

MSG No. 156.52 P_c3m1 [Type IV, trigonal]

Table 1: Wyckoff site: 2a, site symmetry: 3m.

No.	position	mapping
1	[0, 0, z]	[1,2,3,4,5,6]
2	[0, 0, $z + \frac{1}{2}$]	[7,8,9,10,11,12]

Table 2: Wyckoff site: 2b, site symmetry: 3m.

No.	position	mapping
1	[$\frac{1}{3}$, $\frac{2}{3}$, z]	[1,2,3,4,5,6]
2	[$\frac{1}{3}$, $\frac{2}{3}$, $z + \frac{1}{2}$]	[7,8,9,10,11,12]

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

No.	position	mapping
1	[$\frac{2}{3}$, $\frac{1}{3}$, z]	[1,2,3,4,5,6]
2	[$\frac{2}{3}$, $\frac{1}{3}$, $z + \frac{1}{2}$]	[7,8,9,10,11,12]

Table 4: Wyckoff site: 6d, site symmetry: .m.

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

Table 5: Wyckoff site: 12e, 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, y, z]	[4]
5	[-y, -x, z]	[5]
6	[x, x - y, z]	[6]

continued ...

Table 5

No.	position	mapping
7	$[x, y, z + \frac{1}{2}]$	[7]
8	$[-y, x - y, z + \frac{1}{2}]$	[8]
9	$[-x + y, -x, z + \frac{1}{2}]$	[9]
10	$[-x + y, y, z + \frac{1}{2}]$	[10]
11	$[-y, -x, z + \frac{1}{2}]$	[11]
12	$[x, x - y, z + \frac{1}{2}]$	[12]