

MSG No. 148.20 $R_I\bar{3}$ [Type IV, trigonal]

Table 1: Wyckoff site: 6a, site symmetry: -3..

No.	position	mapping
1	[0, 0, 0]	[1,2,3,4,5,6]
2	[\frac{2}{3}, \frac{1}{3}, \frac{1}{3}]	[7,8,9,10,11,12]
3	[\frac{1}{3}, \frac{2}{3}, \frac{2}{3}]	[13,14,15,16,17,18]
4	[0, 0, \frac{1}{2}]	[19,20,21,22,23,24]
5	[\frac{2}{3}, \frac{1}{3}, \frac{5}{6}]	[25,26,27,28,29,30]
6	[\frac{1}{3}, \frac{2}{3}, \frac{1}{6}]	[31,32,33,34,35,36]

Table 2: Wyckoff site: 6b, site symmetry: -3'..

No.	position	mapping
1	[0, 0, \frac{1}{4}]	[1,2,3,22,23,24]
2	[0, 0, \frac{3}{4}]	[4,5,6,19,20,21]
3	[\frac{2}{3}, \frac{1}{3}, \frac{7}{12}]	[7,8,9,28,29,30]
4	[\frac{2}{3}, \frac{1}{3}, \frac{1}{12}]	[10,11,12,25,26,27]
5	[\frac{1}{3}, \frac{2}{3}, \frac{11}{12}]	[13,14,15,34,35,36]
6	[\frac{1}{3}, \frac{2}{3}, \frac{5}{12}]	[16,17,18,31,32,33]

Table 3: Wyckoff site: 12c, site symmetry: 3..

No.	position	mapping
1	[0, 0, z]	[1,2,3]
2	[0, 0, -z]	[4,5,6]
3	[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{3}]	[7,8,9]
4	[\frac{2}{3}, \frac{1}{3}, \frac{1}{3} - z]	[10,11,12]
5	[\frac{1}{3}, \frac{2}{3}, z + \frac{2}{3}]	[13,14,15]
6	[\frac{1}{3}, \frac{2}{3}, \frac{2}{3} - z]	[16,17,18]
7	[0, 0, z + \frac{1}{2}]	[19,20,21]
8	[0, 0, \frac{1}{2} - z]	[22,23,24]
9	[\frac{2}{3}, \frac{1}{3}, z + \frac{5}{6}]	[25,26,27]
10	[\frac{2}{3}, \frac{1}{3}, \frac{5}{6} - z]	[28,29,30]
11	[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{6}]	[31,32,33]
12	[\frac{1}{3}, \frac{2}{3}, \frac{1}{6} - z]	[34,35,36]

Table 4: Wyckoff site: 18d, site symmetry: -1'

No.	position	mapping
1	$[\frac{1}{2}, 0, \frac{1}{4}]$	[1,22]
2	$[0, \frac{1}{2}, \frac{1}{4}]$	[2,23]
3	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[3,24]
4	$[\frac{1}{2}, 0, \frac{3}{4}]$	[4,19]
5	$[0, \frac{1}{2}, \frac{3}{4}]$	[5,20]
6	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[6,21]
7	$[\frac{1}{6}, \frac{1}{3}, \frac{7}{12}]$	[7,28]
8	$[\frac{2}{3}, \frac{5}{6}, \frac{7}{12}]$	[8,29]
9	$[\frac{1}{6}, \frac{5}{6}, \frac{7}{12}]$	[9,30]
10	$[\frac{1}{6}, \frac{1}{3}, \frac{1}{12}]$	[10,25]
11	$[\frac{2}{3}, \frac{5}{6}, \frac{1}{12}]$	[11,26]
12	$[\frac{1}{6}, \frac{5}{6}, \frac{1}{12}]$	[12,27]
13	$[\frac{5}{6}, \frac{2}{3}, \frac{11}{12}]$	[13,34]
14	$[\frac{1}{3}, \frac{1}{6}, \frac{11}{12}]$	[14,35]
15	$[\frac{5}{6}, \frac{1}{6}, \frac{11}{12}]$	[15,36]
16	$[\frac{5}{6}, \frac{2}{3}, \frac{5}{12}]$	[16,31]
17	$[\frac{1}{3}, \frac{1}{6}, \frac{5}{12}]$	[17,32]
18	$[\frac{5}{6}, \frac{1}{6}, \frac{5}{12}]$	[18,33]

