SG No. 129 D_{4h}^{7} $P4/nmm$ [tetragonal]

* plus set: $+[0,\ 0,\ 0]$

Table 1: Wyckoff site: `2a`, site symmetry: `-4m2`

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

Table 2: Wyckoff site: `2b`, site symmetry: `-4m2`

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

Table 3: Wyckoff site: `2c`, site symmetry: `4mm`

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

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

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

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

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

Table 6: Wyckoff site: `4f`, site symmetry: `2mm.`

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

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

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

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

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

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

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

continued ...

Table 9

No.	position	mapping
8	$\left[-y,\ \frac{3}{4},\ -z\right]$	[8,12]

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

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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