SG No. 137 D_{4h}^{15} $P4_2/nmc$ [tetragonal]

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

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

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

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

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

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

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

Table 4: Wyckoff site: `4d`, site symmetry: `2mm.`

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

Table 5: Wyckoff site: `8e`, site symmetry: `-1`

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

continued ...

Table 5

No.	position	mapping
6	$\left[\frac{1}{2}, 0, 0\right]$	[6,14]
7	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[7,15]
8	$\left[0, 0, \frac{1}{2}\right]$	[8,16]

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

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

Table 7: Wyckoff site: 8g, 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	$\left[\frac{1}{2} - y, \frac{1}{4}, z + \frac{1}{2}\right]$	[3,15]
4	$\left[y, \frac{1}{4}, z + \frac{1}{2}\right]$	[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	$\left[y + \frac{1}{2}, \frac{3}{4}, \frac{1}{2} - z\right]$	[7,11]
8	$\left[-y, \frac{3}{4}, \frac{1}{2} - z\right]$	[8,12]

Table 8: Wyckoff site: 16h, 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	$\left[\frac{1}{2} - y, x, z + \frac{1}{2}\right]$	[3]
4	$\left[y, \frac{1}{2} - x, z + \frac{1}{2}\right]$	[4]
5	$\left[-x, y + \frac{1}{2}, -z\right]$	[5]
6	$\left[x + \frac{1}{2}, -y, -z\right]$	[6]
7	$\left[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z\right]$	[7]
8	$\left[-y, -x, \frac{1}{2} - z\right]$	[8]

continued ...

Table 8

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