MSG No. 138.528 P_c4_2/ncm [Type IV, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `-4'm'2`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x,\ x,\ z]$	`[1,16]`

continued ...

Table 10

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

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	$\left[x+\frac{1}{2},\ -y,\ \frac{1}{2}-z\right]$	[4]
5	$\left[-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[5]
6	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	[6]
7	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ -z\right]$	[7]
8	$[-y,\ -x,\ -z]$	[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	$\left[\frac{1}{2}-x,\ y,\ z+\frac{1}{2}\right]$	[12]
13	$\left[x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[13]
14	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ -z\right]$	[14]
15	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z\right]$	[15]
16	$[y,\ x,\ z]$	[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	$\left[x+\frac{1}{2},\ -y,\ -z\right]$	[20]
21	$\left[-x,\ y+\frac{1}{2},\ -z\right]$	[21]
22	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[22]
23	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	[23]
24	$\left[-y,\ -x,\ \frac{1}{2}-z\right]$	[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	$\left[\frac{1}{2}-x,\,y,\,z\right]$	[28]
29	$\left[x,\,\frac{1}{2}-y,\,z\right]$	[29]
30	$\left[x+\frac{1}{2},\,y+\frac{1}{2},\,\frac{1}{2}-z\right]$	[30]
31	$\left[\frac{1}{2}-y,\,\frac{1}{2}-x,\,z+\frac{1}{2}\right]$	[31]
32	$\left[y,\,x,\,z+\frac{1}{2}\right]$	[32]