MSG No. 165.96 $P_c\bar{3}c1$ [Type IV, trigonal]

Table 1: Wyckoff site: `2a`, site symmetry: `-3m'`.

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `3m'`.

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

Table 4: Wyckoff site: `4d`, site symmetry: `3m'`.

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

Table 5: Wyckoff site: `6e`, site symmetry: `.2'/m'`.

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

Table 6: Wyckoff site: `6f`, site symmetry: `.2/m'.`

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

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

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

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

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

Table 9: Wyckoff site: `12i`, site symmetry: `.m'.`

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

Table 10: Wyckoff site: `24j`, site symmetry: `1`

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