

MSG No. 60.421 *Pbcn'* [Type III, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: **4c**, site symmetry: **.2'**.

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

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

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