

MSG No. 133.470 P_I4_2/nbc [Type IV, tetragonal]

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

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

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

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

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	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[4,5,15,16,23,24,28,29]
4	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[7,8,12,13,20,21,31,32]

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

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

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

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

continued ...

Table 5

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

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	$[\frac{3}{4}, \frac{1}{4}, -z]$	[4,5,23,24]
4	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[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	$[\frac{1}{4}, \frac{3}{4}, z]$	[12,13,31,32]
8	$[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[15,16,28,29]

Table 7: Wyckoff site: 8g, site symmetry: 2.m'm'

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

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

No.	position	mapping
1	$[x, x, \frac{3}{4}]$	[1,7,30,32]
2	$[\frac{1}{2} - x, x, \frac{1}{4}]$	[2,5,27,28]
3	$[x, \frac{1}{2} - x, \frac{1}{4}]$	[3,4,26,29]
4	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{3}{4}]$	[6,8,25,31]
5	$[-x, -x, \frac{1}{4}]$	[9,15,22,24]

continued ...

Table 8

No.	position	mapping
6	$[x + \frac{1}{2}, -x, \frac{3}{4}]$	[10,13,19,20]
7	$[-x, x + \frac{1}{2}, \frac{3}{4}]$	[11,12,18,21]
8	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}]$	[14,16,17,23]

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

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

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

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

continued ...

Table 10

No.	position	mapping
16	$[x, \frac{1}{4}, \frac{1}{2}]$	[29,30]

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

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	$[x, \frac{1}{2} - y, \frac{1}{4}]$	[4,29]
5	$[\frac{1}{2} - x, y, \frac{1}{4}]$	[5,28]
6	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{3}{4}]$	[6,25]
7	$[y, x, \frac{3}{4}]$	[7,32]
8	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{3}{4}]$	[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	$[-x, y + \frac{1}{2}, \frac{3}{4}]$	[12,21]
13	$[x + \frac{1}{2}, -y, \frac{3}{4}]$	[13,20]
14	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{4}]$	[14,17]
15	$[-y, -x, \frac{1}{4}]$	[15,24]
16	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}]$	[16,23]

Table 12: Wyckoff site: 16l, site symmetry: $..m'$

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

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