SG No. 138 D_{4h}^{16} $P4_2/ncm$ [tetragonal]

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

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

Table 2: Wyckoff site: 4b, site symmetry: -4..

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

Table 3: Wyckoff site: 4c, 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	$\left[\frac{1}{2}, 0, 0\right]$	[3,6,11,14]
4	$\left[0, \frac{1}{2}, 0\right]$	[4,5,12,13]

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	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[3,6,11,14]
4	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[4,5,12,13]

Table 5: Wyckoff site: 4e, site symmetry: 2.mm

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, z\right]$	[1,2,15,16]

continued ...

Table 5

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

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

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

Table 7: Wyckoff site: 8g, 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	$\left[x+\frac{1}{2},\ x,\ 0\right]$	[3,6]
4	$\left[-x,\ \frac{1}{2}-x,\ 0\right]$	[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	$\left[\frac{1}{2}-x,\ -x,\ 0\right]$	[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	$\left[x,\ -x,\ 0\right]$	[1,8]
2	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ 0\right]$	[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	$\left[-x,\ x,\ 0\right]$	[9,16]
6	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ 0\right]$	[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	$[x,\,x,\,z]$	`[1,16]`
2	$\left[\frac{1}{2}-x,\,\frac{1}{2}-x,\,z\right]$	`[2,15]`
3	$\left[\frac{1}{2}-x,\,x,\,z+\frac{1}{2}\right]$	`[3,14]`
4	$\left[x,\,\frac{1}{2}-x,\,z+\frac{1}{2}\right]$	`[4,13]`
5	$\left[-x,\,x+\frac{1}{2},\,\frac{1}{2}-z\right]$	`[5,12]`
6	$\left[x+\frac{1}{2},\,-x,\,\frac{1}{2}-z\right]$	`[6,11]`
7	$\left[x+\frac{1}{2},\,x+\frac{1}{2},\,-z\right]$	`[7,10]`
8	$[-x,\,-x,\,-z]$	`[8,9]`

Table 10: Wyckoff site: `16j`, 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	$\left[-x,\,y+\frac{1}{2},\,\frac{1}{2}-z\right]$	`[5]`
6	$\left[x+\frac{1}{2},\,-y,\,\frac{1}{2}-z\right]$	`[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	$\left[y+\frac{1}{2},\,-x,\,\frac{1}{2}-z\right]$	`[11]`
12	$\left[-y,\,x+\frac{1}{2},\,\frac{1}{2}-z\right]$	`[12]`
13	$\left[x,\,\frac{1}{2}-y,\,z+\frac{1}{2}\right]$	`[13]`
14	$\left[\frac{1}{2}-x,\,y,\,z+\frac{1}{2}\right]$	`[14]`
15	$\left[\frac{1}{2}-y,\,\frac{1}{2}-x,\,z\right]$	`[15]`
16	$[y,\,x,\,z]$	`[16]`