MSG No. 86.68 $P4_2/n1'$ [Type II, tetragonal]

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

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `-11'`

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `2..1'`

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

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

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

Table 7: Wyckoff site: `8g`, site symmetry: `11'`

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