MSG No. 137.516 P_c4_2/nmc [Type IV, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `-4'm2'`

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

Table 2: Wyckoff site: `4b`, 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	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[17,22,23,24,26,27,28,29]
4	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[18,19,20,21,25,30,31,32]

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

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

Table 4: Wyckoff site: `8d`, site symmetry: `..2'/m'`

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

Table 5: Wyckoff site: `8e`, site symmetry: `..2/m'`

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

Table 6: Wyckoff site: `8f`, 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	$\left[\frac{3}{4},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	`[17,22,28,29]`
6	$\left[\frac{1}{4},\ \frac{3}{4},\ z\right]$	`[18,19,31,32]`
7	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	`[20,21,25,30]`
8	$\left[\frac{3}{4},\ \frac{1}{4},\ -z\right]$	`[23,24,26,27]`

Table 7: Wyckoff site: `16g`, site symmetry: `..2'`

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

Table 8: Wyckoff site: `16h`, site symmetry: `..2`

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

Table 9: Wyckoff site: `16i`, site symmetry: `.m.`

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

Table 10: Wyckoff site: `16j`, site symmetry: `..m'`

No.	position	mapping
1	$[x,\ x,\ z]$	`[1,32]`

continued ...

Table 10

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

Table 11: Wyckoff site: 32k, 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	$\left[x,\ y,\ z+\frac{1}{2}\right]$	[17]
18	$\left[\frac{1}{2}-y,\ x,\ z\right]$	[18]
19	$\left[y,\ \frac{1}{2}-x,\ z\right]$	[19]
20	$\left[x+\frac{1}{2},\ -y,\ \frac{1}{2}-z\right]$	[20]
21	$\left[-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[21]
22	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[22]
23	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ -z\right]$	[23]
24	$[-y,\ -x,\ -z]$	[24]
25	$\left[-x,\ -y,\ \frac{1}{2}-z\right]$	[25]

continued ...

Table 11

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