

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: .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..

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..

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]