

MSG No. 147.13 $P\bar{3}$ [Type I, trigonal]

Table 1: Wyckoff site: **1a**, site symmetry: -3..

No.	position	mapping
1	[0, 0, 0]	[1,2,3,4,5,6]

Table 2: Wyckoff site: **1b**, site symmetry: -3..

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

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

No.	position	mapping
1	[0, 0, z]	[1,2,3]
2	[0, 0, $-z$]	[4,5,6]

Table 4: Wyckoff site: **2d**, site symmetry: 3..

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

Table 5: Wyckoff site: **3e**, site symmetry: -1

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

Table 6: Wyckoff site: **3f**, site symmetry: -1

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

Table 7: Wyckoff site: 6g, site symmetry: 1

No.	position	mapping
1	[x, y, z]	[1]
2	[$-y, x - y, z$]	[2]
3	[$-x + y, -x, z$]	[3]
4	[$-x, -y, -z$]	[4]
5	[$y, -x + y, -z$]	[5]
6	[$x - y, x, -z$]	[6]