

SG No. 162  $D_{3d}^1$   $P\bar{3}1m$  [ trigonal ]

\* plus set:  $+ [0, 0, 0]$

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:  $3.2$

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

Table 4: Wyckoff site: 2d, site symmetry:  $3.2$

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

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

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

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

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

3	$[\frac{1}{2}, \frac{1}{2}, 0]$	[3,6,9,12]
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Table 7: Wyckoff site: 3g, site symmetry:  $\dots 2/m$

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

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

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

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

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

Table 11: Wyckoff site: 6k, site symmetry:  $\cdot \cdot m$ 

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

Table 12: Wyckoff site: 12l, site symmetry: 1

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