

MSG No. 129.420 P_c4/nmm [Type IV, tetragonal]

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: 4mm

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

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

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

Table 5: Wyckoff site: **8e**, site symmetry: $\dots 2^1/m$

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

Table 6: Wyckoff site: **8f**, site symmetry: $2mm$.

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

Table 7: Wyckoff site: **16g**, site symmetry: $\dots 2$

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

Table 8: Wyckoff site: 16h, site symmetry: $\dots 2'$

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

Table 9: Wyckoff site: 16i, site symmetry: $.m.$

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

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

No.	position	mapping
1	$[x, x, z]$	[1,16]

continued ...

Table 10

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

Table 11: Wyckoff site: 32k, 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	$[x + \frac{1}{2}, -y, -z]$	[4]
5	$[-x, y + \frac{1}{2}, -z]$	[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	$[y + \frac{1}{2}, -x, -z]$	[10]
11	$[-y, x + \frac{1}{2}, -z]$	[11]
12	$[\frac{1}{2} - x, y, z]$	[12]
13	$[x, \frac{1}{2} - y, z]$	[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	$[x, y, z + \frac{1}{2}]$	[17]
18	$[\frac{1}{2} - y, x, z + \frac{1}{2}]$	[18]
19	$[y, \frac{1}{2} - x, z + \frac{1}{2}]$	[19]
20	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	[20]
21	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[21]
22	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[22]
23	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[23]
24	$[-y, -x, \frac{1}{2} - z]$	[24]
25	$[-x, -y, \frac{1}{2} - z]$	[25]

continued ...

Table 11

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