

SG No. 189 D_{3h}^3 $P\bar{6}2m$ [hexagonal]

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

Table 1: Wyckoff site: 1a, site symmetry: $-62m$

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: $-62m$

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: $-6..$

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: $-6..$

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: $m2m$

No.	position	mapping
1	$[x, 0, 0]$	$[1, 4, 8, 11]$
2	$[0, x, 0]$	$[2, 5, 7, 10]$

3	$[-x, -x, 0]$	$[3, 6, 9, 12]$
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Table 7: Wyckoff site: **3g**, site symmetry: **m2m**

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

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: **. . m**

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

Table 10: Wyckoff site: **6j**, site symmetry: **m. .**

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

Table 11: Wyckoff site: $6k$, site symmetry: $m . .$

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

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	$[x, y, -z]$	[4]
5	$[-y, x - y, -z]$	[5]
6	$[-x + y, -x, -z]$	[6]
7	$[y, x, -z]$	[7]
8	$[x - y, -y, -z]$	[8]
9	$[-x, -x + y, -z]$	[9]
10	$[y, x, z]$	[10]
11	$[x - y, -y, z]$	[11]
12	$[-x, -x + y, z]$	[12]