MSG No. 201.19 $Pn\bar{3}1'$ [Type II, cubic]

Table 1: Wyckoff site: 2a, site symmetry: 23.1'

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

Table 2: Wyckoff site: 4b, site symmetry: .-3'.1'

No.	position	mapping
1	$[0, 0, 0]$	[1,5,6,13,17,18,25,29,30,37,41,42]
2	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[2,10,11,14,22,23,26,34,35,38,46,47]
3	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[3,7,12,15,19,24,27,31,36,39,43,48]
4	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[4,8,9,16,20,21,28,32,33,40,44,45]

Table 3: Wyckoff site: 4c, site symmetry: .-3'.1'

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[1,5,6,13,17,18,25,29,30,37,41,42]
2	$\left[\frac{1}{2}, 0, 0\right]$	[2,10,11,14,22,23,26,34,35,38,46,47]
3	$\left[0, \frac{1}{2}, 0\right]$	[3,7,12,15,19,24,27,31,36,39,43,48]
4	$\left[0, 0, \frac{1}{2}\right]$	[4,8,9,16,20,21,28,32,33,40,44,45]

Table 4: Wyckoff site: 6d, site symmetry: 222..1'

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

Table 5: Wyckoff site: 8e, site symmetry: .3.1'

No.	position	mapping
1	$[x, x, x]$	[1,5,6,25,29,30]
2	$\left[x, \frac{1}{2}-x, \frac{1}{2}-x\right]$	[2,10,11,26,34,35]

continued ...

Table 5

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

Table 6: Wyckoff site: 12f, site symmetry: 2..1'

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

Table 7: Wyckoff site: 12g, site symmetry: 2..1'

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

Table 8: Wyckoff site: 24h, site symmetry: 11'

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