MSG No. 52.320 $\quad P_Inna$ $\quad$ [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{4}, 0, z\right]$	`[1,4,14,15]`
2	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{2} - z\right]$	`[2,3,13,16]`

continued ...

Table 5

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

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

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

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

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

Table 8: Wyckoff site: 8h, site symmetry: .m'.

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

Table 9: Wyckoff site: `8i`, site symmetry: `m'..`

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

Table 10: Wyckoff site: `16j`, site symmetry: `1`

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