

MSG No. 197.7 *I*23 [ Type I, cubic ]

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

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

Table 2: Wyckoff site: 6b, site symmetry: 222..

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

Table 3: Wyckoff site: 8c, site symmetry: .3.

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

Table 4: Wyckoff site: 12d, site symmetry: 2..

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

*continued ...*

Table 4

No.	position	mapping
10	$[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$	[18,21]
11	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$	[19,23]
12	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[20,22]

Table 5: Wyckoff site: 12e, site symmetry: 2..

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

Table 6: Wyckoff site: 24f, 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	$[z, x, y]$	[5]
6	$[y, z, x]$	[6]
7	$[-y, z, -x]$	[7]
8	$[-z, -x, y]$	[8]
9	$[-y, -z, x]$	[9]
10	$[z, -x, -y]$	[10]
11	$[y, -z, -x]$	[11]
12	$[-z, x, -y]$	[12]
13	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[13]
14	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[14]
15	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[15]
16	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[16]
17	$[z + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}]$	[17]
18	$[y + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}]$	[18]
19	$[\frac{1}{2} - y, z + \frac{1}{2}, \frac{1}{2} - x]$	[19]

continued ...

Table 6

No.	position	mapping
20	$[\frac{1}{2} - z, \frac{1}{2} - x, y + \frac{1}{2}]$	[20]
21	$[\frac{1}{2} - y, \frac{1}{2} - z, x + \frac{1}{2}]$	[21]
22	$[z + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - y]$	[22]
23	$[y + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - x]$	[23]
24	$[\frac{1}{2} - z, x + \frac{1}{2}, \frac{1}{2} - y]$	[24]