MSG No. 222.99 $Pn\bar{3}n1'$ [Type II, cubic]

Table 1: Wyckoff site: 2a, site symmetry: 4321'

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

Table 2: Wyckoff site: 6b, site symmetry: 42.21'

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

Table 3: Wyckoff site: 8c, site symmetry: .-3'.1'

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

Table 4: Wyckoff site: 12d, site symmetry: -4..1'

No.	position	mapping
1	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	[1,8,26,27,49,56,74,75]
2	$\left[0, \frac{1}{4}, \frac{3}{4}\right]$	[2,3,25,32,50,51,73,80]
3	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[4,16,43,47,52,64,91,95]
4	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[5,15,42,45,53,63,90,93]
5	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	[6,11,41,48,54,59,89,96]
6	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[7,12,44,46,55,60,92,94]
7	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	[9,10,37,38,57,58,85,86]

continued …

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Table 4

No.	position	mapping
8	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[13,14,33,34,61,62,81,82]
9	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	[17,24,30,35,65,72,78,83]
10	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[18,21,29,39,66,69,77,87]
11	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[19,23,28,40,67,71,76,88]
12	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[20,22,31,36,68,70,79,84]

Table 5: Wyckoff site: 12e, site symmetry: 4..1'

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

Table 6: Wyckoff site: 16f, site symmetry: .3.1'

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

Table 7: Wyckoff site: `24g`, site symmetry: `2..1'`

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

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

No.	position	mapping
1	$\left[\frac{1}{4}, y, y\right]$	[1,13,49,61]
2	$\left[\frac{1}{4}, \frac{1}{2} - y, y\right]$	[2,10,50,58]
3	$\left[\frac{1}{4}, y, \frac{1}{2} - y\right]$	[3,9,51,57]
4	$\left[y, y, \frac{1}{4}\right]$	[4,18,52,66]
5	$\left[\frac{1}{2} - y, y, \frac{1}{4}\right]$	[5,19,53,67]
6	$\left[\frac{1}{2} - y, \frac{1}{4}, y\right]$	[6,20,54,68]
7	$\left[y, \frac{1}{4}, y\right]$	[7,17,55,65]
8	$\left[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{2} - y\right]$	[8,14,56,62]
9	$\left[y, \frac{1}{4}, \frac{1}{2} - y\right]$	[11,22,59,70]
10	$\left[\frac{1}{2} - y, \frac{1}{4}, \frac{1}{2} - y\right]$	[12,24,60,72]
11	$\left[y, \frac{1}{2} - y, \frac{1}{4}\right]$	[15,23,63,71]
12	$\left[\frac{1}{2} - y, \frac{1}{2} - y, \frac{1}{4}\right]$	[16,21,64,69]
13	$\left[\frac{3}{4}, -y, -y\right]$	[25,37,73,85]
14	$\left[\frac{3}{4}, y + \frac{1}{2}, -y\right]$	[26,34,74,82]
15	$\left[\frac{3}{4}, -y, y + \frac{1}{2}\right]$	[27,33,75,81]

continued ...

Table 8

No.	position	mapping
16	$\left[-y, -y, \frac{3}{4}\right]$	[28,42,76,90]
17	$\left[y+\frac{1}{2}, -y, \frac{3}{4}\right]$	[29,43,77,91]
18	$\left[y+\frac{1}{2}, \frac{3}{4}, -y\right]$	[30,44,78,92]
19	$\left[-y, \frac{3}{4}, -y\right]$	[31,41,79,89]
20	$\left[\frac{3}{4}, y+\frac{1}{2}, y+\frac{1}{2}\right]$	[32,38,80,86]
21	$\left[-y, \frac{3}{4}, y+\frac{1}{2}\right]$	[35,46,83,94]
22	$\left[y+\frac{1}{2}, \frac{3}{4}, y+\frac{1}{2}\right]$	[36,48,84,96]
23	$\left[-y, y+\frac{1}{2}, \frac{3}{4}\right]$	[39,47,87,95]
24	$\left[y+\frac{1}{2}, y+\frac{1}{2}, \frac{3}{4}\right]$	[40,45,88,93]

