MSG No. 177.154 P_c622 [Type IV, hexagonal]

Table 1: Wyckoff site: `2a`, site symmetry: `622`

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

Table 2: Wyckoff site: `2b`, site symmetry: `62'2'`

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	$\left[\frac{1}{3},\ \frac{2}{3},\ 0\right]$	`[1,3,5,10,11,12]`
2	$\left[\frac{2}{3},\ \frac{1}{3},\ 0\right]$	`[2,4,6,7,8,9]`
3	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{2}\right]$	`[13,15,17,22,23,24]`
4	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{2}\right]$	`[14,16,18,19,20,21]`

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `6..`

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

Table 6: Wyckoff site: `6f`, site symmetry: `222`

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

Table 7: Wyckoff site: `6g`, site symmetry: `22'2'`

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{2}, 0, z\right]$	`[1,4]`
2	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[2,5]`
3	$\left[0, \frac{1}{2}, z\right]$	`[3,6]`
4	$\left[\frac{1}{2}, 0, -z\right]$	`[7,11]`
5	$\left[0, \frac{1}{2}, -z\right]$	`[8,12]`
6	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	`[9,10]`
7	$\left[\frac{1}{2}, 0, z+\frac{1}{2}\right]$	`[13,16]`

continued ...

Table 9

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

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

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

Table 11: Wyckoff site: 12k, site symmetry: .2'.

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

Table 12: Wyckoff site: `12l`, site symmetry: `..2`

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

Table 13: Wyckoff site: `12m`, site symmetry: `..2'`

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

Table 14: Wyckoff site: `24n`, site symmetry: `1`

No.	position	mapping
1	$[x, y, z]$	`[1]`
2	$[x-y, x, z]$	`[2]`
3	$[-y, x-y, z]$	`[3]`
4	$[-x, -y, z]$	`[4]`
5	$[-x+y, -x, z]$	`[5]`
6	$[y, -x+y, z]$	`[6]`
7	$[x-y, -y, -z]$	`[7]`
8	$[y, x, -z]$	`[8]`
9	$[-x, -x+y, -z]$	`[9]`

continued ...

Table 14

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