

SG No. 217 T_d^3 $I\bar{4}3m$ [cubic]

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

Table 1: Wyckoff site: 2a, site symmetry: $-43m$

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: 6b, site symmetry: $-42.m$

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

Table 3: Wyckoff site: 8c, site symmetry: $.3m$

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

Table 4: Wyckoff site: 12d, site symmetry: $-4..$

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

Table 5: Wyckoff site: 12e, site symmetry: $2.mm$

No.	position	mapping
1	$[x, 0, 0]$	$[1, 4, 17, 20]$
2	$[-x, 0, 0]$	$[2, 3, 18, 19]$
3	$[0, x, 0]$	$[5, 8, 13, 16]$

continued ...

Table 5

No.	position	mapping
4	$[0, -x, 0]$	$[6, 7, 14, 15]$
5	$[0, 0, x]$	$[9, 12, 21, 24]$
6	$[0, 0, -x]$	$[10, 11, 22, 23]$

Table 6: Wyckoff site: 24f, site symmetry: $2..$

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

Table 7: Wyckoff site: 24g, site symmetry: $..m$

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

Table 8: Wyckoff site: **48h**, 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	$[y, x, z]$	[13]
14	$[-y, -x, z]$	[14]
15	$[y, -x, -z]$	[15]
16	$[-y, x, -z]$	[16]
17	$[x, z, y]$	[17]
18	$[-x, z, -y]$	[18]
19	$[-x, -z, y]$	[19]
20	$[x, -z, -y]$	[20]
21	$[z, y, x]$	[21]
22	$[z, -y, -x]$	[22]
23	$[-z, y, -x]$	[23]
24	$[-z, -y, x]$	[24]