

SG No. 193 D_{6h}^3 $P6_3/mcm$ [hexagonal]

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

Table 1: Wyckoff site: 2a, site symmetry: -62m

No.	position	mapping
1	[0, 0, $\frac{1}{4}$]	[1, 2, 3, 7, 8, 9, 16, 17, 18, 22, 23, 24]
2	[0, 0, $\frac{3}{4}$]	[4, 5, 6, 10, 11, 12, 13, 14, 15, 19, 20, 21]

Table 2: Wyckoff site: 2b, site symmetry: -3.m

No.	position	mapping
1	[0, 0, 0]	[1, 2, 3, 10, 11, 12, 13, 14, 15, 22, 23, 24]
2	[0, 0, $\frac{1}{2}$]	[4, 5, 6, 7, 8, 9, 16, 17, 18, 19, 20, 21]

Table 3: Wyckoff site: 4c, site symmetry: -6..

No.	position	mapping
1	[$\frac{1}{3}$, $\frac{2}{3}$, $\frac{1}{4}$]	[1, 2, 3, 16, 17, 18]
2	[$\frac{2}{3}$, $\frac{1}{3}$, $\frac{3}{4}$]	[4, 5, 6, 13, 14, 15]
3	[$\frac{2}{3}$, $\frac{1}{3}$, $\frac{1}{4}$]	[7, 8, 9, 22, 23, 24]
4	[$\frac{1}{3}$, $\frac{2}{3}$, $\frac{3}{4}$]	[10, 11, 12, 19, 20, 21]

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

No.	position	mapping
1	[$\frac{1}{3}$, $\frac{2}{3}$, 0]	[1, 2, 3, 10, 11, 12]
2	[$\frac{2}{3}$, $\frac{1}{3}$, $\frac{1}{2}$]	[4, 5, 6, 7, 8, 9]
3	[$\frac{2}{3}$, $\frac{1}{3}$, 0]	[13, 14, 15, 22, 23, 24]
4	[$\frac{1}{3}$, $\frac{2}{3}$, $\frac{1}{2}$]	[16, 17, 18, 19, 20, 21]

Table 5: Wyckoff site: 4e, site symmetry: 3.m

No.	position	mapping
1	[0, 0, z]	[1, 2, 3, 22, 23, 24]
2	[0, 0, $z + \frac{1}{2}$]	[4, 5, 6, 19, 20, 21]
3	[0, 0, $\frac{1}{2} - z$]	[7, 8, 9, 16, 17, 18]
4	[0, 0, -z]	[10, 11, 12, 13, 14, 15]

Table 6: Wyckoff site: 6f, site symmetry: $\dots 2/m$

No.	position	mapping
1	$[\frac{1}{2}, 0, 0]$	[1, 11, 13, 23]
2	$[0, \frac{1}{2}, 0]$	[2, 10, 14, 22]
3	$[\frac{1}{2}, \frac{1}{2}, 0]$	[3, 12, 15, 24]
4	$[\frac{1}{2}, 0, \frac{1}{2}]$	[4, 8, 16, 20]
5	$[0, \frac{1}{2}, \frac{1}{2}]$	[5, 7, 17, 19]
6	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[6, 9, 18, 21]

Table 7: Wyckoff site: 6g, site symmetry: $m\bar{2}m$

No.	position	mapping
1	$[x, 0, \frac{1}{4}]$	[1, 8, 16, 23]
2	$[0, x, \frac{1}{4}]$	[2, 7, 17, 22]
3	$[-x, -x, \frac{1}{4}]$	[3, 9, 18, 24]
4	$[-x, 0, \frac{3}{4}]$	[4, 11, 13, 20]
5	$[0, -x, \frac{3}{4}]$	[5, 10, 14, 19]
6	$[x, x, \frac{3}{4}]$	[6, 12, 15, 21]

Table 8: Wyckoff site: 8h, site symmetry: $3\dots$

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, z]$	[1, 2, 3]
2	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[4, 5, 6]
3	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$	[7, 8, 9]
4	$[\frac{1}{3}, \frac{2}{3}, -z]$	[10, 11, 12]
5	$[\frac{2}{3}, \frac{1}{3}, -z]$	[13, 14, 15]
6	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	[16, 17, 18]
7	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	[19, 20, 21]
8	$[\frac{2}{3}, \frac{1}{3}, z]$	[22, 23, 24]

