

# MSG No. 164.86 $P\bar{3}m11'$ [ Type II, trigonal ]

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

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$

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

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$

Table 3: Wyckoff site: 2c, site symmetry: 3m.1'

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 10, 11, 12, 13, 14, 15, 22, 23, 24]$
2	$[0, 0, -z]$	$[4, 5, 6, 7, 8, 9, 16, 17, 18, 19, 20, 21]$

Table 4: Wyckoff site: 2d, site symmetry: 3m.1'

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, z]$	$[1, 2, 3, 10, 11, 12, 13, 14, 15, 22, 23, 24]$
2	$[\frac{2}{3}, \frac{1}{3}, -z]$	$[4, 5, 6, 7, 8, 9, 16, 17, 18, 19, 20, 21]$

Table 5: Wyckoff site: 3e, site symmetry: .2/m.1'

No.	position	mapping
1	$[\frac{1}{2}, 0, 0]$	$[1, 4, 7, 10, 13, 16, 19, 22]$
2	$[0, \frac{1}{2}, 0]$	$[2, 5, 8, 11, 14, 17, 20, 23]$
3	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[3, 6, 9, 12, 15, 18, 21, 24]$

Table 6: Wyckoff site: 3f, site symmetry: .2/m.1'

No.	position	mapping
1	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[1, 4, 7, 10, 13, 16, 19, 22]$
2	$[0, \frac{1}{2}, \frac{1}{2}]$	$[2, 5, 8, 11, 14, 17, 20, 23]$
3	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[3, 6, 9, 12, 15, 18, 21, 24]$

Table 7: Wyckoff site: 6g, site symmetry: .2.1'

No.	position	mapping
1	[ $x, 0, 0$ ]	[1,4,13,16]
2	[ $0, x, 0$ ]	[2,5,14,17]
3	[ $-x, -x, 0$ ]	[3,6,15,18]
4	[ $-x, 0, 0$ ]	[7,10,19,22]
5	[ $0, -x, 0$ ]	[8,11,20,23]
6	[ $x, x, 0$ ]	[9,12,21,24]

Table 8: Wyckoff site: 6h, site symmetry: .2.1'

No.	position	mapping
1	[ $x, 0, \frac{1}{2}$ ]	[1,4,13,16]
2	[ $0, x, \frac{1}{2}$ ]	[2,5,14,17]
3	[ $-x, -x, \frac{1}{2}$ ]	[3,6,15,18]
4	[ $-x, 0, \frac{1}{2}$ ]	[7,10,19,22]
5	[ $0, -x, \frac{1}{2}$ ]	[8,11,20,23]
6	[ $x, x, \frac{1}{2}$ ]	[9,12,21,24]

Table 9: Wyckoff site: 6i, site symmetry: .m.1'

No.	position	mapping
1	[ $x, -x, z$ ]	[1,11,13,23]
2	[ $x, 2x, z$ ]	[2,12,14,24]
3	[ $-2x, -x, z$ ]	[3,10,15,22]
4	[ $2x, x, -z$ ]	[4,9,16,21]
5	[ $-x, x, -z$ ]	[5,7,17,19]
6	[ $-x, -2x, -z$ ]	[6,8,18,20]

Table 10: Wyckoff site: 12j, site symmetry: 11'

No.	position	mapping
1	[ $x, y, z$ ]	[1,13]
2	[ $-y, x - y, z$ ]	[2,14]
3	[ $-x + y, -x, z$ ]	[3,15]
4	[ $x - y, -y, -z$ ]	[4,16]
5	[ $y, x, -z$ ]	[5,17]
6	[ $-x, -x + y, -z$ ]	[6,18]
7	[ $-x, -y, -z$ ]	[7,19]
8	[ $y, -x + y, -z$ ]	[8,20]
9	[ $x - y, x, -z$ ]	[9,21]

*continued ...*

Table 10

No.	position	mapping
10	$[-x + y, y, z]$	[10,22]
11	$[-y, -x, z]$	[11,23]
12	$[x, x - y, z]$	[12,24]