MSG No. 53.330 P_amna [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `m2'm'`

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

continued ...

Table 5

No.	position	mapping
3	$\left[\frac{1}{2}, y, \frac{1}{4}\right]$	[3,8,9,14]
4	$\left[\frac{1}{2}, -y, \frac{3}{4}\right]$	[4,7,10,13]

Table 6: Wyckoff site: 4f, site symmetry: m'2m'

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

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

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

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

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

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

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

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

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

Table 11: Wyckoff site: `8k`, site symmetry: `..m'`

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

Table 12: Wyckoff site: `16l`, site symmetry: `1`

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

continued ...

Table 12

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