

SG No. 51 D_{2h}^5 $Pmma$ [orthorhombic]

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

Table 1: Wyckoff site: 2a, site symmetry: $.2/m$.

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

Table 2: Wyckoff site: 2b, site symmetry: $.2/m$.

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

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

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

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

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

Table 5: Wyckoff site: 2e, site symmetry: $mm2$

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

Table 6: Wyckoff site: 2f, site symmetry: mm2

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

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

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

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

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

Table 9: Wyckoff site: 4i, site symmetry: .m.

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

Table 10: Wyckoff site: 4j, site symmetry: .m.

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

Table 11: Wyckoff site: $4k$, site symmetry: m .

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

Table 12: Wyckoff site: $8l$, site symmetry: 1

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