

MSG No. 71.538  $I_cmmm$  [ Type IV, orthorhombic ]

Table 1: Wyckoff site: **4a**, site symmetry: **mmm**

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

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

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

Table 3: Wyckoff site: **4c**, site symmetry: **mmm'**

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

Table 4: Wyckoff site: **4d**, site symmetry: **mmm'**

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

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

No.	position	mapping
1	[\frac{1}{4}, \frac{1}{4}, 0]	[1,8,28,29]
2	[\frac{1}{4}, \frac{3}{4}, 0]	[2,7,27,30]

*continued ...*

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry:  $\dots 2'/m'$ 

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

Table 7: Wyckoff site: 8g, site symmetry:  $2\bar{m}m$ 

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

Table 8: Wyckoff site: 8h, site symmetry:  $2'mm'$ 

No.	position	mapping
1	$[x, 0, \frac{1}{4}]$	[1,7,18,24]
2	$[x, 0, \frac{3}{4}]$	[2,8,17,23]
3	$[-x, 0, \frac{3}{4}]$	[3,5,20,22]
4	$[-x, 0, \frac{1}{4}]$	[4,6,19,21]
5	$[x + \frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[9,15,26,32]

*continued ...*

Table 8

No.	position	mapping
6	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[10, 16, 25, 31]
7	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{4}]$	[11, 13, 28, 30]
8	$[\frac{1}{2} - x, \frac{1}{2}, \frac{3}{4}]$	[12, 14, 27, 29]

Table 9: Wyckoff site: 8i, site symmetry:  $\text{m}\bar{2}\text{m}$ 

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

Table 10: Wyckoff site: 8j, site symmetry:  $\text{m}2'\bar{\text{m}}'$ 

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

Table 11: Wyckoff site: 8k, site symmetry:  $\text{mm}2$ 

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

Table 12: Wyckoff site: 81, site symmetry:  $\text{mm}2$ 

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

Table 13: Wyckoff site: 16m, site symmetry:  $\dots 2'$ 

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

Table 14: Wyckoff site: 16n, site symmetry:  $\text{m}\dots$ 

No.	position	mapping
1	$[0, y, z]$	[1, 6]
2	$[0, -y, -z]$	[2, 5]
3	$[0, y, -z]$	[3, 8]
4	$[0, -y, z]$	[4, 7]
5	$[\frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9, 14]
6	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[10, 13]
7	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[11, 16]
8	$[\frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[12, 15]
9	$[0, y, z + \frac{1}{2}]$	[17, 22]

continued ...

Table 14

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

Table 15: Wyckoff site: 16o, site symmetry: .m.

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

Table 16: Wyckoff site: 16p, site symmetry: ..m

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

continued ...

Table 16

No.	position	mapping
12	$[-x, -y, \frac{1}{2}]$	[20,21]
13	$[x + \frac{1}{2}, y + \frac{1}{2}, 0]$	[25,32]
14	$[x + \frac{1}{2}, \frac{1}{2} - y, 0]$	[26,31]
15	$[\frac{1}{2} - x, y + \frac{1}{2}, 0]$	[27,30]
16	$[\frac{1}{2} - x, \frac{1}{2} - y, 0]$	[28,29]

Table 17: Wyckoff site: 16q, site symmetry: .m'

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

Table 18: Wyckoff site: 32r, site symmetry: 1

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

continued ...

Table 18

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