

MSG No. 162.74  $P\bar{3}1m1'$  [ Type II, trigonal ]

Table 1: Wyckoff site: 1a, site symmetry:  $-3.m1'$

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:  $-3.m1'$

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:  $3.21'$

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

Table 4: Wyckoff site: 2d, site symmetry:  $3.21'$

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

Table 5: Wyckoff site: 2e, site symmetry:  $3.m1'$

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 6: Wyckoff site: 3f, site symmetry:  $..2/m1'$

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

Table 7: Wyckoff site:  $3g$ , site symmetry:  $..2/m1'$ 

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

Table 8: Wyckoff site:  $4h$ , site symmetry:  $3..1'$ 

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

Table 9: Wyckoff site:  $6i$ , site symmetry:  $..21'$ 

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

Table 10: Wyckoff site:  $6j$ , site symmetry:  $..21'$ 

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

Table 11: Wyckoff site:  $6k$ , site symmetry:  $..m1'$ 

No.	position	mapping
1	$[x, 0, z]$	[1, 11, 13, 23]

*continued ...*

Table 11

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

Table 12: Wyckoff site: 12l, 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	$[x, x - y, -z]$	$[4, 16]$
5	$[-x + y, y, -z]$	$[5, 17]$
6	$[-y, -x, -z]$	$[6, 18]$
7	$[-x, -y, -z]$	$[7, 19]$
8	$[y, -x + y, -z]$	$[8, 20]$
9	$[x - y, x, -z]$	$[9, 21]$
10	$[-x, -x + y, z]$	$[10, 22]$
11	$[x - y, -y, z]$	$[11, 23]$
12	$[y, x, z]$	$[12, 24]$