MSG No. 53.333 P_Amna [Type IV, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `2'22'`

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

Table 2: Wyckoff site: `4b`, site symmetry: `2'22'`

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

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

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

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

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

Table 5: Wyckoff site: `4e`, 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]`

continued ...

Table 5

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

Table 6: Wyckoff site: 4f, site symmetry: 2/m..

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `2'..`

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

Table 10: Wyckoff site: `8j`, site symmetry: `2'..`

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

Table 11: Wyckoff site: `8k`, 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	$\left[x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[9,10]`
6	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ 0\right]$	`[11,12]`
7	$\left[-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[13,14]`
8	$\left[x+\frac{1}{2},\ \frac{1}{2},\ 0\right]$	`[15,16]`

Table 12: Wyckoff site: `8l`, 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]`

continued ...

Table 12

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

Table 13: Wyckoff site: 16m, 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]
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	$\left[x, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[9]
10	$\left[x, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[10]
11	$\left[\frac{1}{2}-x, y+\frac{1}{2}, -z\right]$	[11]
12	$\left[\frac{1}{2}-x, \frac{1}{2}-y, z\right]$	[12]
13	$\left[-x, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[13]
14	$\left[-x, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[14]
15	$\left[x+\frac{1}{2}, \frac{1}{2}-y, z\right]$	[15]
16	$\left[x+\frac{1}{2}, y+\frac{1}{2}, -z\right]$	[16]