MSG No. 137.517 P_C4_2/nmc [Type IV, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `m'mm.`

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

Table 2: Wyckoff site: `4b`, site symmetry: `-4'm2'`

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

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

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

Table 4: Wyckoff site: `4d`, site symmetry: `-4m2`

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

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

No.	position	mapping
1	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[1,7,22,24]`
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	`[2,5,19,20]`

continued ...

Table 5

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

Table 6: Wyckoff site: `8f`, site symmetry: `2'/m'..`

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

Table 7: Wyckoff site: `8g`, site symmetry: `2mm.`

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

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

No.	position	mapping
1	$\left[\frac{3}{4},\ \frac{1}{4},\ z\right]$	`[1,6,12,13]`
2	$\left[\frac{1}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	`[2,3,15,16]`
3	$\left[\frac{1}{4},\ \frac{3}{4},\ -z\right]$	`[4,5,9,14]`
4	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	`[7,8,10,11]`
5	$\left[\frac{1}{4},\ \frac{3}{4},\ z\right]$	`[17,22,28,29]`

continued ...

Table 8

No.	position	mapping
6	$\left[\frac{3}{4}, \frac{1}{4}, z+\frac{1}{2}\right]$	[18,19,31,32]
7	$\left[\frac{3}{4}, \frac{1}{4}, -z\right]$	[20,21,25,30]
8	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}-z\right]$	[23,24,26,27]

Table 9: Wyckoff site: 8i, site symmetry: m'm2'.

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

Table 10: Wyckoff site: 8j, site symmetry: m'm2'.

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

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

No.	position	mapping
1	$\left[\frac{1}{2}, 0, z\right]$	[1,22]
2	$\left[\frac{1}{2}, \frac{1}{2}, z+\frac{1}{2}\right]$	[2,19]
3	$\left[0, 0, z+\frac{1}{2}\right]$	[3,18]
4	$[0, 0, -z]$	[4,21]
5	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	[5,20]
6	$\left[0, \frac{1}{2}, z\right]$	[6,17]
7	$\left[\frac{1}{2}, 0, \frac{1}{2}-z\right]$	[7,24]
8	$\left[0, \frac{1}{2}, \frac{1}{2}-z\right]$	[8,23]

continued ...

Table 11

No.	position	mapping
9	$\left[\frac{1}{2}, 0, -z\right]$	[9,30]
10	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z\right]$	[10,27]
11	$\left[0, 0, \frac{1}{2} - z\right]$	[11,26]
12	$[0, 0, z]$	[12,29]
13	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	[13,28]
14	$\left[0, \frac{1}{2}, -z\right]$	[14,25]
15	$\left[\frac{1}{2}, 0, z + \frac{1}{2}\right]$	[15,32]
16	$\left[0, \frac{1}{2}, z + \frac{1}{2}\right]$	[16,31]

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

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

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

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

continued ...

Table 13

No.	position	mapping
11	$\left[x,\ -x,\ \frac{1}{4}\right]$	[19,20]
12	$\left[-x,\ \frac{1}{2}-x,\ \frac{3}{4}\right]$	[22,24]
13	$\left[\frac{1}{2}-x,\ -x,\ \frac{1}{4}\right]$	[25,31]
14	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{3}{4}\right]$	[26,29]
15	$\left[-x,\ x,\ \frac{3}{4}\right]$	[27,28]
16	$\left[x,\ x+\frac{1}{2},\ \frac{1}{4}\right]$	[30,32]

Table 14: Wyckoff site: 16n, site symmetry: m'..

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

Table 15: Wyckoff site: 16o, site symmetry: .m.

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

continued ...

Table 15

No.	position	mapping
13	$\left[\frac{3}{4}, y, -z\right]$	[21,30]
14	$\left[\frac{1}{4}, -y, z\right]$	[22,29]
15	$\left[y, \frac{3}{4}, \frac{1}{2} - z\right]$	[23,26]
16	$\left[\frac{1}{2} - y, \frac{3}{4}, \frac{1}{2} - z\right]$	[24,27]

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

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