$	$-\frac{11\sqrt{6}}{168}$	$-\frac{11\sqrt{6}}{168}$	$-\frac{11\sqrt{6}}{168}$	$\frac{13\sqrt{6}}{168}$	$-\frac{\sqrt{6}}{84}$	$-\frac{11\sqrt{6}}{168}$	$\frac{13\sqrt{6}}{168}$	$-\frac{\sqrt{6}}{84}$

continued ...

Table 19

[illegible]

continued ...

Table 19

[illegible]

continued ...

Table 19

[illegible]

continued ...

[illegible]

19

Table 19

[illegible]

continued ...

Table 19

[illegible]

continued ...

symbol	1	2	3	4	5	6	7	8	9	10
	$-\frac{\sqrt{2}}{7}$	$-\frac{\sqrt{2}}{7}$	$-\frac{\sqrt{2}}{7}$	$-\frac{\sqrt{2}}{7}$	$\frac{3\sqrt{2}}{56}$	$\frac{3\sqrt{2}}{56}$	$\frac{3\sqrt{2}}{56}$	$\frac{3\sqrt{2}}{56}$	$-\frac{5\sqrt{2}}{56}$	$\frac{\sqrt{2}}{7}$
	$-\frac{3\sqrt{2}}{56}$	$-\frac{5\sqrt{2}}{56}$	$\frac{\sqrt{2}}{7}$	$-\frac{3\sqrt{2}}{56}$	$-\frac{5\sqrt{2}}{56}$	$-\frac{5\sqrt{2}}{56}$	$-\frac{5\sqrt{2}}{56}$	$-\frac{5\sqrt{2}}{56}$	$\frac{5\sqrt{2}}{56}$	$\frac{3\sqrt{2}}{56}$
	$-\frac{\sqrt{2}}{7}$	$\frac{5\sqrt{2}}{56}$	$\frac{3\sqrt{2}}{56}$	$-\frac{\sqrt{2}}{7}$	$\frac{\sqrt{2}}{7}$	$\frac{\sqrt{2}}{7}$	$\frac{\sqrt{2}}{7}$	$\frac{\sqrt{2}}{7}$	$-\frac{3\sqrt{2}}{56}$	$-\frac{3\sqrt{2}}{56}$
	$-\frac{3\sqrt{2}}{56}$	$-\frac{3\sqrt{2}}{56}$	$\frac{5\sqrt{2}}{56}$	$-\frac{\sqrt{2}}{7}$	$\frac{3\sqrt{2}}{56}$	$\frac{5\sqrt{2}}{56}$	$-\frac{\sqrt{2}}{7}$	$\frac{3\sqrt{2}}{56}$		
$\mathbb{Q}_{7,0}^{(T_{2u},1)}$	$-\frac{1}{14}$	$\frac{1}{14}$	$-\frac{1}{14}$	$\frac{1}{14}$	$\frac{3}{28}$	$\frac{3}{14}$	$-\frac{1}{14}$	$-\frac{3}{28}$	$-\frac{3}{14}$	$-\frac{1}{14}$
	$-\frac{3}{14}$	$\frac{3}{14}$	$-\frac{3}{14}$	$\frac{3}{14}$	$-\frac{3}{28}$	$\frac{3}{28}$	$\frac{3}{28}$	$-\frac{3}{28}$	$-\frac{3}{28}$	$\frac{1}{14}$
	$\frac{3}{14}$	$\frac{3}{28}$	$\frac{1}{14}$	$-\frac{3}{14}$	$\frac{1}{14}$	$-\frac{1}{14}$	$\frac{1}{14}$	$-\frac{1}{14}$	$-\frac{3}{28}$	$-\frac{3}{14}$
	$\frac{1}{14}$	$\frac{3}{28}$	$\frac{3}{14}$	$\frac{1}{14}$	$\frac{3}{14}$	$-\frac{3}{14}$	$\frac{3}{14}$	$-\frac{3}{14}$	$\frac{3}{28}$	$-\frac{3}{28}$
	$-\frac{3}{28}$	$\frac{3}{28}$	$\frac{3}{28}$	$-\frac{1}{14}$	$-\frac{3}{14}$	$-\frac{3}{28}$	$-\frac{1}{14}$	$\frac{3}{14}$		
$\mathbb{Q}_{7,1}^{(T_{2u},1)}$	$-\frac{3}{28}$	$\frac{3}{28}$	$\frac{3}{28}$	$-\frac{3}{28}$	$\frac{1}{14}$	$-\frac{3}{28}$	$\frac{3}{14}$	$-\frac{1}{14}$	$-\frac{3}{28}$	$-\frac{3}{14}$
	$-\frac{1}{14}$	$\frac{1}{14}$	$\frac{1}{14}$	$-\frac{1}{14}$	$-\frac{3}{14}$	$-\frac{3}{14}$	$\frac{3}{14}$	$\frac{3}{14}$	$\frac{1}{14}$	$-\frac{3}{14}$
