

MSG No. 208.44  $P4_232$  [ Type I, cubic ]

Table 1: Wyckoff site: 2a, site symmetry: 23.

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

Table 2: Wyckoff site: 4b, site symmetry: .32

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

Table 3: Wyckoff site: 4c, site symmetry: .32

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

Table 4: Wyckoff site: 6d, site symmetry: 222..

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

Table 5: Wyckoff site: 6e, site symmetry: 2.22

No.	position	mapping
1	[\frac{1}{4}, 0, \frac{1}{2}]	[1,8,13,14]
2	[\frac{3}{4}, 0, \frac{1}{2}]	[2,3,9,10]

*continued ...*

Table 5

No.	position	mapping
3	$[0, \frac{1}{2}, \frac{1}{4}]$	[4,16,18,21]
4	$[0, \frac{1}{2}, \frac{3}{4}]$	[5,15,19,23]
5	$[\frac{1}{2}, \frac{3}{4}, 0]$	[6,11,20,22]
6	$[\frac{1}{2}, \frac{1}{4}, 0]$	[7,12,17,24]

Table 6: Wyckoff site: 6f, site symmetry: 2.22

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

Table 7: Wyckoff site: 8g, site symmetry: .3.

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

Table 8: Wyckoff site: 12h, site symmetry: 2..

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

*continued ...*

Table 8

No.	position	mapping
10	$[0, 0, x]$	[18,21]
11	$[0, 0, -x]$	[19,23]
12	$[0, -x, 0]$	[20,22]

Table 9: Wyckoff site: 12i, site symmetry: 2..

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

Table 10: Wyckoff site: 12j, site symmetry: 2..

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

Table 11: Wyckoff site: 12k, site symmetry: . . 2

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

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

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

Table 13: Wyckoff site: 24m, site symmetry: 1

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

continued ...

Table 13

No.	position	mapping
10	$[-x, -y, z]$	[10]
11	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[11]
12	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[12]
13	$[\frac{1}{2} - x, z + \frac{1}{2}, y + \frac{1}{2}]$	[13]
14	$[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - y]$	[14]
15	$[z + \frac{1}{2}, \frac{1}{2} - y, x + \frac{1}{2}]$	[15]
16	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2} - x]$	[16]
17	$[z, x, y]$	[17]
18	$[y, z, x]$	[18]
19	$[-y, z, -x]$	[19]
20	$[-z, -x, y]$	[20]
21	$[-y, -z, x]$	[21]
22	$[z, -x, -y]$	[22]
23	$[y, -z, -x]$	[23]
24	$[-z, x, -y]$	[24]