MSG No. 15.91 C_a2/c [Type IV, monoclinic]

Table 1: Wyckoff site: `8a`, site symmetry: `-1`

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

Table 2: Wyckoff site: `8b`, site symmetry: `-1`

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, y, z]$	`[1]`
2	$\left[-x, y, \frac{1}{2}-z\right]$	`[2]`
3	$[-x, -y, -z]$	`[3]`

continued ...

Table 7

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