	$\frac{3}{28}$	$-\frac{1}{14}$	$\frac{3}{14}$	$\frac{3}{28}$	$\frac{3}{28}$	$-\frac{3}{28}$	$-\frac{3}{28}$	$\frac{3}{28}$	$-\frac{1}{14}$	$\frac{3}{28}$
	$-\frac{3}{14}$	$\frac{1}{14}$	$\frac{3}{28}$	$\frac{3}{14}$	$\frac{1}{14}$	$-\frac{1}{14}$	$-\frac{1}{14}$	$\frac{1}{14}$	$\frac{3}{14}$	$\frac{3}{14}$
	$-\frac{3}{14}$	$-\frac{3}{14}$	$-\frac{1}{14}$	$\frac{3}{14}$	$-\frac{3}{28}$	$\frac{1}{14}$	$-\frac{3}{14}$	$-\frac{3}{28}$		
$\mathbb{Q}_{7,2}^{(T_{2u},1)}$	$-\frac{3}{14}$	$-\frac{3}{14}$	$\frac{3}{14}$	$\frac{3}{14}$	$-\frac{3}{14}$	$\frac{1}{14}$	$\frac{3}{28}$	$-\frac{3}{14}$	$-\frac{1}{14}$	$-\frac{3}{28}$
	$-\frac{3}{28}$	$-\frac{3}{28}$	$\frac{3}{28}$	$\frac{3}{28}$	$-\frac{1}{14}$	$\frac{1}{14}$	$-\frac{1}{14}$	$\frac{1}{14}$	$\frac{3}{14}$	$\frac{3}{28}$
	$-\frac{1}{14}$	$\frac{3}{14}$	$-\frac{3}{28}$	$\frac{1}{14}$	$\frac{3}{14}$	$\frac{3}{14}$	$-\frac{3}{14}$	$-\frac{3}{14}$	$\frac{3}{14}$	$-\frac{1}{14}$
	$-\frac{3}{28}$	$\frac{3}{14}$	$\frac{1}{14}$	$\frac{3}{28}$	$\frac{3}{28}$	$\frac{3}{28}$	$-\frac{3}{28}$	$-\frac{3}{28}$	$\frac{1}{14}$	$-\frac{1}{14}$
	$\frac{1}{14}$	$-\frac{1}{14}$	$-\frac{3}{14}$	$-\frac{3}{28}$	$\frac{1}{14}$	$-\frac{3}{14}$	$\frac{3}{28}$	$-\frac{1}{14}$		
$\mathbb{Q}_{8,0}^{(T_{1g},1)}$	$-\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$
	$-\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{28}$	$-\frac{3\sqrt{14}}{56}$
	$-\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$	$-\frac{3\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{56}$

continued ...

Table 19

symbol	1	2	3	4	5	6	7	8	9	10
	$-\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{28}$	$-\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$
	$\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{28}$	$-\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{56}$	$-\frac{3\sqrt{14}}{56}$
	$-\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$-\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{28}$	$\frac{\sqrt{14}}{28}$	$-\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$
	$-\frac{3\sqrt{14}}{56}$	$\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{28}$	$\frac{3\sqrt{14}}{56}$	$-\frac{\sqrt{14}}{56}$	$\frac{\sqrt{14}}{28}$	$-\frac{3\sqrt{14}}{56}$		
$Q_9^{(A_{1u})}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$
	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$
	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$
	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$
	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$	$-\frac{\sqrt{3}}{12}$		