MSG No. 133.468 P_c4_2/nbc [Type IV, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `4'22'`

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `-4'2m'`

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

Table 4: Wyckoff site: `4d`, site symmetry: `-42'm'`

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

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

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[1,9,23,31]`
2	$\left[0, \frac{1}{2}, 0\right]$	`[2,10,21,29]`

continued ...

Table 5

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

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

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

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

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

Table 8: Wyckoff site: 8h, site symmetry: 2.m'm'

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{3}{4}, z\right]$	[1,6,31,32]
2	$\left[\frac{3}{4}, \frac{1}{4}, z+\frac{1}{2}\right]$	[2,3,28,29]
3	$\left[\frac{1}{4}, \frac{3}{4}, -z\right]$	[4,5,26,27]
4	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}-z\right]$	[7,8,25,30]
5	$\left[\frac{3}{4}, \frac{1}{4}, -z\right]$	[9,14,23,24]

continued ...

Table 8

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

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

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

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

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

continued ...

Table 10

No.	position	mapping
16	$\left[x+\frac{1}{2},\, x+\frac{1}{2},\, \frac{3}{4}\right]$	[30,32]

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

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

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

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

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

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

Table 14: Wyckoff site: 32n, 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	$\left[\frac{1}{2}-x,\ y,\ -z\right]$	[5]
6	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	[6]
7	$\left[y,\ x,\ \frac{1}{2}-z\right]$	[7]
8	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[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	$\left[-x,\ y+\frac{1}{2},\ z\right]$	[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	$\left[-y,\ -x,\ z+\frac{1}{2}\right]$	[15]
16	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[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	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}-z\right]$	[21]
22	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[22]
23	$[y,\ x,\ -z]$	[23]

continued ...

Table 14

No.	position	mapping
24	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ -z\right]$	[24]
25	$\left[-x,\ -y,\ \frac{1}{2}-z\right]$	[25]
26	$\left[y+\frac{1}{2},\ -x,\ -z\right]$	[26]
27	$\left[-y,\ x+\frac{1}{2},\ -z\right]$	[27]
28	$\left[-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[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	$\left[-y,\ -x,\ z\right]$	[31]
32	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z\right]$	[32]