MSG No. 130.424 $P4/ncc1'$ [Type II, tetragonal]

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

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `4..1'`

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

Table 4: Wyckoff site: `8d`, site symmetry: `-11'`

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

Table 5: Wyckoff site: `8e`, site symmetry: `2..1'`

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

Table 6: Wyckoff site: `8f`, site symmetry: `..21'`

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

Table 7: Wyckoff site: `16g`, 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	$\left[x + \frac{1}{2}, -y, \frac{1}{2} - z\right]$	`[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	$\left[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z\right]$	`[7,23]`
8	$\left[-y, -x, \frac{1}{2} - z\right]$	`[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	$\left[\frac{1}{2} - x, y, z + \frac{1}{2}\right]$	`[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	$\left[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}\right]$	`[15,31]`
16	$\left[y, x, z + \frac{1}{2}\right]$	`[16,32]`