MSG No. 129.412 $P4/nmm1'$ [Type II, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: -4m21'

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[1,6,7,8,10,11,12,13,17,22,23,24,26,27,28,29]
2	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[2,3,4,5,9,14,15,16,18,19,20,21,25,30,31,32]

Table 2: Wyckoff site: 2b, site symmetry: -4m21'

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[1,6,7,8,10,11,12,13,17,22,23,24,26,27,28,29]
2	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[2,3,4,5,9,14,15,16,18,19,20,21,25,30,31,32]

Table 3: Wyckoff site: 2c, site symmetry: 4mm1'

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, z\right]$	[1,2,3,6,12,13,15,16,17,18,19,22,28,29,31,32]
2	$\left[\frac{3}{4}, \frac{3}{4}, -z\right]$	[4,5,7,8,9,10,11,14,20,21,23,24,25,26,27,30]

Table 4: Wyckoff site: 4d, site symmetry: ..2/m1'

No.	position	mapping
1	$[0, 0, 0]$	[1,8,9,16,17,24,25,32]
2	$\left[\frac{1}{2}, 0, 0\right]$	[2,4,10,12,18,20,26,28]
3	$\left[0, \frac{1}{2}, 0\right]$	[3,5,11,13,19,21,27,29]
4	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[6,7,14,15,22,23,30,31]

Table 5: Wyckoff site: 4e, site symmetry: ..2/m1'

No.	position	mapping
1	$\left[0, 0, \frac{1}{2}\right]$	[1,8,9,16,17,24,25,32]
2	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[2,4,10,12,18,20,26,28]
3	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[3,5,11,13,19,21,27,29]
4	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[6,7,14,15,22,23,30,31]

Table 6: Wyckoff site: `4f`, site symmetry: `2mm.1'`

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, z\right]$	[1,6,12,13,17,22,28,29]
2	$\left[\frac{1}{4}, \frac{3}{4}, z\right]$	[2,3,15,16,18,19,31,32]
3	$\left[\frac{1}{4}, \frac{3}{4}, -z\right]$	[4,5,9,14,20,21,25,30]
4	$\left[\frac{3}{4}, \frac{1}{4}, -z\right]$	[7,8,10,11,23,24,26,27]

Table 7: Wyckoff site: `8g`, site symmetry: `..21'`

No.	position	mapping
1	$[x, -x, 0]$	[1,8,17,24]
2	$\left[x+\frac{1}{2}, x, 0\right]$	[2,4,18,20]
3	$\left[-x, \frac{1}{2}-x, 0\right]$	[3,5,19,21]
4	$\left[\frac{1}{2}-x, x+\frac{1}{2}, 0\right]$	[6,7,22,23]
5	$[-x, x, 0]$	[9,16,25,32]
6	$\left[\frac{1}{2}-x, -x, 0\right]$	[10,12,26,28]
7	$\left[x, x+\frac{1}{2}, 0\right]$	[11,13,27,29]
8	$\left[x+\frac{1}{2}, \frac{1}{2}-x, 0\right]$	[14,15,30,31]

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

No.	position	mapping
1	$\left[x, -x, \frac{1}{2}\right]$	[1,8,17,24]
2	$\left[x+\frac{1}{2}, x, \frac{1}{2}\right]$	[2,4,18,20]
3	$\left[-x, \frac{1}{2}-x, \frac{1}{2}\right]$	[3,5,19,21]
4	$\left[\frac{1}{2}-x, x+\frac{1}{2}, \frac{1}{2}\right]$	[6,7,22,23]
5	$\left[-x, x, \frac{1}{2}\right]$	[9,16,25,32]
6	$\left[\frac{1}{2}-x, -x, \frac{1}{2}\right]$	[10,12,26,28]
7	$\left[x, x+\frac{1}{2}, \frac{1}{2}\right]$	[11,13,27,29]
8	$\left[x+\frac{1}{2}, \frac{1}{2}-x, \frac{1}{2}\right]$	[14,15,30,31]

Table 9: Wyckoff site: `8i`, site symmetry: `.m.1'`

No.	position	mapping
1	$\left[\frac{1}{4}, y, z\right]$	[1,12,17,28]
2	$\left[\frac{1}{2}-y, \frac{1}{4}, z\right]$	[2,15,18,31]
3	$\left[y, \frac{1}{4}, z\right]$	[3,16,19,32]
4	$\left[\frac{3}{4}, -y, -z\right]$	[4,9,20,25]
5	$\left[\frac{3}{4}, y+\frac{1}{2}, -z\right]$	[5,14,21,30]
6	$\left[\frac{1}{4}, \frac{1}{2}-y, z\right]$	[6,13,22,29]
7	$\left[y+\frac{1}{2}, \frac{3}{4}, -z\right]$	[7,10,23,26]

continued ...

Table 9

No.	position	mapping
8	$\left[-y, \frac{3}{4}, -z\right]$	[8,11,24,27]

Table 10: Wyckoff site: 8j, site symmetry: ..m1'

No.	position	mapping
1	$[x, x, z]$	[1,16,17,32]
2	$\left[\frac{1}{2} - x, x, z\right]$	[2,12,18,28]
3	$\left[x, \frac{1}{2} - x, z\right]$	[3,13,19,29]
4	$\left[x + \frac{1}{2}, -x, -z\right]$	[4,10,20,26]
5	$\left[-x, x + \frac{1}{2}, -z\right]$	[5,11,21,27]
6	$\left[\frac{1}{2} - x, \frac{1}{2} - x, z\right]$	[6,15,22,31]
7	$\left[x + \frac{1}{2}, x + \frac{1}{2}, -z\right]$	[7,14,23,30]
8	$[-x, -x, -z]$	[8,9,24,25]

Table 11: Wyckoff site: 16k, site symmetry: 11'

No.	position	mapping
1	$[x, y, z]$	[1,17]
2	$\left[\frac{1}{2} - y, x, z\right]$	[2,18]
3	$\left[y, \frac{1}{2} - x, z\right]$	[3,19]
4	$\left[x + \frac{1}{2}, -y, -z\right]$	[4,20]
5	$\left[-x, y + \frac{1}{2}, -z\right]$	[5,21]
6	$\left[\frac{1}{2} - x, \frac{1}{2} - y, z\right]$	[6,22]
7	$\left[y + \frac{1}{2}, x + \frac{1}{2}, -z\right]$	[7,23]
8	$[-y, -x, -z]$	[8,24]
9	$[-x, -y, -z]$	[9,25]
10	$\left[y + \frac{1}{2}, -x, -z\right]$	[10,26]
11	$\left[-y, x + \frac{1}{2}, -z\right]$	[11,27]
12	$\left[\frac{1}{2} - x, y, z\right]$	[12,28]
13	$\left[x, \frac{1}{2} - y, z\right]$	[13,29]
14	$\left[x + \frac{1}{2}, y + \frac{1}{2}, -z\right]$	[14,30]
15	$\left[\frac{1}{2} - y, \frac{1}{2} - x, z\right]$	[15,31]
16	$[y, x, z]$	[16,32]