

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:  $\bar{3}.2/m$

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:  $\bar{3}2/m$

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:  $3\bar{2}$

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:  $\bar{3}2$

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:  $\bar{3}2$

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:  $\bar{6}m$ 

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:  $121$ , site symmetry:  $1$ 

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-y, x - y, z]$	$[2]$
3	$[-x + y, -x, z]$	$[3]$
4	$[-y, -x, -z]$	$[4]$
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	$[-x, -x + y, z]$	$[12]$