SG No. 67 D_{2h}^{21} $Cmme$ [orthorhombic]

* plus set: $+[0,\ 0,\ 0]$, $+\left[\frac{1}{2},\ \frac{1}{2},\ 0\right]$

Table 1: Wyckoff site: `4a`, site symmetry: `222`

No.	position	mapping
1	$\left[\frac{1}{4},\ 0,\ 0\right]$	`[1,2,3,4]`
2	$\left[\frac{3}{4},\ 0,\ 0\right]$	`[5,6,7,8]`

Table 2: Wyckoff site: `4b`, site symmetry: `222`

No.	position	mapping
1	$\left[\frac{1}{4},\ 0,\ \frac{1}{2}\right]$	`[1,2,3,4]`
2	$\left[\frac{3}{4},\ 0,\ \frac{1}{2}\right]$	`[5,6,7,8]`

Table 3: Wyckoff site: `4c`, site symmetry: `2/m..`

No.	position	mapping
1	$[0,\ 0,\ 0]$	`[1,4,5,8]`
2	$\left[0,\ \frac{1}{2},\ 0\right]$	`[2,3,6,7]`

Table 4: Wyckoff site: `4d`, site symmetry: `2/m..`

No.	position	mapping
1	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[1,4,5,8]`
2	$\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[2,3,6,7]`

Table 5: Wyckoff site: `4e`, site symmetry: `.2/m.`

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{4},\ 0\right]$	`[1,3,5,7]`
2	$\left[\frac{3}{4},\ \frac{1}{4},\ 0\right]$	`[2,4,6,8]`

Table 6: Wyckoff site: `4f`, site symmetry: `.2/m.`

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$	`[1,3,5,7]`
2	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	`[2,4,6,8]`

Table 7: Wyckoff site: `4g`, site symmetry: `mm2`

No.	position	mapping
1	$\left[0, \frac{1}{4}, z\right]$	`[1,2,7,8]`
2	$\left[0, \frac{3}{4}, -z\right]$	`[3,4,5,6]`

Table 8: Wyckoff site: `8h`, site symmetry: `2..`

No.	position	mapping
1	$[x, 0, 0]$	`[1,4]`
2	$\left[-x, \frac{1}{2}, 0\right]$	`[2,3]`
3	$[-x, 0, 0]$	`[5,8]`
4	$\left[x, \frac{1}{2}, 0\right]$	`[6,7]`

Table 9: Wyckoff site: `8i`, site symmetry: `2..`

No.	position	mapping
1	$\left[x, 0, \frac{1}{2}\right]$	`[1,4]`
2	$\left[-x, \frac{1}{2}, \frac{1}{2}\right]$	`[2,3]`
3	$\left[-x, 0, \frac{1}{2}\right]$	`[5,8]`
4	$\left[x, \frac{1}{2}, \frac{1}{2}\right]$	`[6,7]`

Table 10: Wyckoff site: `8j`, site symmetry: `.2.`

No.	position	mapping
1	$\left[\frac{1}{4}, y, 0\right]$	`[1,3]`
2	$\left[\frac{3}{4}, \frac{1}{2} - y, 0\right]$	`[2,4]`
3	$\left[\frac{3}{4}, -y, 0\right]$	`[5,7]`
4	$\left[\frac{1}{4}, y + \frac{1}{2}, 0\right]$	`[6,8]`

Table 11: Wyckoff site: `8k`, site symmetry: `.2.`

No.	position	mapping
1	$\left[\frac{1}{4},\, y,\, \frac{1}{2}\right]$	`[1,3]`
2	$\left[\frac{3}{4},\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	`[2,4]`
3	$\left[\frac{3}{4},\, -y,\, \frac{1}{2}\right]$	`[5,7]`
4	$\left[\frac{1}{4},\, y+\frac{1}{2},\, \frac{1}{2}\right]$	`[6,8]`

Table 12: Wyckoff site: `8l`, site symmetry: `..2`

No.	position	mapping
1	$\left[\frac{1}{4},\, 0,\, z\right]$	`[1,2]`
2	$\left[\frac{3}{4},\, \frac{1}{2},\, -z\right]$	`[3,4]`
3	$\left[\frac{3}{4},\, 0,\, -z\right]$	`[5,6]`
4	$\left[\frac{1}{4},\, \frac{1}{2},\, z\right]$	`[7,8]`

Table 13: Wyckoff site: `8m`, site symmetry: `m..`

No.	position	mapping
1	$[0,\, y,\, z]$	`[1,8]`
2	$\left[0,\, \frac{1}{2}-y,\, z\right]$	`[2,7]`
3	$\left[0,\, y+\frac{1}{2},\, -z\right]$	`[3,6]`
4	$[0,\, -y,\, -z]$	`[4,5]`

Table 14: Wyckoff site: `8n`, site symmetry: `.m.`

No.	position	mapping
1	$\left[x,\, \frac{1}{4},\, z\right]$	`[1,7]`
2	$\left[-x,\, \frac{1}{4},\, z\right]$	`[2,8]`
3	$\left[-x,\, \frac{3}{4},\, -z\right]$	`[3,5]`
4	$\left[x,\, \frac{3}{4},\, -z\right]$	`[4,6]`

Table 15: Wyckoff site: `16o`, site symmetry: `1`

No.	position	mapping
1	$[x,\, y,\, z]$	`[1]`
2	$\left[-x,\, \frac{1}{2}-y,\, z\right]$	`[2]`
3	$\left[-x,\, y+\frac{1}{2},\, -z\right]$	`[3]`
4	$[x,\, -y,\, -z]$	`[4]`

continued ...

Table 15

No.	position	mapping
5	$[-x,\, -y,\, -z]$	[5]
6	$\left[x,\, y+\frac{1}{2},\, -z\right]$	[6]
7	$\left[x,\, \frac{1}{2}-y,\, z\right]$	[7]
8	$[-x,\, y,\, z]$	[8]