MSG No. 208.45 $P4_232'$ [Type II, cubic]

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: .321'

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

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

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

Table 5: Wyckoff site: 6e, site symmetry: 2.221'

No.	position	mapping
1	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	[1,8,13,14,25,32,37,38]
2	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	[2,3,9,10,26,27,33,34]

continued ...

Table 5

No.	position	mapping
3	$\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$	[4,16,18,21,28,40,42,45]
4	$\left[0,\ \frac{1}{2},\ \frac{3}{4}\right]$	[5,15,19,23,29,39,43,47]
5	$\left[\frac{1}{2},\ \frac{3}{4},\ 0\right]$	[6,11,20,22,30,35,44,46]
6	$\left[\frac{1}{2},\ \frac{1}{4},\ 0\right]$	[7,12,17,24,31,36,41,48]

Table 6: Wyckoff site: 6f, site symmetry: 2.221'

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

Table 7: Wyckoff site: 8g, site symmetry: .3.1'

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

Table 8: Wyckoff site: 12h, site symmetry: 2..1'

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

continued ...

Table 8

No.	position	mapping
10	$[0,\ 0,\ x]$	`[18,21,42,45]`
11	$[0,\ 0,\ -x]$	`[19,23,43,47]`
12	$[0,\ -x,\ 0]$	`[20,22,44,46]`

Table 9: Wyckoff site: `12i`, site symmetry: `2..1'`

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

Table 10: Wyckoff site: `12j`, site symmetry: `2..1'`

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

Table 11: Wyckoff site: `12k`, site symmetry: `..21'`

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

Table 12: Wyckoff site: `12l`, site symmetry: `..21'`

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

Table 13: Wyckoff site: `24m`, site symmetry: `11'`

No.	position	mapping
1	$[x,\ y,\ z]$	`[1,25]`
2	$\left[x+\frac{1}{2},\ \frac{1}{2}-z,\ y+\frac{1}{2}\right]$	`[2,26]`
3	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ \frac{1}{2}-y\right]$	`[3,27]`
4	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-x\right]$	`[4,28]`
5	$\left[\frac{1}{2}-z,\ y+\frac{1}{2},\ x+\frac{1}{2}\right]$	`[5,29]`
6	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	`[6,30]`
7	$\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	`[7,31]`
8	$[x,\ -y,\ -z]$	`[8,32]`
9	$[-x,\ y,\ -z]$	`[9,33]`

continued ...

Table 13

No.	position	mapping
10	$[-x, -y, z]$	[10,34]
11	$\left[y+\frac{1}{2}, x+\frac{1}{2}, \frac{1}{2}-z\right]$	[11,35]
12	$\left[\frac{1}{2}-y, \frac{1}{2}-x, \frac{1}{2}-z\right]$	[12,36]
13	$\left[\frac{1}{2}-x, z+\frac{1}{2}, y+\frac{1}{2}\right]$	[13,37]
14	$\left[\frac{1}{2}-x, \frac{1}{2}-z, \frac{1}{2}-y\right]$	[14,38]
15	$\left[z+\frac{1}{2}, \frac{1}{2}-y, x+\frac{1}{2}\right]$	[15,39]
16	$\left[\frac{1}{2}-z, \frac{1}{2}-y, \frac{1}{2}-x\right]$	[16,40]
17	$[z, x, y]$	[17,41]
18	$[y, z, x]$	[18,42]
19	$[-y, z, -x]$	[19,43]
20	$[-z, -x, y]$	[20,44]
21	$[-y, -z, x]$	[21,45]
22	$[z, -x, -y]$	[22,46]
23	$[y, -z, -x]$	[23,47]
24	$[-z, x, -y]$	[24,48]