MSG No. 97.156 I_c422 [Type IV, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `422`

No.	position	mapping
1	$[0, 0, 0]$	`[1,2,3,4,5,6,7,8]`
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[9,10,11,12,13,14,15,16]`
3	$\left[0, 0, \frac{1}{2}\right]$	`[17,18,19,20,21,22,23,24]`
4	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[25,26,27,28,29,30,31,32]`

Table 2: Wyckoff site: `4b`, site symmetry: `42'2'`

No.	position	mapping
1	$\left[0, 0, \frac{1}{4}\right]$	`[1,2,3,6,20,21,23,24]`
2	$\left[0, 0, \frac{3}{4}\right]$	`[4,5,7,8,17,18,19,22]`
3	$\left[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}\right]$	`[9,10,11,14,28,29,31,32]`
4	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	`[12,13,15,16,25,26,27,30]`

Table 3: Wyckoff site: `4c`, site symmetry: `4'22'`

No.	position	mapping
1	$\left[0, \frac{1}{2}, 0\right]$	`[1,4,5,6,26,27,31,32]`
2	$\left[\frac{1}{2}, 0, 0\right]$	`[2,3,7,8,25,28,29,30]`
3	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[9,12,13,14,18,19,23,24]`
4	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[10,11,15,16,17,20,21,22]`

Table 4: Wyckoff site: `4d`, site symmetry: `4'2'2`

No.	position	mapping
1	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[1,6,15,16,20,21,26,27]`
2	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[2,3,12,13,23,24,25,30]`
3	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	`[4,5,10,11,17,22,31,32]`
4	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[7,8,9,14,18,19,28,29]`

Table 5: Wyckoff site: `8e`, site symmetry: `2.22`

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	`[1,7,30,32]`
2	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	`[2,5,27,28]`

continued ...

Table 5

No.	position	mapping
3	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[3,4,26,29]
4	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	[6,8,25,31]
5	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[9,15,22,24]
6	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[10,13,19,20]
7	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[11,12,18,21]
8	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[14,16,17,23]

Table 6: Wyckoff site: 8f, site symmetry: 2.22

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[1,16,23,30]
2	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[2,12,21,27]
3	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[3,13,20,26]
4	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[4,10,19,29]
5	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[5,11,18,28]
6	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[6,15,24,25]
7	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[7,14,17,32]
8	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[8,9,22,31]

Table 7: Wyckoff site: 8g, site symmetry: 4..

No.	position	mapping
1	$[0, 0, z]$	[1,2,3,6]
2	$[0, 0, -z]$	[4,5,7,8]
3	$\left[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}\right]$	[9,10,11,14]
4	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z\right]$	[12,13,15,16]
5	$\left[0, 0, z + \frac{1}{2}\right]$	[17,18,19,22]
6	$\left[0, 0, \frac{1}{2} - z\right]$	[20,21,23,24]
7	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	[25,26,27,30]
8	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	[28,29,31,32]

Table 8: Wyckoff site: 8h, site symmetry: 4'..

No.	position	mapping
1	$\left[0, \frac{1}{2}, z\right]$	[1,6,26,27]
2	$\left[\frac{1}{2}, 0, z\right]$	[2,3,25,30]
3	$\left[0, \frac{1}{2}, -z\right]$	[4,5,31,32]
4	$\left[\frac{1}{2}, 0, -z\right]$	[7,8,28,29]
5	$\left[\frac{1}{2}, 0, z + \frac{1}{2}\right]$	[9,14,18,19]

continued ...

Table 8

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

Table 9: Wyckoff site: `16i`, site symmetry: `2'..`

No.	position	mapping
1	$\left[\frac{3}{4},\ \frac{1}{4},\ z\right]$	`[1,30]`
2	$\left[\frac{3}{4},\ \frac{3}{4},\ z\right]$	`[2,27]`
3	$\left[\frac{1}{4},\ \frac{1}{4},\ z\right]$	`[3,26]`
4	$\left[\frac{3}{4},\ \frac{3}{4},\ -z\right]$	`[4,29]`
5	$\left[\frac{1}{4},\ \frac{1}{4},\ -z\right]$	`[5,28]`
6	$\left[\frac{1}{4},\ \frac{3}{4},\ z\right]$	`[6,25]`
7	$\left[\frac{1}{4},\ \frac{3}{4},\ -z\right]$	`[7,32]`
8	$\left[\frac{3}{4},\ \frac{1}{4},\ -z\right]$	`[8,31]`
9	$\left[\frac{1}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	`[9,22]`
10	$\left[\frac{1}{4},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	`[10,19]`
11	$\left[\frac{3}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	`[11,18]`
12	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	`[12,21]`
13	$\left[\frac{3}{4},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	`[13,20]`
14	$\left[\frac{3}{4},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	`[14,17]`
15	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	`[15,24]`
16	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	`[16,23]`

