

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: . . 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: ..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: ..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:  $\dots \text{m}$ 

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]