SG No. 139 D_{4h}^{17} $I4/mmm$ [tetragonal]

* plus set: $+[0,\ 0,\ 0]$, $+\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$

Table 1: Wyckoff site: `2a`, site symmetry: `4/mmm`

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

Table 2: Wyckoff site: `2b`, site symmetry: `4/mmm`

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

Table 3: Wyckoff site: `4c`, site symmetry: `mmm.`

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

Table 4: Wyckoff site: `4d`, site symmetry: `-4m2`

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

Table 5: Wyckoff site: `4e`, site symmetry: `4mm`

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

Table 6: Wyckoff site: `8f`, site symmetry: `..2/m`

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

continued ...

Table 6

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `m2m.`

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

Table 10: Wyckoff site: `8j`, site symmetry: `m2m.`

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

Table 11: Wyckoff site: `16k`, site symmetry: `..2`

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

Table 12: Wyckoff site: `16l`, site symmetry: `m..`

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

Table 13: Wyckoff site: `16m`, site symmetry: `..m`

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

Table 14: Wyckoff site: `16n`, site symmetry: `.m.`

No.	position	mapping
1	$[0,\ y,\ z]$	`[1,14]`
2	$[0,\ -y,\ z]$	`[2,13]`
3	$[-y,\ 0,\ z]$	`[3,15]`

continued ...

Table 14

No.	position	mapping
4	$[y, 0, z]$	[4,16]
5	$[0, y, -z]$	[5,10]
6	$[0, -y, -z]$	[6,9]
7	$[y, 0, -z]$	[7,11]
8	$[-y, 0, -z]$	[8,12]

Table 15: Wyckoff site: 32o, site symmetry: 1

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