

# 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:  $\dots 2/m1'$

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:  $\dots 2/m1'$ 

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:  $3\dots 1'$ 

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:  $\dots 21'$ 

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:  $\dots 21'$ 

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:  $\dots m1'$ 

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: 121, 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]