SG No. 225 O_h^5 $Fm\bar{3}m$ [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-3m`

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,` `25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48]`

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

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,` `25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48]`

Table 3: Wyckoff site: `8c`, site symmetry: `-43m`

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[1,2,3,4,5,6,7,8,9,10,11,12,37,38,39,40,41,42,43,44,45,46,47,48]`
2	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36]`

Table 4: Wyckoff site: `24d`, site symmetry: `m.mm`

No.	position	mapping
1	$\left[0, \frac{1}{4}, \frac{1}{4}\right]$	`[1,4,18,19,25,28,42,43]`
2	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	`[2,3,17,20,26,27,41,44]`
3	$\left[\frac{1}{4}, 0, \frac{1}{4}\right]$	`[5,8,14,15,29,32,38,39]`
4	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	`[6,7,13,16,30,31,37,40]`
5	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	`[9,12,21,24,33,36,45,48]`
6	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	`[10,11,22,23,34,35,46,47]`

Table 5: Wyckoff site: `24e`, site symmetry: `4m.m`

No.	position	mapping
1	$[x, 0, 0]$	`[1,4,17,20,26,27,42,43]`
2	$[-x, 0, 0]$	`[2,3,18,19,25,28,41,44]`
3	$[0, x, 0]$	`[5,8,13,16,30,31,38,39]`
4	$[0, -x, 0]$	`[6,7,14,15,29,32,37,40]`
5	$[0, 0, x]$	`[9,12,22,23,34,35,45,48]`

continued ...

1

Table 5

No.	position	mapping
6	$[0, 0, -x]$	[10,11,21,24,33,36,46,47]

Table 6: Wyckoff site: `32f`, site symmetry: `.3m`

No.	position	mapping
1	$[x, x, x]$	[1,5,9,38,43,48]
2	$[-x, -x, x]$	[2,7,12,37,41,45]
3	$[-x, x, -x]$	[3,8,10,39,44,46]
4	$[x, -x, -x]$	[4,6,11,40,42,47]
5	$[x, x, -x]$	[13,17,21,26,31,36]
6	$[-x, -x, -x]$	[14,19,24,25,29,33]
7	$[x, -x, x]$	[15,20,22,27,32,34]
8	$[-x, x, x]$	[16,18,23,28,30,35]

Table 7: Wyckoff site: `48g`, site symmetry: `2.mm`

No.	position	mapping
1	$\left[x, \frac{1}{4}, \frac{1}{4}\right]$	[1,4,42,43]
2	$\left[-x, \frac{3}{4}, \frac{1}{4}\right]$	[2,3,41,44]
3	$\left[\frac{1}{4}, x, \frac{1}{4}\right]$	[5,8,38,39]
4	$\left[\frac{1}{4}, -x, \frac{3}{4}\right]$	[6,7,37,40]
5	$\left[\frac{1}{4}, \frac{1}{4}, x\right]$	[9,12,45,48]
6	$\left[\frac{3}{4}, \frac{1}{4}, -x\right]$	[10,11,46,47]
7	$\left[\frac{1}{4}, x, \frac{3}{4}\right]$	[13,16,30,31]
8	$\left[\frac{3}{4}, -x, \frac{3}{4}\right]$	[14,15,29,32]
9	$\left[x, \frac{1}{4}, \frac{3}{4}\right]$	[17,20,26,27]
10	$\left[-x, \frac{1}{4}, \frac{1}{4}\right]$	[18,19,25,28]
11	$\left[\frac{1}{4}, \frac{1}{4}, -x\right]$	[21,24,33,36]
12	$\left[\frac{1}{4}, \frac{3}{4}, x\right]$	[22,23,34,35]

Table 8: Wyckoff site: `48h`, site symmetry: `m.m2`

No.	position	mapping
1	$[0, y, y]$	[1,18,28,43]
2	$[0, -y, y]$	[2,20,27,41]
3	$[0, y, -y]$	[3,17,26,44]
4	$[0, -y, -y]$	[4,19,25,42]
5	$[y, 0, y]$	[5,15,32,38]
6	$[y, 0, -y]$	[6,13,31,40]

continued …

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Table 8

No.	position	mapping
7	$[-y, 0, y]$	[7,16,30,37]
8	$[-y, 0, -y]$	[8,14,29,39]
9	$[y, y, 0]$	[9,21,36,48]
10	$[-y, y, 0]$	[10,23,35,46]
11	$[y, -y, 0]$	[11,22,34,47]
12	$[-y, -y, 0]$	[12,24,33,45]

