SG No. 50 D_{2h}^4 *Pban* [orthorhombic]

* plus set: + [0, 0, 0]

Table 1: Wyckoff site: 2a, site symmetry: 222

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: 222

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

Table 4: Wyckoff site: 2d, site symmetry: 222

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

Table 5: Wyckoff site: 4e, site symmetry: -1

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

Table 6: Wyckoff site: `4f`, site symmetry: `-1`

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

Table 7: Wyckoff site: `4g`, site symmetry: `2..`

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

Table 8: Wyckoff site: `4h`, site symmetry: `2..`

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

Table 9: Wyckoff site: `4i`, site symmetry: `.2.`

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

Table 10: Wyckoff site: `4j`, site symmetry: `.2.`

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

Table 11: Wyckoff site: `4k`, site symmetry: `..2`

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

Table 12: Wyckoff site: `4l`, site symmetry: `..2`

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

Table 13: Wyckoff site: `8m`, site symmetry: `1`

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