SG No. 141 D_{4h}^{19} $I4_1/amd$ [tetragonal]

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

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

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

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

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

Table 3: Wyckoff site: `8c`, site symmetry: `.2/m.`

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

Table 4: Wyckoff site: `8d`, site symmetry: `.2/m.`

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

Table 5: Wyckoff site: `8e`, site symmetry: `2mm.`

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

Table 6: Wyckoff site: `16f`, site symmetry: `.2.`

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

Table 7: Wyckoff site: `16g`, site symmetry: `..2`

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

Table 8: Wyckoff site: `16h`, site symmetry: `.m.`

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

Table 9: Wyckoff site: `32i`, site symmetry: `1`

No.	position	mapping
1	$[x,\ y,\ z]$	`[1]`
2	$\left[\frac{1}{2}-x,\ -y,\ z+\frac{1}{2}\right]$	`[2]`
3	$\left[\frac{1}{4}-y,\ x+\frac{3}{4},\ z+\frac{1}{4}\right]$	`[3]`

continued ...

Table 9

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