Table 9: Wyckoff site: `48i`, site symmetry: `m.m2`

No.	position	mapping
1	$\left[\frac{1}{2}, y, y\right]$	[1,18,28,43]
2	$\left[\frac{1}{2}, -y, y\right]$	[2,20,27,41]
3	$\left[\frac{1}{2}, y, -y\right]$	[3,17,26,44]
4	$\left[\frac{1}{2}, -y, -y\right]$	[4,19,25,42]
5	$\left[y, \frac{1}{2}, y\right]$	[5,15,32,38]
6	$\left[y, \frac{1}{2}, -y\right]$	[6,13,31,40]
7	$\left[-y, \frac{1}{2}, y\right]$	[7,16,30,37]
8	$\left[-y, \frac{1}{2}, -y\right]$	[8,14,29,39]
9	$\left[y, y, \frac{1}{2}\right]$	[9,21,36,48]
10	$\left[-y, y, \frac{1}{2}\right]$	[10,23,35,46]
11	$\left[y, -y, \frac{1}{2}\right]$	[11,22,34,47]
12	$\left[-y, -y, \frac{1}{2}\right]$	[12,24,33,45]

Table 10: Wyckoff site: `96j`, site symmetry: `m..`

No.	position	mapping
1	$[0, y, z]$	[1,28]
2	$[0, -y, z]$	[2,27]
3	$[0, y, -z]$	[3,26]
4	$[0, -y, -z]$	[4,25]
5	$[z, 0, y]$	[5,32]
6	$[z, 0, -y]$	[6,31]
7	$[-z, 0, y]$	[7,30]
8	$[-z, 0, -y]$	[8,29]
9	$[y, z, 0]$	[9,36]
10	$[-y, z, 0]$	[10,35]
11	$[y, -z, 0]$	[11,34]
12	$[-y, -z, 0]$	[12,33]
13	$[y, 0, -z]$	[13,40]
14	$[-y, 0, -z]$	[14,39]
15	$[y, 0, z]$	[15,38]
16	$[-y, 0, z]$	[16,37]

continued …

Table 10

No.	position	mapping
17	$[0, z, -y]$	[17,44]
18	$[0, z, y]$	[18,43]
19	$[0, -z, -y]$	[19,42]
20	$[0, -z, y]$	[20,41]
21	$[z, y, 0]$	[21,48]
22	$[z, -y, 0]$	[22,47]
23	$[-z, y, 0]$	[23,46]
24	$[-z, -y, 0]$	[24,45]

Table 11: Wyckoff site: `96k`, site symmetry: `..m`

No.	position	mapping
1	$[x, x, z]$	[1,38]
2	$[-x, -x, z]$	[2,37]
3	$[-x, x, -z]$	[3,39]
4	$[x, -x, -z]$	[4,40]
5	$[z, x, x]$	[5,48]
6	$[z, -x, -x]$	[6,47]
7	$[-z, -x, x]$	[7,45]
8	$[-z, x, -x]$	[8,46]
9	$[x, z, x]$	[9,43]
10	$[-x, z, -x]$	[10,44]
11	$[x, -z, -x]$	[11,42]
12	$[-x, -z, x]$	[12,41]
13	$[x, x, -z]$	[13,26]
14	$[-x, -x, -z]$	[14,25]
15	$[x, -x, z]$	[15,27]
16	$[-x, x, z]$	[16,28]
17	$[x, z, -x]$	[17,36]
18	$[-x, z, x]$	[18,35]
19	$[-x, -z, -x]$	[19,33]
20	$[x, -z, x]$	[20,34]
21	$[z, x, -x]$	[21,31]
22	$[z, -x, x]$	[22,32]
23	$[-z, x, x]$	[23,30]
24	$[-z, -x, -x]$	[24,29]

Table 12: Wyckoff site: `192l`, site symmetry: `1`

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-x, -y, z]$	[2]

continued ...

Table 12

No.	position	mapping
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]
25	$[-x, -y, -z]$	[25]
26	$[x, y, -z]$	[26]
27	$[x, -y, z]$	[27]
28	$[-x, y, z]$	[28]
29	$[-z, -x, -y]$	[29]
30	$[-z, x, y]$	[30]
31	$[z, x, -y]$	[31]
32	$[z, -x, y]$	[32]
33	$[-y, -z, -x]$	[33]
34	$[y, -z, x]$	[34]
35	$[-y, z, x]$	[35]
36	$[y, z, -x]$	[36]
37	$[-y, -x, z]$	[37]
38	$[y, x, z]$	[38]
39	$[-y, x, -z]$	[39]
40	$[y, -x, -z]$	[40]
41	$[-x, -z, y]$	[41]
42	$[x, -z, -y]$	[42]
43	$[x, z, y]$	[43]
44	$[-x, z, -y]$	[44]
45	$[-z, -y, x]$	[45]
46	$[-z, y, -x]$	[46]
47	$[z, -y, -x]$	[47]
48	$[z, y, x]$	[48]