

MSG No. 61.434 *Pbca1'* [Type II, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: -11'

No.	position	mapping
1	[0, 0, 0]	[1,5,9,13]
2	[\frac{1}{2}, \frac{1}{2}, 0]	[2,6,10,14]
3	[0, \frac{1}{2}, \frac{1}{2}]	[3,7,11,15]
4	[\frac{1}{2}, 0, \frac{1}{2}]	[4,8,12,16]

Table 2: Wyckoff site: 4b, site symmetry: -11'

No.	position	mapping
1	[0, 0, \frac{1}{2}]	[1,5,9,13]
2	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]	[2,6,10,14]
3	[0, \frac{1}{2}, 0]	[3,7,11,15]
4	[\frac{1}{2}, 0, 0]	[4,8,12,16]

Table 3: Wyckoff site: 8c, site symmetry: 11'

No.	position	mapping
1	[x, y, z]	[1,9]
2	[x + \frac{1}{2}, \frac{1}{2} - y, -z]	[2,10]
3	[-x, y + \frac{1}{2}, \frac{1}{2} - z]	[3,11]
4	[\frac{1}{2} - x, -y, z + \frac{1}{2}]	[4,12]
5	[-x, -y, -z]	[5,13]
6	[\frac{1}{2} - x, y + \frac{1}{2}, z]	[6,14]
7	[x, \frac{1}{2} - y, z + \frac{1}{2}]	[7,15]
8	[x + \frac{1}{2}, y, \frac{1}{2} - z]	[8,16]