

MSG No. 138.530 P_I4_2/ncm [Type IV, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: 4'2'2

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: m'.mm

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

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

No.	position	mapping
1	$[0, \frac{1}{2}, 0]$	[1,7,9,15]
2	$[0, 0, \frac{1}{2}]$	[2,5,10,13]

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 4' ..

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

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

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

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

No.	position	mapping
1	$[x, x, \frac{3}{4}]$	[1, 16, 23, 30]
2	$[\frac{1}{2} - x, x, \frac{1}{4}]$	[2, 12, 21, 27]
3	$[x, \frac{1}{2} - x, \frac{1}{4}]$	[3, 13, 20, 26]
4	$[x + \frac{1}{2}, -x, \frac{3}{4}]$	[4, 10, 19, 29]
5	$[-x, x + \frac{1}{2}, \frac{3}{4}]$	[5, 11, 18, 28]

continued ...

Table 8

No.	position	mapping
6	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{3}{4}]$	[6,15,24,25]
7	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}]$	[7,14,17,32]
8	$[-x, -x, \frac{1}{4}]$	[8,9,22,31]

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

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

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

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

continued ...

Table 10

No.	position	mapping
16	$[\frac{1}{4}, x, 0]$	[16,27]

Table 11: Wyckoff site: 16k, site symmetry: $m' \dots$

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

Table 12: Wyckoff site: 16l, site symmetry: $\dots m$

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

Table 13: Wyckoff site: 32m, site symmetry: 1

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