

MSG No. 201.20 $Pn'3'$ [Type III, cubic]

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

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

Table 2: Wyckoff site: 4b, site symmetry: .-3'.

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

Table 3: Wyckoff site: 4c, site symmetry: .-3'.

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: .3.

No.	position	mapping
1	[x, x, x]	[1,5,6]
2	$[x, \frac{1}{2} - x, \frac{1}{2} - x]$	[2,10,11]

continued ...

Table 5

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

Table 6: Wyckoff site: 12f, site symmetry: 2..

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

Table 7: Wyckoff site: 12g, site symmetry: 2..

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

Table 8: Wyckoff site: 24h, site symmetry: 1

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