MSG No. 214.68 $I4_1321'$ [Type II, cubic]

Table 1: Wyckoff site: 8a, site symmetry: .321'

No.	position	mapping
1	$\left[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}\right]$	[1,12,14,16,17,18,49,60,62,64,65,66]
2	$\left[\frac{3}{8}, \frac{1}{8}, \frac{7}{8}\right]$	[2,7,9,15,19,24,50,55,57,63,67,72]
3	$\left[\frac{7}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[3,4,10,11,20,21,51,52,58,59,68,69]
4	$\left[\frac{1}{8}, \frac{7}{8}, \frac{3}{8}\right]$	[5,6,8,13,22,23,53,54,56,61,70,71]
5	$\left[\frac{5}{8}, \frac{5}{8}, \frac{5}{8}\right]$	[25,36,38,40,41,42,73,84,86,88,89,90]
6	$\left[\frac{7}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[26,31,33,39,43,48,74,79,81,87,91,96]
7	$\left[\frac{3}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[27,28,34,35,44,45,75,76,82,83,92,93]
8	$\left[\frac{5}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[29,30,32,37,46,47,77,78,80,85,94,95]

Table 2: Wyckoff site: 8b, site symmetry: .321'

No.	position	mapping
1	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[1,17,18,36,38,40,49,65,66,84,86,88]
2	$\left[\frac{1}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[2,7,15,33,43,48,50,55,63,81,91,96]
3	$\left[\frac{5}{8}, \frac{1}{8}, \frac{3}{8}\right]$	[3,4,11,34,44,45,51,52,59,82,92,93]
4	$\left[\frac{3}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[5,6,13,32,46,47,53,54,61,80,94,95]
5	$\left[\frac{7}{8}, \frac{1}{8}, \frac{5}{8}\right]$	[8,22,23,29,30,37,56,70,71,77,78,85]
6	$\left[\frac{5}{8}, \frac{7}{8}, \frac{1}{8}\right]$	[9,19,24,26,31,39,57,67,72,74,79,87]
7	$\left[\frac{1}{8}, \frac{5}{8}, \frac{7}{8}\right]$	[10,20,21,27,28,35,58,68,69,75,76,83]
8	$\left[\frac{3}{8}, \frac{3}{8}, \frac{3}{8}\right]$	[12,14,16,25,41,42,60,62,64,73,89,90]

Table 3: Wyckoff site: 12c, site symmetry: 2.221'

No.	position	mapping
1	$\left[\frac{1}{8}, 0, \frac{1}{4}\right]$	[1,8,13,14,49,56,61,62]
2	$\left[\frac{3}{8}, 0, \frac{3}{4}\right]$	[2,9,27,34,50,57,75,82]
3	$\left[\frac{7}{8}, \frac{1}{2}, \frac{1}{4}\right]$	[3,10,26,33,51,58,74,81]
4	$\left[0, \frac{1}{4}, \frac{1}{8}\right]$	[4,16,18,21,52,64,66,69]
5	$\left[0, \frac{3}{4}, \frac{3}{8}\right]$	[5,23,39,43,53,71,87,91]
6	$\left[\frac{1}{4}, \frac{7}{8}, \frac{1}{2}\right]$	[6,22,35,44,54,70,83,92]
7	$\left[\frac{1}{4}, \frac{1}{8}, 0\right]$	[7,12,17,24,55,60,65,72]
8	$\left[\frac{3}{4}, \frac{3}{8}, 0\right]$	[11,20,30,46,59,68,78,94]
9	$\left[\frac{1}{2}, \frac{1}{4}, \frac{7}{8}\right]$	[15,19,29,47,63,67,77,95]
10	$\left[\frac{5}{8}, \frac{1}{2}, \frac{3}{4}\right]$	[25,32,37,38,73,80,85,86]
11	$\left[\frac{1}{2}, \frac{3}{4}, \frac{5}{8}\right]$	[28,40,42,45,76,88,90,93]
12	$\left[\frac{3}{4}, \frac{5}{8}, \frac{1}{2}\right]$	[31,36,41,48,79,84,89,96]

