MSG No. 130.431 $P4/n'c'c'$ [Type III, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `2.22`

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[1,6,7,8]`
2	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[2,3,4,5]`
3	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[9,14,15,16]`
4	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[10,11,12,13]`

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

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	`[1,6,10,11]`
2	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	`[2,3,9,14]`
3	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	`[4,5,15,16]`
4	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	`[7,8,12,13]`

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

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, z\right]$	`[1,2,3,6]`
2	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z\right]$	`[4,5,7,8]`
3	$\left[\frac{3}{4}, \frac{3}{4}, -z\right]$	`[9,10,11,14]`
4	$\left[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}\right]$	`[12,13,15,16]`

Table 4: Wyckoff site: `8d`, site symmetry: `-1'`

No.	position	mapping
1	$[0, 0, 0]$	`[1,9]`
2	$\left[\frac{1}{2}, 0, 0\right]$	`[2,10]`
3	$\left[0, \frac{1}{2}, 0\right]$	`[3,11]`
4	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[4,12]`
5	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[5,13]`
6	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[6,14]`
7	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[7,15]`
8	$\left[0, 0, \frac{1}{2}\right]$	`[8,16]`

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

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, z\right]$	`[1,6]`
2	$\left[\frac{1}{4}, \frac{3}{4}, z\right]$	`[2,3]`
3	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - z\right]$	`[4,5]`
4	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z\right]$	`[7,8]`
5	$\left[\frac{1}{4}, \frac{3}{4}, -z\right]$	`[9,14]`
6	$\left[\frac{3}{4}, \frac{1}{4}, -z\right]$	`[10,11]`
7	$\left[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}\right]$	`[12,13]`
8	$\left[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}\right]$	`[15,16]`

Table 6: Wyckoff site: `8f`, site symmetry: `..2`

No.	position	mapping
1	$\left[x, -x, \frac{1}{4}\right]$	`[1,8]`
2	$\left[x + \frac{1}{2}, x, \frac{1}{4}\right]$	`[2,4]`
3	$\left[-x, \frac{1}{2} - x, \frac{1}{4}\right]$	`[3,5]`
4	$\left[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{4}\right]$	`[6,7]`
5	$\left[-x, x, \frac{3}{4}\right]$	`[9,16]`
6	$\left[\frac{1}{2} - x, -x, \frac{3}{4}\right]$	`[10,12]`
7	$\left[x, x + \frac{1}{2}, \frac{3}{4}\right]$	`[11,13]`
8	$\left[x + \frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}\right]$	`[14,15]`

Table 7: Wyckoff site: `16g`, site symmetry: `1`

No.	position	mapping
1	$[x, y, z]$	`[1]`
2	$\left[\frac{1}{2} - y, x, z\right]$	`[2]`
3	$\left[y, \frac{1}{2} - x, z\right]$	`[3]`
4	$\left[x + \frac{1}{2}, -y, \frac{1}{2} - z\right]$	`[4]`
5	$\left[-x, y + \frac{1}{2}, \frac{1}{2} - z\right]$	`[5]`
6	$\left[\frac{1}{2} - x, \frac{1}{2} - y, z\right]$	`[6]`
7	$\left[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z\right]$	`[7]`
8	$\left[-y, -x, \frac{1}{2} - z\right]$	`[8]`
9	$[-x, -y, -z]$	`[9]`
10	$\left[y + \frac{1}{2}, -x, -z\right]$	`[10]`
11	$\left[-y, x + \frac{1}{2}, -z\right]$	`[11]`
12	$\left[\frac{1}{2} - x, y, z + \frac{1}{2}\right]$	`[12]`
13	$\left[x, \frac{1}{2} - y, z + \frac{1}{2}\right]$	`[13]`
14	$\left[x + \frac{1}{2}, y + \frac{1}{2}, -z\right]$	`[14]`
15	$\left[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}\right]$	`[15]`
16	$\left[y, x, z + \frac{1}{2}\right]$	`[16]`