

SG No. 202 T_h^3 $Fm\bar{3}$ [cubic]

* plus set: $+ [0, 0, 0]$, $+ [0, \frac{1}{2}, \frac{1}{2}]$, $+ [\frac{1}{2}, 0, \frac{1}{2}]$, $+ [\frac{1}{2}, \frac{1}{2}, 0]$

Table 1: Wyckoff site: 4a, site symmetry: $m-3$.

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

Table 2: Wyckoff site: 4b, site symmetry: $m-3$.

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

Table 3: Wyckoff site: 8c, site symmetry: 23 .

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

Table 4: Wyckoff site: 24d, site symmetry: $2/m..$

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

Table 5: Wyckoff site: 24e, site symmetry: $mm2..$

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

Table 6: Wyckoff site: **32f**, site symmetry: $\bar{3}$.

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

Table 7: Wyckoff site: **48g**, site symmetry: $2\bar{3}$.

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

Table 8: Wyckoff site: **48h**, site symmetry: $m\bar{3}$.

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

Table 9: Wyckoff site: **96i**, site symmetry: **1**

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