Table 4: Wyckoff site: `12d`, site symmetry: `2.221'`

No.	position	mapping
1	$\left[\frac{5}{8}, 0, \frac{1}{4}\right]$	`[1,8,13,14,49,56,61,62]`
2	$\left[\frac{7}{8}, 0, \frac{3}{4}\right]$	`[2,9,27,34,50,57,75,82]`
3	$\left[\frac{3}{8}, \frac{1}{2}, \frac{1}{4}\right]$	`[3,10,26,33,51,58,74,81]`
4	$\left[0, \frac{1}{4}, \frac{5}{8}\right]$	`[4,16,18,21,52,64,66,69]`
5	$\left[0, \frac{3}{4}, \frac{7}{8}\right]$	`[5,23,39,43,53,71,87,91]`
6	$\left[\frac{1}{4}, \frac{3}{8}, \frac{1}{2}\right]$	`[6,22,35,44,54,70,83,92]`
7	$\left[\frac{1}{4}, \frac{5}{8}, 0\right]$	`[7,12,17,24,55,60,65,72]`
8	$\left[\frac{3}{4}, \frac{7}{8}, 0\right]$	`[11,20,30,46,59,68,78,94]`
9	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{8}\right]$	`[15,19,29,47,63,67,77,95]`
10	$\left[\frac{1}{8}, \frac{1}{2}, \frac{3}{4}\right]$	`[25,32,37,38,73,80,85,86]`
11	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{8}\right]$	`[28,40,42,45,76,88,90,93]`
12	$\left[\frac{3}{4}, \frac{1}{8}, \frac{1}{2}\right]$	`[31,36,41,48,79,84,89,96]`

Table 5: Wyckoff site: `16e`, site symmetry: `.3.1'`

No.	position	mapping
1	$[x, x, x]$	`[1,17,18,49,65,66]`
2	$\left[x + \frac{1}{4}, \frac{1}{4} - x, x + \frac{3}{4}\right]$	`[2,7,15,50,55,63]`
3	$\left[x + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{4} - x\right]$	`[3,4,11,51,52,59]`
4	$\left[\frac{1}{4} - x, x + \frac{3}{4}, x + \frac{1}{4}\right]$	`[5,6,13,53,54,61]`
5	$\left[x, -x, \frac{1}{2} - x\right]$	`[8,22,23,56,70,71]`
6	$\left[\frac{1}{2} - x, x, -x\right]$	`[9,19,24,57,67,72]`
7	$\left[-x, \frac{1}{2} - x, x\right]$	`[10,20,21,58,68,69]`
8	$\left[\frac{1}{4} - x, \frac{1}{4} - x, \frac{1}{4} - x\right]$	`[12,14,16,60,62,64]`
9	$\left[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}\right]$	`[25,41,42,73,89,90]`
10	$\left[x + \frac{3}{4}, \frac{3}{4} - x, x + \frac{1}{4}\right]$	`[26,31,39,74,79,87]`
11	$\left[x + \frac{1}{4}, x + \frac{3}{4}, \frac{3}{4} - x\right]$	`[27,28,35,75,76,83]`
12	$\left[\frac{3}{4} - x, x + \frac{1}{4}, x + \frac{3}{4}\right]$	`[29,30,37,77,78,85]`
13	$\left[x + \frac{1}{2}, \frac{1}{2} - x, -x\right]$	`[32,46,47,80,94,95]`
14	$\left[-x, x + \frac{1}{2}, \frac{1}{2} - x\right]$	`[33,43,48,81,91,96]`
15	$\left[\frac{1}{2} - x, -x, x + \frac{1}{2}\right]$	`[34,44,45,82,92,93]`
16	$\left[\frac{3}{4} - x, \frac{3}{4} - x, \frac{3}{4} - x\right]$	`[36,38,40,84,86,88]`

Table 6: Wyckoff site: `24f`, site symmetry: `2..1'`

No.	position	mapping
1	$\left[x, 0, \frac{1}{4}\right]$	`[1,8,49,56]`
2	$\left[x + \frac{1}{4}, 0, \frac{3}{4}\right]$	`[2,27,50,75]`
3	$\left[x + \frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	`[3,26,51,74]`
4	$\left[0, \frac{1}{4}, \frac{1}{4} - x\right]$	`[4,16,52,64]`
5	$\left[0, \frac{3}{4}, x + \frac{1}{4}\right]$	`[5,39,53,87]`

continued ...

