MSG No. 207.41 $P4321'$ [Type II, cubic]

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

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

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

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

Table 3: Wyckoff site: 3c, site symmetry: 42.21'

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

Table 4: Wyckoff site: 3d, site symmetry: 42.21'

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

Table 5: Wyckoff site: 6e, site symmetry: 4..1'

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

Table 6: Wyckoff site: `6f`, site symmetry: `4..1'`

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

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

No.	position	mapping
1	$[x, x, x]$	`[1,17,18,25,41,42]`
2	$[x, -x, x]$	`[2,7,15,26,31,39]`
3	$[x, x, -x]$	`[3,4,11,27,28,35]`
4	$[-x, x, x]$	`[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	$[-x, -x, -x]$	`[12,14,16,36,38,40]`

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

No.	position	mapping
1	$\left[x, \frac{1}{2}, 0\right]$	`[1,8,25,32]`
2	$\left[x, 0, \frac{1}{2}\right]$	`[2,3,26,27]`
3	$\left[0, \frac{1}{2}, -x\right]$	`[4,16,28,40]`
4	$\left[0, \frac{1}{2}, x\right]$	`[5,15,29,39]`
5	$\left[\frac{1}{2}, x, 0\right]$	`[6,11,30,35]`
6	$\left[\frac{1}{2}, -x, 0\right]$	`[7,12,31,36]`
7	$\left[-x, \frac{1}{2}, 0\right]$	`[9,10,33,34]`
8	$\left[-x, 0, \frac{1}{2}\right]$	`[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 9: Wyckoff site: `12i`, site symmetry: `..21'`

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

Table 10: Wyckoff site: `12j`, site symmetry: `..21'`

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

Table 11: Wyckoff site: `24k`, site symmetry: `11'`

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

continued ...

Table 11

No.	position	mapping
10	$[-x, -y, z]$	[10,34]
11	$[y, x, -z]$	[11,35]
12	$[-y, -x, -z]$	[12,36]
13	$[-x, z, y]$	[13,37]
14	$[-x, -z, -y]$	[14,38]
15	$[z, -y, x]$	[15,39]
16	$[-z, -y, -x]$	[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]