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

No.	position	mapping
1	$[x, y, z]$	[1,49]
2	$\left[x, \frac{1}{2}-z, y\right]$	[2,50]
3	$\left[x, z, \frac{1}{2}-y\right]$	[3,51]
4	$\left[z, y, \frac{1}{2}-x\right]$	[4,52]
5	$\left[\frac{1}{2}-z, y, x\right]$	[5,53]
6	$\left[\frac{1}{2}-y, x, z\right]$	[6,54]
7	$\left[y, \frac{1}{2}-x, z\right]$	[7,55]
8	$\left[x, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[8,56]
9	$\left[\frac{1}{2}-x, y, \frac{1}{2}-z\right]$	[9,57]
10	$\left[\frac{1}{2}-x, \frac{1}{2}-y, z\right]$	[10,58]
11	$\left[y, x, \frac{1}{2}-z\right]$	[11,59]
12	$\left[\frac{1}{2}-y, \frac{1}{2}-x, \frac{1}{2}-z\right]$	[12,60]
13	$\left[\frac{1}{2}-x, z, y\right]$	[13,61]
14	$\left[\frac{1}{2}-x, \frac{1}{2}-z, \frac{1}{2}-y\right]$	[14,62]
15	$\left[z, \frac{1}{2}-y, x\right]$	[15,63]
16	$\left[\frac{1}{2}-z, \frac{1}{2}-y, \frac{1}{2}-x\right]$	[16,64]
17	$[z, x, y]$	[17,65]
18	$[y, z, x]$	[18,66]
19	$\left[\frac{1}{2}-y, z, \frac{1}{2}-x\right]$	[19,67]
20	$\left[\frac{1}{2}-z, \frac{1}{2}-x, y\right]$	[20,68]
21	$\left[\frac{1}{2}-y, \frac{1}{2}-z, x\right]$	[21,69]
22	$\left[z, \frac{1}{2}-x, \frac{1}{2}-y\right]$	[22,70]
23	$\left[y, \frac{1}{2}-z, \frac{1}{2}-x\right]$	[23,71]
24	$\left[\frac{1}{2}-z, x, \frac{1}{2}-y\right]$	[24,72]
25	$[-x, -y, -z]$	[25,73]
26	$\left[-x, z+\frac{1}{2}, -y\right]$	[26,74]
27	$\left[-x, -z, y+\frac{1}{2}\right]$	[27,75]
28	$\left[-z, -y, x+\frac{1}{2}\right]$	[28,76]
29	$\left[z+\frac{1}{2}, -y, -x\right]$	[29,77]
30	$\left[y+\frac{1}{2}, -x, -z\right]$	[30,78]
31	$\left[-y, x+\frac{1}{2}, -z\right]$	[31,79]

Table 9

No.	position	mapping
32	$\left[-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[32,80]
33	$\left[x+\frac{1}{2},\, -y,\, z+\frac{1}{2}\right]$	[33,81]
34	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, -z\right]$	[34,82]
35	$\left[-y,\, -x,\, z+\frac{1}{2}\right]$	[35,83]
36	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[36,84]
37	$\left[x+\frac{1}{2},\, -z,\, -y\right]$	[37,85]
38	$\left[x+\frac{1}{2},\, z+\frac{1}{2},\, y+\frac{1}{2}\right]$	[38,86]
39	$\left[-z,\, y+\frac{1}{2},\, -x\right]$	[39,87]
40	$\left[z+\frac{1}{2},\, y+\frac{1}{2},\, x+\frac{1}{2}\right]$	[40,88]
41	$\left[-z,\, -x,\, -y\right]$	[41,89]
42	$\left[-y,\, -z,\, -x\right]$	[42,90]
43	$\left[y+\frac{1}{2},\, -z,\, x+\frac{1}{2}\right]$	[43,91]
44	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, -y\right]$	[44,92]
45	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, -x\right]$	[45,93]
46	$\left[-z,\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$	[46,94]
47	$\left[-y,\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[47,95]
48	$\left[z+\frac{1}{2},\, -x,\, y+\frac{1}{2}\right]$	[48,96]