

MSG No. 212.60 $P4_3321'$ [Type II, cubic]

Table 1: Wyckoff site: 4a, site symmetry: .321'

No.	position	mapping
1	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$	[1,12,14,16,17,18,25,36,38,40,41,42]
2	$[\frac{7}{8}, \frac{5}{8}, \frac{3}{8}]$	[2,7,9,15,19,24,26,31,33,39,43,48]
3	$[\frac{3}{8}, \frac{7}{8}, \frac{5}{8}]$	[3,4,10,11,20,21,27,28,34,35,44,45]
4	$[\frac{5}{8}, \frac{3}{8}, \frac{7}{8}]$	[5,6,8,13,22,23,29,30,32,37,46,47]

Table 2: Wyckoff site: 4b, site symmetry: .321'

No.	position	mapping
1	$[\frac{5}{8}, \frac{5}{8}, \frac{5}{8}]$	[1,12,14,16,17,18,25,36,38,40,41,42]
2	$[\frac{3}{8}, \frac{1}{8}, \frac{7}{8}]$	[2,7,9,15,19,24,26,31,33,39,43,48]
3	$[\frac{7}{8}, \frac{3}{8}, \frac{1}{8}]$	[3,4,10,11,20,21,27,28,34,35,44,45]
4	$[\frac{1}{8}, \frac{7}{8}, \frac{3}{8}]$	[5,6,8,13,22,23,29,30,32,37,46,47]

Table 3: Wyckoff site: 8c, site symmetry: .3.1'

No.	position	mapping
1	$[x, x, x]$	[1,17,18,25,41,42]
2	$[x + \frac{3}{4}, \frac{3}{4} - x, x + \frac{1}{4}]$	[2,7,15,26,31,39]
3	$[x + \frac{1}{4}, x + \frac{3}{4}, \frac{3}{4} - x]$	[3,4,11,27,28,35]
4	$[\frac{3}{4} - x, x + \frac{1}{4}, x + \frac{3}{4}]$	[5,6,13,29,30,37]
5	$[x + \frac{1}{2}, \frac{1}{2} - x, -x]$	[8,22,23,32,46,47]
6	$[-x, x + \frac{1}{2}, \frac{1}{2} - x]$	[9,19,24,33,43,48]
7	$[\frac{1}{2} - x, -x, x + \frac{1}{2}]$	[10,20,21,34,44,45]
8	$[\frac{1}{4} - x, \frac{1}{4} - x, \frac{1}{4} - x]$	[12,14,16,36,38,40]

Table 4: Wyckoff site: 12d, site symmetry: ..21'

No.	position	mapping
1	$[\frac{1}{8}, y, \frac{1}{4} - y]$	[1,14,25,38]
2	$[\frac{7}{8}, y + \frac{1}{2}, y + \frac{1}{4}]$	[2,9,26,33]
3	$[\frac{3}{8}, -y, \frac{3}{4} - y]$	[3,10,27,34]
4	$[\frac{1}{2} - y, y + \frac{3}{4}, \frac{5}{8}]$	[4,21,28,45]
5	$[y + \frac{1}{2}, y + \frac{1}{4}, \frac{7}{8}]$	[5,23,29,47]
6	$[\frac{3}{4} - y, \frac{3}{8}, -y]$	[6,22,30,46]
7	$[y + \frac{3}{4}, \frac{5}{8}, \frac{1}{2} - y]$	[7,24,31,48]
8	$[\frac{5}{8}, \frac{1}{2} - y, y + \frac{3}{4}]$	[8,13,32,37]
9	$[y + \frac{1}{4}, \frac{7}{8}, y + \frac{1}{2}]$	[11,20,35,44]

continued ...

Table 4

No.	position	mapping
10	$[\frac{1}{4} - y, \frac{1}{8}, y]$	[12,17,36,41]
11	$[-y, \frac{3}{4} - y, \frac{3}{8}]$	[15,19,39,43]
12	$[y, \frac{1}{4} - y, \frac{1}{8}]$	[16,18,40,42]

Table 5: Wyckoff site: 24e, site symmetry: 11'

No.	position	mapping
1	$[x, y, z]$	[1,25]
2	$[x + \frac{3}{4}, \frac{3}{4} - z, y + \frac{1}{4}]$	[2,26]
3	$[x + \frac{1}{4}, z + \frac{3}{4}, \frac{3}{4} - y]$	[3,27]
4	$[z + \frac{1}{4}, y + \frac{3}{4}, \frac{3}{4} - x]$	[4,28]
5	$[\frac{3}{4} - z, y + \frac{1}{4}, x + \frac{3}{4}]$	[5,29]
6	$[\frac{3}{4} - y, x + \frac{1}{4}, z + \frac{3}{4}]$	[6,30]
7	$[y + \frac{3}{4}, \frac{3}{4} - x, z + \frac{1}{4}]$	[7,31]
8	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[8,32]
9	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[9,33]
10	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[10,34]
11	$[y + \frac{1}{4}, x + \frac{3}{4}, \frac{3}{4} - z]$	[11,35]
12	$[\frac{1}{4} - y, \frac{1}{4} - x, \frac{1}{4} - z]$	[12,36]
13	$[\frac{3}{4} - x, z + \frac{1}{4}, y + \frac{3}{4}]$	[13,37]
14	$[\frac{1}{4} - x, \frac{1}{4} - z, \frac{1}{4} - y]$	[14,38]
15	$[z + \frac{3}{4}, \frac{3}{4} - y, x + \frac{1}{4}]$	[15,39]
16	$[\frac{1}{4} - z, \frac{1}{4} - y, \frac{1}{4} - x]$	[16,40]
17	$[z, x, y]$	[17,41]
18	$[y, z, x]$	[18,42]
19	$[-y, z + \frac{1}{2}, \frac{1}{2} - x]$	[19,43]
20	$[\frac{1}{2} - z, -x, y + \frac{1}{2}]$	[20,44]
21	$[\frac{1}{2} - y, -z, x + \frac{1}{2}]$	[21,45]
22	$[z + \frac{1}{2}, \frac{1}{2} - x, -y]$	[22,46]
23	$[y + \frac{1}{2}, \frac{1}{2} - z, -x]$	[23,47]
24	$[-z, x + \frac{1}{2}, \frac{1}{2} - y]$	[24,48]