MSG No. 86.73 P_C4_2/n [Type IV, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `2/m'..`

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[1,4,14,15]`
2	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[2,3,13,16]`

continued ...

Table 5

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

Table 6: Wyckoff site: `4f`, site symmetry: `-4..`

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

Table 7: Wyckoff site: `8g`, site symmetry: `2..`

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

Table 8: Wyckoff site: `8h`, site symmetry: `2..`

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

Table 9: Wyckoff site: `8i`, site symmetry: `2’..`

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

Table 10: Wyckoff site: `8j`, site symmetry: `m’..`

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

Table 11: Wyckoff site: `16k`, site symmetry: `1`

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