

MSG No. 126.384 P_c4/nnc [Type IV, tetragonal]

Table 1: Wyckoff site: **4a**, site symmetry: $42'2'$

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

Table 2: Wyckoff site: **4b**, site symmetry: 422

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

Table 3: Wyckoff site: **4c**, site symmetry: $-42'm'$

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

Table 4: Wyckoff site: **4d**, site symmetry: $-4'2m'$

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

Table 5: Wyckoff site: **8e**, site symmetry: $\dots 2'/m'$

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

continued ...

Table 5

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

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

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

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

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

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

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

continued ...

Table 8

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

Table 9: Wyckoff site: 16i, site symmetry: $\dots 2'$

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

Table 10: Wyckoff site: 16j, site symmetry: $\dots 2$

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

continued ...

Table 10

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

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

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

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

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

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

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

Table 14: Wyckoff site: 32n, site symmetry: 1

No.	position	mapping
1	[x, y, z]	[1]
2	[$\frac{1}{2}$ - y, x, z]	[2]
3	[y, $\frac{1}{2}$ - x, z]	[3]
4	[x, $\frac{1}{2}$ - y, $\frac{1}{2}$ - z]	[4]
5	[$\frac{1}{2}$ - x, y, $\frac{1}{2}$ - 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, -z]	[10]
11	[-y, x + $\frac{1}{2}$, -z]	[11]
12	[-x, y + $\frac{1}{2}$, 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	[-y, -x, z + $\frac{1}{2}$]	[15]
16	[y + $\frac{1}{2}$, x + $\frac{1}{2}$, z + $\frac{1}{2}$]	[16]
17	[x, y, z + $\frac{1}{2}$]	[17]
18	[$\frac{1}{2}$ - y, x, z + $\frac{1}{2}$]	[18]
19	[y, $\frac{1}{2}$ - x, z + $\frac{1}{2}$]	[19]
20	[x, $\frac{1}{2}$ - y, -z]	[20]
21	[$\frac{1}{2}$ - x, y, -z]	[21]
22	[$\frac{1}{2}$ - x, $\frac{1}{2}$ - y, z + $\frac{1}{2}$]	[22]
23	[y, x, -z]	[23]

continued ...

Table 14

No.	position	mapping
24	$[\frac{1}{2} - y, \frac{1}{2} - x, -z]$	[24]
25	$[-x, -y, \frac{1}{2} - z]$	[25]
26	$[y + \frac{1}{2}, -x, \frac{1}{2} - z]$	[26]
27	$[-y, x + \frac{1}{2}, \frac{1}{2} - z]$	[27]
28	$[-x, y + \frac{1}{2}, z]$	[28]
29	$[x + \frac{1}{2}, -y, z]$	[29]
30	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[30]
31	$[-y, -x, z]$	[31]
32	$[y + \frac{1}{2}, x + \frac{1}{2}, z]$	[32]