

MSG No. 164.88  $P\bar{3}'m'1$  [ Type III, trigonal ]

Table 1: Wyckoff site: 1a, site symmetry:  $-3'm'$ .

No.	position	mapping
1	[0, 0, 0]	[1,2,3,4,5,6,7,8,9,10,11,12]

Table 2: Wyckoff site: 1b, site symmetry:  $-3'm'$ .

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

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

No.	position	mapping
1	[0, 0, $z$ ]	[1,2,3,10,11,12]
2	[0, 0, $-z$ ]	[4,5,6,7,8,9]

Table 4: Wyckoff site: 2d, site symmetry:  $3m'$ .

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

Table 5: Wyckoff site: 3e, site symmetry:  $.2/m'$ .

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

Table 6: Wyckoff site: 3f, site symmetry:  $.2/m'$ .

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

Table 7: Wyckoff site: 6g, site symmetry: .2.

No.	position	mapping
1	[ $x, 0, 0$ ]	[1,4]
2	[ $0, x, 0$ ]	[2,5]
3	[ $-x, -x, 0$ ]	[3,6]
4	[ $-x, 0, 0$ ]	[7,10]
5	[ $0, -x, 0$ ]	[8,11]
6	[ $x, x, 0$ ]	[9,12]

Table 8: Wyckoff site: 6h, site symmetry: .2.

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

Table 9: Wyckoff site: 6i, site symmetry: .m'.

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

Table 10: Wyckoff site: 12j, 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]
7	[ $-x, -y, -z$ ]	[7]
8	[ $y, -x + y, -z$ ]	[8]
9	[ $x - y, x, -z$ ]	[9]

continued ...

Table 10

No.	position	mapping
10	$[-x + y, y, z]$	[10]
11	$[-y, -x, z]$	[11]
12	$[x, x - y, z]$	[12]