

MSG No. 88.86 I_c4_1/a [Type IV, tetragonal]

Table 1: Wyckoff site: 8a, site symmetry: $-4..$

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

Table 2: Wyckoff site: 8b, site symmetry: $-4'..$

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

Table 3: Wyckoff site: 16c, site symmetry: -1

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

continued ...

Table 3

No.	position	mapping
16	$[\frac{1}{2}, 0, \frac{1}{2}]$	[28,32]

Table 4: Wyckoff site: **16d**, site symmetry: $-1'$

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

Table 5: Wyckoff site: **16e**, site symmetry: $2'..$

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

Table 6: Wyckoff site: **16f**, site symmetry: **2** .

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

Table 7: Wyckoff site: **32g**, site symmetry: **1**

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

continued ...

Table 7

No.	position	mapping
24	$[x, y + \frac{1}{2}, \frac{1}{2} - z]$	[24]
25	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[25]
26	$[\frac{1}{4} - y, x + \frac{3}{4}, z + \frac{1}{4}]$	[26]
27	$[y + \frac{3}{4}, \frac{3}{4} - x, z + \frac{1}{4}]$	[27]
28	$[\frac{1}{2} - x, -y, z]$	[28]
29	$[\frac{1}{2} - x, \frac{1}{2} - y, -z]$	[29]
30	$[y + \frac{3}{4}, \frac{1}{4} - x, \frac{3}{4} - z]$	[30]
31	$[\frac{1}{4} - y, x + \frac{1}{4}, \frac{3}{4} - z]$	[31]
32	$[x + \frac{1}{2}, y, -z]$	[32]