MSG No. 138.520 $P4_2/ncm1'$ [Type II, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `2.221'`

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `..2/m1'`

No.	position	mapping
1	$\left[0, 0, \frac{1}{2}\right]$	`[1,8,9,16,17,24,25,32]`
2	$\left[\frac{1}{2}, 0, 0\right]$	`[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	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[6,7,14,15,22,23,30,31]`

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	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[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	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[6,7,14,15,22,23,30,31]`

Table 5: Wyckoff site: `4e`, site symmetry: `2.mm1'`

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, z\right]$	`[1,6,15,16,17,22,31,32]`
2	$\left[\frac{1}{4}, \frac{1}{4}, z+\frac{1}{2}\right]$	`[2,3,12,13,18,19,28,29]`

continued ...

Table 5

No.	position	mapping
3	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z\right]$	[4,5,10,11,20,21,26,27]
4	$\left[\frac{3}{4}, \frac{3}{4}, -z\right]$	[7,8,9,14,23,24,25,30]

Table 6: Wyckoff site: 8f, site symmetry: 2..1'

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

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

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

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

No.	position	mapping
1	$[x, -x, 0]$	[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	$\left[\frac{1}{2} - x, x + \frac{1}{2}, 0\right]$	[6,7,22,23]
5	$[-x, x, 0]$	[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	$\left[x + \frac{1}{2}, \frac{1}{2} - x, 0\right]$	[14,15,30,31]

Table 9: Wyckoff site: `8i`, site symmetry: `..m1'`

No.	position	mapping
1	$[x,\ x,\ z]$	`[1,16,17,32]`
2	$\left[\frac{1}{2}-x,\ x,\ z+\frac{1}{2}\right]$	`[2,12,18,28]`
3	$\left[x,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	`[3,13,19,29]`
4	$\left[x+\frac{1}{2},\ -x,\ \frac{1}{2}-z\right]$	`[4,10,20,26]`
5	$\left[-x,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	`[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 10: Wyckoff site: `16j`, site symmetry: `11'`

No.	position	mapping
1	$[x,\ y,\ z]$	`[1,17]`
2	$\left[\frac{1}{2}-y,\ x,\ z+\frac{1}{2}\right]$	`[2,18]`
3	$\left[y,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	`[3,19]`
4	$\left[x+\frac{1}{2},\ -y,\ \frac{1}{2}-z\right]$	`[4,20]`
5	$\left[-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	`[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	$\left[y+\frac{1}{2},\ -x,\ \frac{1}{2}-z\right]$	`[10,26]`
11	$\left[-y,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	`[11,27]`
12	$\left[\frac{1}{2}-x,\ y,\ z+\frac{1}{2}\right]$	`[12,28]`
13	$\left[x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	`[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]`