MSG No. 197.8 $I231'$ [Type II, cubic]

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

No.	position	mapping
1	$[0,\ 0,\ 0]$	[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	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	[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: 6b, site symmetry: 222..1'

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

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

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

Table 4: Wyckoff site: 12d, site symmetry: 2..1'

No.	position	mapping
1	$[x,\ 0,\ 0]$	[1,2,25,26]
2	$[-x,\ 0,\ 0]$	[3,4,27,28]
3	$[0,\ x,\ 0]$	[5,12,29,36]
4	$[0,\ 0,\ x]$	[6,9,30,33]
5	$[0,\ 0,\ -x]$	[7,11,31,35]
6	$[0,\ -x,\ 0]$	[8,10,32,34]
7	$\left[x+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	[13,14,37,38]
8	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	[15,16,39,40]
9	$\left[\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}\right]$	[17,24,41,48]

continued ...

Table 4

No.	position	mapping
10	$\left[\frac{1}{2}, \frac{1}{2}, x+\frac{1}{2}\right]$	`[18,21,42,45]`
11	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}-x\right]$	`[19,23,43,47]`
12	$\left[\frac{1}{2}, \frac{1}{2}-x, \frac{1}{2}\right]$	`[20,22,44,46]`

Table 5: Wyckoff site: `12e`, site symmetry: `2..1'`

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

Table 6: Wyckoff site: `24f`, site symmetry: `11'`

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

continued ...

Table 6

No.	position	mapping
20	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ y+\frac{1}{2}\right]$	[20,44]
21	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ x+\frac{1}{2}\right]$	[21,45]
22	$\left[z+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-y\right]$	[22,46]
23	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[23,47]
24	$\left[\frac{1}{2}-z,\ x+\frac{1}{2},\ \frac{1}{2}-y\right]$	[24,48]