MSG No. 116.297 $P_C\bar{4}c2$ [Type IV, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `2.22`

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

Table 2: Wyckoff site: `4b`, site symmetry: `2.22`

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

Table 3: Wyckoff site: `4c`, site symmetry: `2.2'2'`

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

Table 4: Wyckoff site: `4d`, site symmetry: `2.22`

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

Table 5: Wyckoff site: `4e`, site symmetry: `-4..`

No.	position	mapping
1	$[0,\ 0,\ 0]$	`[1,2,5,6]`
2	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[3,4,7,8]`

continued ...

Table 5

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

Table 6: Wyckoff site: `4f`, site symmetry: `-4’..`

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

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

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

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

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

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

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

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

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

Table 11: Wyckoff site: `8k`, site symmetry: `2..`

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

Table 12: Wyckoff site: `8l`, site symmetry: `2..`

No.	position	mapping
1	$\left[0,\ \frac{1}{2},\ z\right]$	`[1,2]`
2	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$	`[3,4]`
3	$\left[\frac{1}{2},\ 0,\ -z\right]$	`[5,6]`

continued ...

Table 12

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

Table 13: Wyckoff site: 8m, site symmetry: 2'..

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

Table 14: Wyckoff site: 16n, site symmetry: 1

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