Table 6

No.	position	mapping
6	$\left[\frac{1}{4},\, x+\frac{3}{4},\, \frac{1}{2}\right]$	[6,35,54,83]
7	$\left[\frac{1}{4},\, \frac{1}{4}-x,\, 0\right]$	[7,12,55,60]
8	$\left[\frac{1}{2}-x,\, 0,\, \frac{3}{4}\right]$	[9,34,57,82]
9	$\left[-x,\, \frac{1}{2},\, \frac{1}{4}\right]$	[10,33,58,81]
10	$\left[\frac{3}{4},\, x+\frac{1}{4},\, 0\right]$	[11,30,59,78]
11	$\left[\frac{1}{4}-x,\, 0,\, \frac{1}{4}\right]$	[13,14,61,62]
12	$\left[\frac{1}{2},\, \frac{1}{4},\, x+\frac{3}{4}\right]$	[15,29,63,77]
13	$\left[\frac{1}{4},\, x,\, 0\right]$	[17,24,65,72]
14	$\left[0,\, \frac{1}{4},\, x\right]$	[18,21,66,69]
15	$\left[\frac{1}{2},\, \frac{1}{4},\, -x\right]$	[19,47,67,95]
16	$\left[\frac{3}{4},\, \frac{1}{2}-x,\, 0\right]$	[20,46,68,94]
17	$\left[\frac{1}{4},\, -x,\, \frac{1}{2}\right]$	[22,44,70,92]
18	$\left[0,\, \frac{3}{4},\, \frac{1}{2}-x\right]$	[23,43,71,91]
19	$\left[x+\frac{1}{2},\, \frac{1}{2},\, \frac{3}{4}\right]$	[25,32,73,80]
20	$\left[\frac{1}{2},\, \frac{3}{4},\, \frac{3}{4}-x\right]$	[28,40,76,88]
21	$\left[\frac{3}{4},\, \frac{3}{4}-x,\, \frac{1}{2}\right]$	[31,36,79,84]
22	$\left[\frac{3}{4}-x,\, \frac{1}{2},\, \frac{3}{4}\right]$	[37,38,85,86]
23	$\left[\frac{3}{4},\, x+\frac{1}{2},\, \frac{1}{2}\right]$	[41,48,89,96]
24	$\left[\frac{1}{2},\, \frac{3}{4},\, x+\frac{1}{2}\right]$	[42,45,90,93]

Table 7: Wyckoff site: 24g, site symmetry: ..21'

No.	position	mapping
1	$\left[\frac{1}{8},\, y,\, y+\frac{1}{4}\right]$	[1,13,49,61]
2	$\left[\frac{3}{8},\, -y,\, y+\frac{3}{4}\right]$	[2,34,50,82]
3	$\left[\frac{7}{8},\, y+\frac{1}{2},\, \frac{1}{4}-y\right]$	[3,33,51,81]
4	$\left[y,\, y+\frac{1}{4},\, \frac{1}{8}\right]$	[4,18,52,66]
5	$\left[-y,\, y+\frac{3}{4},\, \frac{3}{8}\right]$	[5,43,53,91]
6	$\left[\frac{1}{4}-y,\, \frac{7}{8},\, y+\frac{1}{2}\right]$	[6,44,54,92]
7	$\left[y+\frac{1}{4},\, \frac{1}{8},\, y\right]$	[7,17,55,65]
8	$\left[\frac{1}{8},\, -y,\, \frac{1}{4}-y\right]$	[8,14,56,62]
9	$\left[\frac{3}{8},\, y,\, \frac{3}{4}-y\right]$	[9,27,57,75]
10	$\left[\frac{7}{8},\, \frac{1}{2}-y,\, y+\frac{1}{4}\right]$	[10,26,58,74]
11	$\left[y+\frac{3}{4},\, \frac{3}{8},\, -y\right]$	[11,46,59,94]
12	$\left[\frac{1}{4}-y,\, \frac{1}{8},\, -y\right]$	[12,24,60,72]
13	$\left[y+\frac{1}{2},\, \frac{1}{4}-y,\, \frac{7}{8}\right]$	[15,47,63,95]
14	$\left[-y,\, \frac{1}{4}-y,\, \frac{1}{8}\right]$	[16,21,64,69]
15	$\left[\frac{1}{2}-y,\, y+\frac{1}{4},\, \frac{7}{8}\right]$	[19,29,67,77]
16	$\left[\frac{3}{4}-y,\, \frac{3}{8},\, y\right]$	[20,30,68,78]
17	$\left[y+\frac{1}{4},\, \frac{7}{8},\, \frac{1}{2}-y\right]$	[22,35,70,83]
18	$\left[y,\, \frac{3}{4}-y,\, \frac{3}{8}\right]$	[23,39,71,87]
19	$\left[\frac{5}{8},\, y+\frac{1}{2},\, y+\frac{3}{4}\right]$	[25,37,73,85]
20	$\left[y+\frac{1}{2},\, y+\frac{3}{4},\, \frac{5}{8}\right]$	[28,42,76,90]
21	$\left[y+\frac{3}{4},\, \frac{5}{8},\, y+\frac{1}{2}\right]$	[31,41,79,89]

continued ...

