

SG No. 211 O^5 $I432$ [cubic]

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

Table 1: Wyckoff site: 2a, site symmetry: 432

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: 42.2

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: .32

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

Table 4: Wyckoff site: 12d, site symmetry: 2.22

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	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[9, 12, 21, 24]$
6	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[10, 11, 22, 23]$

Table 5: Wyckoff site: 12e, site symmetry: 4..

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, 22, 23]
6	[0, 0, -x]	[10, 11, 21, 24]

Table 6: Wyckoff site: 16f, 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: 24g, 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	[\mathbf{\frac{1}{2}}, 0, x]	[9, 12]
6	[\mathbf{\frac{1}{2}}, 0, -x]	[10, 11]
7	[\mathbf{\frac{1}{2}}, x, 0]	[13, 16]
8	[\mathbf{\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 8: Wyckoff site: 24h, site symmetry: ..2

No.	position	mapping
1	[0, y, y]	[1, 18]
2	[0, -y, y]	[2, 20]
3	[0, y, -y]	[3, 17]
4	[0, -y, -y]	[4, 19]

continued ...

Table 8

No.	position	mapping
5	$[y, 0, y]$	[5,15]
6	$[y, 0, -y]$	[6,13]
7	$[-y, 0, y]$	[7,16]
8	$[-y, 0, -y]$	[8,14]
9	$[y, y, 0]$	[9,21]
10	$[-y, y, 0]$	[10,23]
11	$[y, -y, 0]$	[11,22]
12	$[-y, -y, 0]$	[12,24]

Table 9: Wyckoff site: 24i, site symmetry: . . 2

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

Table 10: Wyckoff site: 48j, 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]

continued ...

Table 10

No.	position	mapping
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]