

SG No. 62 D_{2h}^{16} $Pnma$ [orthorhombic]

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

Table 1: Wyckoff site: 4a, site symmetry: -1

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

Table 2: Wyckoff site: 4b, site symmetry: -1

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

Table 3: Wyckoff site: 4c, site symmetry: .m.

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

Table 4: Wyckoff site: 8d, site symmetry: 1

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