MSG No. 218.83 $P\bar{4}'3n'$ [Type III, cubic]

Table 1: Wyckoff site: 2a, site symmetry: 23.

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

Table 2: Wyckoff site: 6b, site symmetry: 222..

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

Table 3: Wyckoff site: 6c, site symmetry: -4'..

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

Table 4: Wyckoff site: 6d, site symmetry: -4'..

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

Table 5: Wyckoff site: `8e`, site symmetry: `.3.`

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

Table 6: Wyckoff site: `12f`, site symmetry: `2..`

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

Table 7: Wyckoff site: `12g`, site symmetry: `2..`

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

Table 8: Wyckoff site: `12h`, site symmetry: `2..`

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

Table 9: Wyckoff site: `24i`, 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	$[y,\ z,\ x]$	`[6]`
7	$[-y,\ z,\ -x]$	`[7]`
8	$[-z,\ -x,\ y]$	`[8]`
9	$[-y,\ -z,\ x]$	`[9]`
10	$[z,\ -x,\ -y]$	`[10]`
11	$[y,\ -z,\ -x]$	`[11]`
12	$[-z,\ x,\ -y]$	`[12]`
13	$\left[\frac{1}{2}-x,\ z+\frac{1}{2},\ \frac{1}{2}-y\right]$	`[13]`
14	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ y+\frac{1}{2}\right]$	`[14]`
15	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ x+\frac{1}{2}\right]$	`[15]`
16	$\left[z+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-x\right]$	`[16]`
17	$\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	`[17]`
18	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	`[18]`
19	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	`[19]`
20	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	`[20]`
21	$\left[x+\frac{1}{2},\ \frac{1}{2}-z,\ \frac{1}{2}-y\right]$	`[21]`
22	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	`[22]`
23	$\left[\frac{1}{2}-z,\ y+\frac{1}{2},\ \frac{1}{2}-x\right]$	`[23]`
24	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ x+\frac{1}{2}\right]$	`[24]`