MSG No. 195.3 P_I23 [Type IV, 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	$\left[\frac{1}{2},\ 0,\ 0\right]$	`[13,14,15,16]`
5	$\left[0,\ \frac{1}{2},\ 0\right]$	`[17,20,22,24]`
6	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[18,19,21,23]`

Table 3: Wyckoff site: `8c`, 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	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ x+\frac{1}{2}\right]$	`[13,17,18]`
6	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$	`[14,22,23]`
7	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ \frac{1}{2}-x\right]$	`[15,19,24]`
8	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ x+\frac{1}{2}\right]$	`[16,20,21]`

Table 4: Wyckoff site: `12d`, 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	$\left[x+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[13,14]`
8	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[15,16]`
9	$\left[\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[17,24]`

continued ...

Table 4

No.	position	mapping
10	$\left[\frac{1}{2}, \frac{1}{2}, x+\frac{1}{2}\right]$	`[18,21]`
11	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}-x\right]$	`[19,23]`
12	$\left[\frac{1}{2}, \frac{1}{2}-x, \frac{1}{2}\right]$	`[20,22]`

Table 5: Wyckoff site: `12e`, 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	$\left[x+\frac{1}{2}, 0, \frac{1}{2}\right]$	`[13,14]`
8	$\left[\frac{1}{2}-x, 0, \frac{1}{2}\right]$	`[15,16]`
9	$\left[\frac{1}{2}, x+\frac{1}{2}, 0\right]$	`[17,24]`
10	$\left[0, \frac{1}{2}, x+\frac{1}{2}\right]$	`[18,21]`
11	$\left[0, \frac{1}{2}, \frac{1}{2}-x\right]$	`[19,23]`
12	$\left[\frac{1}{2}, \frac{1}{2}-x, 0\right]$	`[20,22]`

Table 6: Wyckoff site: `24f`, 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	$\left[x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}\right]$	`[13]`
14	$\left[x+\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}-z\right]$	`[14]`
15	$\left[\frac{1}{2}-x, y+\frac{1}{2}, \frac{1}{2}-z\right]$	`[15]`
16	$\left[\frac{1}{2}-x, \frac{1}{2}-y, z+\frac{1}{2}\right]$	`[16]`
17	$\left[z+\frac{1}{2}, x+\frac{1}{2}, y+\frac{1}{2}\right]$	`[17]`
18	$\left[y+\frac{1}{2}, z+\frac{1}{2}, x+\frac{1}{2}\right]$	`[18]`
19	$\left[\frac{1}{2}-y, z+\frac{1}{2}, \frac{1}{2}-x\right]$	`[19]`

continued ...

Table 6

No.	position	mapping
20	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ y+\frac{1}{2}\right]$	[20]
21	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ x+\frac{1}{2}\right]$	[21]
22	$\left[z+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-y\right]$	[22]
23	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[23]
24	$\left[\frac{1}{2}-z,\ x+\frac{1}{2},\ \frac{1}{2}-y\right]$	[24]