

MSG No. 45.235 *Iba2* [Type I, orthorhombic]

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

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

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

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

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

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