SG No. 200 T_{h}^{1} $Pm\bar{3}$ [cubic]

* plus set: +[0, 0, 0]

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

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]

Table 3: Wyckoff site: 3c, site symmetry: mmm..

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

Table 4: Wyckoff site: 3d, site symmetry: mmm..

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

Table 5: Wyckoff site: 6e, 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: `6f`, site symmetry: `mm2..`

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

Table 7: Wyckoff site: `6g`, site symmetry: `mm2..`

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

Table 8: Wyckoff site: `6h`, site symmetry: `mm2..`

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

Table 9: Wyckoff site: `8i`, 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 10: Wyckoff site: `12j`, 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 11: Wyckoff site: `12k`, site symmetry: `m..`

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

Table 12: Wyckoff site: `24l`, 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]`

continued ...

Table 12

No.	position	mapping
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]