Table 7

No.	position	mapping
22	$\left[\frac{5}{8}, \frac{1}{2}-y, \frac{3}{4}-y\right]$	[32,38,80,86]
23	$\left[\frac{3}{4}-y, \frac{5}{8}, \frac{1}{2}-y\right]$	[36,48,84,96]
24	$\left[\frac{1}{2}-y, \frac{3}{4}-y, \frac{5}{8}\right]$	[40,45,88,93]

Table 8: Wyckoff site: 24h, site symmetry: ..21'

No.	position	mapping
1	$\left[\frac{1}{8}, y, \frac{1}{4}-y\right]$	[1,14,49,62]
2	$\left[\frac{3}{8}, y, y+\frac{3}{4}\right]$	[2,9,50,57]
3	$\left[\frac{7}{8}, \frac{1}{2}-y, \frac{1}{4}-y\right]$	[3,10,51,58]
4	$\left[-y, y+\frac{1}{4}, \frac{1}{8}\right]$	[4,21,52,69]
5	$\left[y, y+\frac{3}{4}, \frac{3}{8}\right]$	[5,23,53,71]
6	$\left[\frac{1}{4}-y, \frac{7}{8}, \frac{1}{2}-y\right]$	[6,22,54,70]
7	$\left[y+\frac{1}{4}, \frac{1}{8}, -y\right]$	[7,24,55,72]
8	$\left[\frac{1}{8}, -y, y+\frac{1}{4}\right]$	[8,13,56,61]
9	$\left[y+\frac{3}{4}, \frac{3}{8}, y\right]$	[11,20,59,68]
10	$\left[\frac{1}{4}-y, \frac{1}{8}, y\right]$	[12,17,60,65]
11	$\left[\frac{1}{2}-y, \frac{1}{4}-y, \frac{7}{8}\right]$	[15,19,63,67]
12	$\left[y, \frac{1}{4}-y, \frac{1}{8}\right]$	[16,18,64,66]
13	$\left[\frac{5}{8}, y+\frac{1}{2}, \frac{3}{4}-y\right]$	[25,38,73,86]
14	$\left[\frac{7}{8}, y+\frac{1}{2}, y+\frac{1}{4}\right]$	[26,33,74,81]
15	$\left[\frac{3}{8}, -y, \frac{3}{4}-y\right]$	[27,34,75,82]
16	$\left[\frac{1}{2}-y, y+\frac{3}{4}, \frac{5}{8}\right]$	[28,45,76,93]
17	$\left[y+\frac{1}{2}, y+\frac{1}{4}, \frac{7}{8}\right]$	[29,47,77,95]
18	$\left[\frac{3}{4}-y, \frac{3}{8}, -y\right]$	[30,46,78,94]
19	$\left[y+\frac{3}{4}, \frac{5}{8}, \frac{1}{2}-y\right]$	[31,48,79,96]
20	$\left[\frac{5}{8}, \frac{1}{2}-y, y+\frac{3}{4}\right]$	[32,37,80,85]
21	$\left[y+\frac{1}{4}, \frac{7}{8}, y+\frac{1}{2}\right]$	[35,44,83,92]
22	$\left[\frac{3}{4}-y, \frac{5}{8}, y+\frac{1}{2}\right]$	[36,41,84,89]
23	$\left[-y, \frac{3}{4}-y, \frac{3}{8}\right]$	[39,43,87,91]
24	$\left[y+\frac{1}{2}, \frac{3}{4}-y, \frac{5}{8}\right]$	[40,42,88,90]

Table 9: Wyckoff site: 48i, site symmetry: 11'

No.	position	mapping
1	$[x, y, z]$	[1,49]
2	$\left[x+\frac{1}{4}, \frac{1}{4}-z, y+\frac{3}{4}\right]$	[2,50]
3	$\left[x+\frac{3}{4}, z+\frac{1}{4}, \frac{1}{4}-y\right]$	[3,51]
4	$\left[z+\frac{3}{4}, y+\frac{1}{4}, \frac{1}{4}-x\right]$	[4,52]
5	$\left[\frac{1}{4}-z, y+\frac{3}{4}, x+\frac{1}{4}\right]$	[5,53]
6	$\left[\frac{1}{4}-y, x+\frac{3}{4}, z+\frac{1}{4}\right]$	[6,54]
7	$\left[y+\frac{1}{4}, \frac{1}{4}-x, z+\frac{3}{4}\right]$	[7,55]

continued ...

