

SG No. 187 D_{3h}^1 $P\bar{6}m2$ [hexagonal]

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

Table 1: Wyckoff site: 1a, site symmetry: $-6m2$

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: $-6m2$

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: 1c, site symmetry: $-6m2$

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

Table 4: Wyckoff site: 1d, site symmetry: $-6m2$

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

Table 5: Wyckoff site: 1e, site symmetry: $-6m2$

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

Table 6: Wyckoff site: 1f, site symmetry: $-6m2$

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

Table 7: Wyckoff site: $2g$, site symmetry: $3m$.

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

Table 8: Wyckoff site: $2h$, site symmetry: $3m$.

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

Table 9: Wyckoff site: $2i$, site symmetry: $3m$.

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

Table 10: Wyckoff site: $3j$, site symmetry: $mm2$

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

Table 11: Wyckoff site: $3k$, site symmetry: $mm2$

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

Table 12: Wyckoff site: $6l$, site symmetry: m .

No.	position	mapping
1	$[x, y, 0]$	$[1, 4]$
2	$[-y, x - y, 0]$	$[2, 5]$

continued ...

Table 12

No.	position	mapping
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 13: Wyckoff site: $6\bar{m}$, 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 14: Wyckoff site: $6n$, site symmetry: $.m.$

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

Table 15: Wyckoff site: $12o$, 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]

continued ...

Table 15

No.	position	mapping
12	$[x, x - y, -z]$	[12]