MSG No. 163.84 $P_c\bar{3}1c$ [Type IV, trigonal]

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

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: 3.2'

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

Table 4: Wyckoff site: 4d, site symmetry: 3.2

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

Table 5: Wyckoff site: 4e, site symmetry: 3.m'

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

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

Table 7: Wyckoff site: `6g`, site symmetry: `..2/m'`

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

Table 8: Wyckoff site: `8h`, site symmetry: `3..`

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

Table 9: Wyckoff site: `12i`, site symmetry: `..2'`

No.	position	mapping
1	$[x, -x, 0]$	[1,18]
2	$[x, 2x, 0]$	[2,16]
3	$[-2x, -x, 0]$	[3,17]
4	$\left[x, 2x, \frac{1}{2}\right]$	[4,14]
5	$\left[-2x, -x, \frac{1}{2}\right]$	[5,15]
6	$\left[x, -x, \frac{1}{2}\right]$	[6,13]
7	$[-x, x, 0]$	[7,24]

continued …

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Table 9

No.	position	mapping
8	$[-x, -2x, 0]$	[8,22]
9	$[2x, x, 0]$	[9,23]
10	$[-x, -2x, \frac{1}{2}]$	[10,20]
11	$[2x, x, \frac{1}{2}]$	[11,21]
12	$[-x, x, \frac{1}{2}]$	[12,19]

Table 10: Wyckoff site: `12j`, site symmetry: `..2`

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

Table 11: Wyckoff site: `12k`, site symmetry: `..m'`

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

Table 12: Wyckoff site: 241, site symmetry: 1

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