

MSG No. 141.553 $I4_1/a'md$ [Type III, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: $-4'm2'$

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

Table 2: Wyckoff site: 4b, site symmetry: $-4'm2'$

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

Table 3: Wyckoff site: 8c, site symmetry: $.2'/m$.

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

Table 4: Wyckoff site: 8d, site symmetry: $.2'/m$.

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

Table 5: Wyckoff site: 8e, site symmetry: $2mm$.

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

Table 6: Wyckoff site: 16f, site symmetry: $.2'$.

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

Table 7: Wyckoff site: 16g, site symmetry: $. .2'$

No.	position	mapping
1	$[x, x + \frac{1}{4}, \frac{7}{8}]$	[1,11]
2	$[-x, x + \frac{3}{4}, \frac{1}{8}]$	[2,10]
3	$[x, \frac{3}{4} - x, \frac{1}{8}]$	[3,9]
4	$[-x, \frac{1}{4} - x, \frac{7}{8}]$	[4,12]
5	$[-x, x + \frac{1}{4}, \frac{7}{8}]$	[5,15]
6	$[x, \frac{1}{4} - x, \frac{7}{8}]$	[6,14]
7	$[-x, \frac{3}{4} - x, \frac{1}{8}]$	[7,13]
8	$[x, x + \frac{3}{4}, \frac{1}{8}]$	[8,16]
9	$[x + \frac{1}{2}, x + \frac{3}{4}, \frac{3}{8}]$	[17,27]

continued ...

Table 7

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

Table 8: Wyckoff site: 16h, site symmetry: .m.

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

Table 9: Wyckoff site: 32i, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[\frac{1}{4} - y, x + \frac{3}{4}, z + \frac{1}{4}]$	[2]
3	$[y + \frac{3}{4}, \frac{3}{4} - x, z + \frac{1}{4}]$	[3]
4	$[-x, \frac{1}{2} - y, z]$	[4]
5	$[-x, y, z]$	[5]
6	$[x, \frac{1}{2} - y, z]$	[6]
7	$[\frac{1}{4} - y, \frac{3}{4} - x, z + \frac{1}{4}]$	[7]
8	$[y + \frac{3}{4}, x + \frac{3}{4}, z + \frac{1}{4}]$	[8]
9	$[x, -y, -z]$	[9]
10	$[-x, y + \frac{1}{2}, -z]$	[10]
11	$[y + \frac{3}{4}, x + \frac{1}{4}, \frac{3}{4} - z]$	[11]

continued ...

Table 9

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