Table 9: Wyckoff site: 12i, site symmetry: $\dots 2$

No.	position	mapping
1	$[x, 2x, 0]$	[1, 11]
2	$[-2x, -x, 0]$	[2, 10]
3	$[x, -x, 0]$	[3, 12]
4	$[-x, -2x, \frac{1}{2}]$	[4, 8]
5	$[2x, x, \frac{1}{2}]$	[5, 7]
6	$[-x, x, \frac{1}{2}]$	[6, 9]
7	$[-x, -2x, 0]$	[13, 23]

continued ...

Table 9

No.	position	mapping
8	$[2x, x, 0]$	[14,22]
9	$[-x, x, 0]$	[15,24]
10	$[x, 2x, \frac{1}{2}]$	[16,20]
11	$[-2x, -x, \frac{1}{2}]$	[17,19]
12	$[x, -x, \frac{1}{2}]$	[18,21]

Table 10: Wyckoff site: 12j, site symmetry: $\mathbf{m..}$

No.	position	mapping
1	$[x, y, \frac{1}{4}]$	[1,16]
2	$[-y, x - y, \frac{1}{4}]$	[2,17]
3	$[-x + y, -x, \frac{1}{4}]$	[3,18]
4	$[-x, -y, \frac{3}{4}]$	[4,13]
5	$[y, -x + y, \frac{3}{4}]$	[5,14]
6	$[x - y, x, \frac{3}{4}]$	[6,15]
7	$[y, x, \frac{1}{4}]$	[7,22]
8	$[x - y, -y, \frac{1}{4}]$	[8,23]
9	$[-x, -x + y, \frac{1}{4}]$	[9,24]
10	$[-y, -x, \frac{3}{4}]$	[10,19]
11	$[-x + y, y, \frac{3}{4}]$	[11,20]
12	$[x, x - y, \frac{3}{4}]$	[12,21]

Table 11: Wyckoff site: 12k, site symmetry: $\mathbf{..m}$

No.	position	mapping
1	$[x, 0, z]$	[1,23]
2	$[0, x, z]$	[2,22]
3	$[-x, -x, z]$	[3,24]
4	$[-x, 0, z + \frac{1}{2}]$	[4,20]
5	$[0, -x, z + \frac{1}{2}]$	[5,19]
6	$[x, x, z + \frac{1}{2}]$	[6,21]
7	$[0, x, \frac{1}{2} - z]$	[7,17]
8	$[x, 0, \frac{1}{2} - z]$	[8,16]
9	$[-x, -x, \frac{1}{2} - z]$	[9,18]
10	$[0, -x, -z]$	[10,14]
11	$[-x, 0, -z]$	[11,13]
12	$[x, x, -z]$	[12,15]

Table 12: Wyckoff site: 241, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x - y, z]$	[2]
3	$[-x + y, -x, z]$	[3]
4	$[-x, -y, z + \frac{1}{2}]$	[4]
5	$[y, -x + y, z + \frac{1}{2}]$	[5]
6	$[x - y, x, z + \frac{1}{2}]$	[6]
7	$[y, x, \frac{1}{2} - z]$	[7]
8	$[x - y, -y, \frac{1}{2} - z]$	[8]
9	$[-x, -x + y, \frac{1}{2} - z]$	[9]
10	$[-y, -x, -z]$	[10]
11	$[-x + y, y, -z]$	[11]
12	$[x, x - y, -z]$	[12]
13	$[-x, -y, -z]$	[13]
14	$[y, -x + y, -z]$	[14]
15	$[x - y, x, -z]$	[15]
16	$[x, y, \frac{1}{2} - z]$	[16]
17	$[-y, x - y, \frac{1}{2} - z]$	[17]
18	$[-x + y, -x, \frac{1}{2} - z]$	[18]
19	$[-y, -x, z + \frac{1}{2}]$	[19]
20	$[-x + y, y, z + \frac{1}{2}]$	[20]
21	$[x, x - y, z + \frac{1}{2}]$	[21]
22	$[y, x, z]$	[22]
23	$[x - y, -y, z]$	[23]
24	$[-x, -x + y, z]$	[24]