Table 10: Wyckoff site: `16j`, site symmetry: `.2.`

No.	position	mapping
1	$[0,\ y,\ 0]$	`[1,5]`
2	$[-y,\ 0,\ 0]$	`[2,8]`
3	$[y,\ 0,\ 0]$	`[3,7]`
4	$[0,\ -y,\ 0]$	`[4,6]`
5	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[9,13]`
6	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[10,16]`
7	$\left[y+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[11,15]`
8	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[12,14]`
9	$\left[0,\ y,\ \frac{1}{2}\right]$	`[17,21]`
10	$\left[-y,\ 0,\ \frac{1}{2}\right]$	`[18,24]`
11	$\left[y,\ 0,\ \frac{1}{2}\right]$	`[19,23]`
12	$\left[0,\ -y,\ \frac{1}{2}\right]$	`[20,22]`
13	$\left[\frac{1}{2},\ y+\frac{1}{2},\ 0\right]$	`[25,29]`
14	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ 0\right]$	`[26,32]`
15	$\left[y+\frac{1}{2},\ \frac{1}{2},\ 0\right]$	`[27,31]`

continued ...

Table 10

No.	position	mapping
16	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	[28,30]

Table 11: Wyckoff site: 16k, site symmetry: .2'.

No.	position	mapping
1	$\left[0,\ y,\ \frac{1}{4}\right]$	[1,21]
2	$\left[-y,\ 0,\ \frac{1}{4}\right]$	[2,24]
3	$\left[y,\ 0,\ \frac{1}{4}\right]$	[3,23]
4	$\left[0,\ -y,\ \frac{3}{4}\right]$	[4,22]
5	$\left[0,\ y,\ \frac{3}{4}\right]$	[5,17]
6	$\left[0,\ -y,\ \frac{1}{4}\right]$	[6,20]
7	$\left[y,\ 0,\ \frac{3}{4}\right]$	[7,19]
8	$\left[-y,\ 0,\ \frac{3}{4}\right]$	[8,18]
9	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[9,29]
10	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ \frac{3}{4}\right]$	[10,32]
11	$\left[y+\frac{1}{2},\ \frac{1}{2},\ \frac{3}{4}\right]$	[11,31]
12	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[12,30]
13	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[13,25]
14	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[14,28]
15	$\left[y+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{4}\right]$	[15,27]
16	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ \frac{1}{4}\right]$	[16,26]

Table 12: Wyckoff site: 16l, site symmetry: ..2

No.	position	mapping
1	$[x,\ x,\ 0]$	[1,7]
2	$[-x,\ x,\ 0]$	[2,5]
3	$[x,\ -x,\ 0]$	[3,4]
4	$[-x,\ -x,\ 0]$	[6,8]
5	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}\right]$	[9,15]
6	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	[10,13]
7	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[11,12]
8	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[14,16]
9	$\left[x,\ x,\ \frac{1}{2}\right]$	[17,23]
10	$\left[-x,\ x,\ \frac{1}{2}\right]$	[18,21]
11	$\left[x,\ -x,\ \frac{1}{2}\right]$	[19,20]
12	$\left[-x,\ -x,\ \frac{1}{2}\right]$	[22,24]
13	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ 0\right]$	[25,31]
14	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ 0\right]$	[26,29]
15	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ 0\right]$	[27,28]
16	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ 0\right]$	[30,32]

Table 13: Wyckoff site: `16m`, site symmetry: `..2`

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ \frac{1}{4}\right]$	`[1,15]`
2	$\left[\frac{1}{2}-x,\ x,\ \frac{1}{4}\right]$	`[2,13]`
3	$\left[x+\frac{1}{2},\ -x,\ \frac{1}{4}\right]$	`[3,12]`
4	$\left[x,\ \frac{1}{2}-x,\ \frac{3}{4}\right]$	`[4,11]`
5	$\left[-x,\ x+\frac{1}{2},\ \frac{3}{4}\right]$	`[5,10]`
6	$\left[-x,\ \frac{1}{2}-x,\ \frac{1}{4}\right]$	`[6,16]`
7	$\left[x+\frac{1}{2},\ x,\ \frac{3}{4}\right]$	`[7,9]`
8	$\left[\frac{1}{2}-x,\ -x,\ \frac{3}{4}\right]$	`[8,14]`
9	$\left[x,\ x+\frac{1}{2},\ \frac{3}{4}\right]$	`[17,31]`
10	$\left[\frac{1}{2}-x,\ x,\ \frac{3}{4}\right]$	`[18,29]`
11	$\left[x+\frac{1}{2},\ -x,\ \frac{3}{4}\right]$	`[19,28]`
12	$\left[x,\ \frac{1}{2}-x,\ \frac{1}{4}\right]$	`[20,27]`
13	$\left[-x,\ x+\frac{1}{2},\ \frac{1}{4}\right]$	`[21,26]`
14	$\left[-x,\ \frac{1}{2}-x,\ \frac{3}{4}\right]$	`[22,32]`
15	$\left[x+\frac{1}{2},\ x,\ \frac{1}{4}\right]$	`[23,25]`
16	$\left[\frac{1}{2}-x,\ -x,\ \frac{1}{4}\right]$	`[24,30]`

