

MSG No. 45.237 *Ib'a2'* [Type III, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: ...2'

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

Table 2: Wyckoff site: 4b, site symmetry: ...2'

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

Table 3: Wyckoff site: 8c, site symmetry: 1

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