Table 5: Wyckoff site: 18e, site symmetry: -1

No.	position	mapping
1	$[\frac{1}{2}, 0, 0]$	[1,4]
2	$[0, \frac{1}{2}, 0]$	[2,5]
3	$[\frac{1}{2}, \frac{1}{2}, 0]$	[3,6]
4	$[\frac{1}{6}, \frac{1}{3}, \frac{1}{3}]$	[7,10]
5	$[\frac{2}{3}, \frac{5}{6}, \frac{1}{3}]$	[8,11]
6	$[\frac{1}{6}, \frac{5}{6}, \frac{1}{3}]$	[9,12]
7	$[\frac{5}{6}, \frac{2}{3}, \frac{2}{3}]$	[13,16]
8	$[\frac{1}{3}, \frac{1}{6}, \frac{2}{3}]$	[14,17]
9	$[\frac{5}{6}, \frac{1}{6}, \frac{2}{3}]$	[15,18]
10	$[\frac{1}{2}, 0, \frac{1}{2}]$	[19,22]
11	$[0, \frac{1}{2}, \frac{1}{2}]$	[20,23]
12	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[21,24]
13	$[\frac{1}{6}, \frac{1}{3}, \frac{5}{6}]$	[25,28]
14	$[\frac{2}{3}, \frac{5}{6}, \frac{5}{6}]$	[26,29]
15	$[\frac{1}{6}, \frac{5}{6}, \frac{5}{6}]$	[27,30]
16	$[\frac{5}{6}, \frac{2}{3}, \frac{1}{6}]$	[31,34]
17	$[\frac{1}{3}, \frac{1}{6}, \frac{1}{6}]$	[32,35]
18	$[\frac{5}{6}, \frac{1}{6}, \frac{1}{6}]$	[33,36]

Table 6: Wyckoff site: 36f, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x - y, z]$	[2]
3	$[-x + y, -x, z]$	[3]
4	$[-x, -y, -z]$	[4]
5	$[y, -x + y, -z]$	[5]
6	$[x - y, x, -z]$	[6]
7	$[x + \frac{2}{3}, y + \frac{1}{3}, z + \frac{1}{3}]$	[7]
8	$[\frac{2}{3} - y, x - y + \frac{1}{3}, z + \frac{1}{3}]$	[8]
9	$[-x + y + \frac{2}{3}, \frac{1}{3} - x, z + \frac{1}{3}]$	[9]
10	$[\frac{2}{3} - x, \frac{1}{3} - y, \frac{1}{3} - z]$	[10]
11	$[y + \frac{2}{3}, -x + y + \frac{1}{3}, \frac{1}{3} - z]$	[11]
12	$[x - y + \frac{2}{3}, x + \frac{1}{3}, \frac{1}{3} - z]$	[12]
13	$[x + \frac{1}{3}, y + \frac{2}{3}, z + \frac{2}{3}]$	[13]
14	$[\frac{1}{3} - y, x - y + \frac{2}{3}, z + \frac{2}{3}]$	[14]
15	$[-x + y + \frac{1}{3}, \frac{2}{3} - x, z + \frac{2}{3}]$	[15]
16	$[\frac{1}{3} - x, \frac{2}{3} - y, \frac{2}{3} - z]$	[16]
17	$[y + \frac{1}{3}, -x + y + \frac{2}{3}, \frac{2}{3} - z]$	[17]
18	$[x - y + \frac{1}{3}, x + \frac{2}{3}, \frac{2}{3} - z]$	[18]
19	$[x, y, z + \frac{1}{2}]$	[19]
20	$[-y, x - y, z + \frac{1}{2}]$	[20]
21	$[-x + y, -x, z + \frac{1}{2}]$	[21]
22	$[-x, -y, \frac{1}{2} - z]$	[22]
23	$[y, -x + y, \frac{1}{2} - z]$	[23]
24	$[x - y, x, \frac{1}{2} - z]$	[24]
25	$[x + \frac{2}{3}, y + \frac{1}{3}, z + \frac{5}{6}]$	[25]
26	$[\frac{2}{3} - y, x - y + \frac{1}{3}, z + \frac{5}{6}]$	[26]
27	$[-x + y + \frac{2}{3}, \frac{1}{3} - x, z + \frac{5}{6}]$	[27]
28	$[\frac{2}{3} - x, \frac{1}{3} - y, \frac{5}{6} - z]$	[28]
29	$[y + \frac{2}{3}, -x + y + \frac{1}{3}, \frac{5}{6} - z]$	[29]
30	$[x - y + \frac{2}{3}, x + \frac{1}{3}, \frac{5}{6} - z]$	[30]
31	$[x + \frac{1}{3}, y + \frac{2}{3}, z + \frac{1}{6}]$	[31]
32	$[\frac{1}{3} - y, x - y + \frac{2}{3}, z + \frac{1}{6}]$	[32]
33	$[-x + y + \frac{1}{3}, \frac{2}{3} - x, z + \frac{1}{6}]$	[33]
34	$[\frac{1}{3} - x, \frac{2}{3} - y, \frac{1}{6} - z]$	[34]
35	$[y + \frac{1}{3}, -x + y + \frac{2}{3}, \frac{1}{6} - z]$	[35]
36	$[x - y + \frac{1}{3}, x + \frac{2}{3}, \frac{1}{6} - z]$	[36]