

MSG No. 162.75 $P\bar{3}'1m$ [Type III, trigonal]

Table 1: Wyckoff site: **1a**, site symmetry: $-3' \cdot m$

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: $-3' \cdot m$

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: $3 \cdot 2'$

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

Table 4: Wyckoff site: **2d**, site symmetry: $3 \cdot 2'$

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

Table 5: Wyckoff site: **2e**, site symmetry: $3 \cdot m$

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

Table 6: Wyckoff site: **3f**, site symmetry: $\dots 2'/m$

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

Table 7: Wyckoff site: 3g, site symmetry: $\dots 2'/\text{m}$

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

Table 8: Wyckoff site: 4h, site symmetry: 3..

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

Table 9: Wyckoff site: 6i, site symmetry: $\dots 2'$

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

Table 10: Wyckoff site: 6j, site symmetry: $\dots 2'$

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

Table 11: Wyckoff site: 6k, site symmetry: $\dots \text{m}$

No.	position	mapping
1	$[x, 0, z]$	[1,5]

continued ...

Table 11

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

Table 12: Wyckoff site: 121, 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 , - x + y , z]	[4]
5	[x - y , - y , z]	[5]
6	[y , x , z]	[6]
7	[x , x - y , - z]	[7]
8	[- x + y , y , - z]	[8]
9	[- y , - x , - z]	[9]
10	[- x , - y , - z]	[10]
11	[y , - x + y , - z]	[11]
12	[x - y , x , - z]	[12]