Table 14: Wyckoff site: `16n`, site symmetry: `..2'`

No.	position	mapping
1	$\left[x,\ x,\ \frac{1}{4}\right]$	`[1,23]`
2	$\left[-x,\ x,\ \frac{1}{4}\right]$	`[2,21]`
3	$\left[x,\ -x,\ \frac{1}{4}\right]$	`[3,20]`
4	$\left[x,\ -x,\ \frac{3}{4}\right]$	`[4,19]`
5	$\left[-x,\ x,\ \frac{3}{4}\right]$	`[5,18]`
6	$\left[-x,\ -x,\ \frac{1}{4}\right]$	`[6,24]`
7	$\left[x,\ x,\ \frac{3}{4}\right]$	`[7,17]`
8	$\left[-x,\ -x,\ \frac{3}{4}\right]$	`[8,22]`
9	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ \frac{3}{4}\right]$	`[9,31]`
10	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ \frac{3}{4}\right]$	`[10,29]`
11	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{3}{4}\right]$	`[11,28]`
12	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{4}\right]$	`[12,27]`
13	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ \frac{1}{4}\right]$	`[13,26]`
14	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ \frac{3}{4}\right]$	`[14,32]`
15	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{4}\right]$	`[15,25]`
16	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ \frac{1}{4}\right]$	`[16,30]`

Table 15: Wyckoff site: `16o`, site symmetry: `..2'`

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ 0\right]$	`[1,31]`

continued ...

Table 15

No.	position	mapping
2	$\left[\frac{1}{2}-x,\ x,\ 0\right]$	[2,29]
3	$\left[x+\frac{1}{2},\ -x,\ 0\right]$	[3,28]
4	$\left[x,\ \frac{1}{2}-x,\ 0\right]$	[4,27]
5	$\left[-x,\ x+\frac{1}{2},\ 0\right]$	[5,26]
6	$\left[-x,\ \frac{1}{2}-x,\ 0\right]$	[6,32]
7	$\left[x+\frac{1}{2},\ x,\ 0\right]$	[7,25]
8	$\left[\frac{1}{2}-x,\ -x,\ 0\right]$	[8,30]
9	$\left[x+\frac{1}{2},\ x,\ \frac{1}{2}\right]$	[9,23]
10	$\left[-x,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	[10,21]
11	$\left[x,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[11,20]
12	$\left[x+\frac{1}{2},\ -x,\ \frac{1}{2}\right]$	[12,19]
13	$\left[\frac{1}{2}-x,\ x,\ \frac{1}{2}\right]$	[13,18]
14	$\left[\frac{1}{2}-x,\ -x,\ \frac{1}{2}\right]$	[14,24]
15	$\left[x,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	[15,17]
16	$\left[-x,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[16,22]

Table 16: Wyckoff site: 32p, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$[-y,\ x,\ z]$	[2]
3	$[y,\ -x,\ z]$	[3]
4	$[x,\ -y,\ -z]$	[4]
5	$[-x,\ y,\ -z]$	[5]
6	$[-x,\ -y,\ z]$	[6]
7	$[y,\ x,\ -z]$	[7]
8	$[-y,\ -x,\ -z]$	[8]
9	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[9]
10	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[10]
11	$\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	[11]
12	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[12]
13	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[13]
14	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[14]
15	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	[15]
16	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[16]
17	$\left[x,\ y,\ z+\frac{1}{2}\right]$	[17]
18	$\left[-y,\ x,\ z+\frac{1}{2}\right]$	[18]
19	$\left[y,\ -x,\ z+\frac{1}{2}\right]$	[19]
20	$\left[x,\ -y,\ \frac{1}{2}-z\right]$	[20]
21	$\left[-x,\ y,\ \frac{1}{2}-z\right]$	[21]
22	$\left[-x,\ -y,\ z+\frac{1}{2}\right]$	[22]
23	$\left[y,\ x,\ \frac{1}{2}-z\right]$	[23]
24	$\left[-y,\ -x,\ \frac{1}{2}-z\right]$	[24]
25	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	[25]

continued ...

Table 16

No.	position	mapping
26	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, z\right]$	[26]
27	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, z\right]$	[27]
28	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$	[28]
29	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, -z\right]$	[29]
30	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z\right]$	[30]
31	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, -z\right]$	[31]
32	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, -z\right]$	[32]