MSG No. 88.81 $I4_1/a$ [Type I, tetragonal]

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

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

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

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

Table 3: Wyckoff site: `8c`, site symmetry: `-1`

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

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

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

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

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

Table 6: Wyckoff site: `16f`, site symmetry: `1`

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