Table 9

No.	position	mapping
8	$\left[x,\, -y,\, \frac{1}{2}-z\right]$	[8,56]
9	$\left[\frac{1}{2}-x,\, y,\, -z\right]$	[9,57]
10	$\left[-x,\, \frac{1}{2}-y,\, z\right]$	[10,58]
11	$\left[y+\frac{3}{4},\, x+\frac{1}{4},\, \frac{1}{4}-z\right]$	[11,59]
12	$\left[\frac{1}{4}-y,\, \frac{1}{4}-x,\, \frac{1}{4}-z\right]$	[12,60]
13	$\left[\frac{1}{4}-x,\, z+\frac{3}{4},\, y+\frac{1}{4}\right]$	[13,61]
14	$\left[\frac{1}{4}-x,\, \frac{1}{4}-z,\, \frac{1}{4}-y\right]$	[14,62]
15	$\left[z+\frac{1}{4},\, \frac{1}{4}-y,\, x+\frac{3}{4}\right]$	[15,63]
16	$\left[\frac{1}{4}-z,\, \frac{1}{4}-y,\, \frac{1}{4}-x\right]$	[16,64]
17	$[z,\, x,\, y]$	[17,65]
18	$[y,\, z,\, x]$	[18,66]
19	$\left[\frac{1}{2}-y,\, z,\, -x\right]$	[19,67]
20	$\left[-z,\, \frac{1}{2}-x,\, y\right]$	[20,68]
21	$\left[-y,\, \frac{1}{2}-z,\, x\right]$	[21,69]
22	$\left[z,\, -x,\, \frac{1}{2}-y\right]$	[22,70]
23	$\left[y,\, -z,\, \frac{1}{2}-x\right]$	[23,71]
24	$\left[\frac{1}{2}-z,\, x,\, -y\right]$	[24,72]
25	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[25,73]
26	$\left[x+\frac{3}{4},\, \frac{3}{4}-z,\, y+\frac{1}{4}\right]$	[26,74]
27	$\left[x+\frac{1}{4},\, z+\frac{3}{4},\, \frac{3}{4}-y\right]$	[27,75]
28	$\left[z+\frac{1}{4},\, y+\frac{3}{4},\, \frac{3}{4}-x\right]$	[28,76]
29	$\left[\frac{3}{4}-z,\, y+\frac{1}{4},\, x+\frac{3}{4}\right]$	[29,77]
30	$\left[\frac{3}{4}-y,\, x+\frac{1}{4},\, z+\frac{3}{4}\right]$	[30,78]
31	$\left[y+\frac{3}{4},\, \frac{3}{4}-x,\, z+\frac{1}{4}\right]$	[31,79]
32	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$	[32,80]
33	$\left[-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[33,81]
34	$\left[\frac{1}{2}-x,\, -y,\, z+\frac{1}{2}\right]$	[34,82]
35	$\left[y+\frac{1}{4},\, x+\frac{3}{4},\, \frac{3}{4}-z\right]$	[35,83]
36	$\left[\frac{3}{4}-y,\, \frac{3}{4}-x,\, \frac{3}{4}-z\right]$	[36,84]
37	$\left[\frac{3}{4}-x,\, z+\frac{1}{4},\, y+\frac{3}{4}\right]$	[37,85]
38	$\left[\frac{3}{4}-x,\, \frac{3}{4}-z,\, \frac{3}{4}-y\right]$	[38,86]
39	$\left[z+\frac{3}{4},\, \frac{3}{4}-y,\, x+\frac{1}{4}\right]$	[39,87]
40	$\left[\frac{3}{4}-z,\, \frac{3}{4}-y,\, \frac{3}{4}-x\right]$	[40,88]
41	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$	[41,89]
42	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[42,90]
43	$\left[-y,\, z+\frac{1}{2},\, \frac{1}{2}-x\right]$	[43,91]
44	$\left[\frac{1}{2}-z,\, -x,\, y+\frac{1}{2}\right]$	[44,92]
45	$\left[\frac{1}{2}-y,\, -z,\, x+\frac{1}{2}\right]$	[45,93]
46	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, -y\right]$	[46,94]
47	$\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, -x\right]$	[47,95]
48	$\left[-z,\, x+\frac{1}{2},\, \frac{1}{2}-y\right]$	[48,96]