SG No. 142 D_{4h}^{20} $I4_1/acd$ [tetragonal]

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

Table 1: Wyckoff site: `8a`, site symmetry: `-4..`

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

Table 2: Wyckoff site: `8b`, site symmetry: `2.22`

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

Table 3: Wyckoff site: `16c`, site symmetry: `-1`

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

Table 4: Wyckoff site: `16d`, site symmetry: `2..`

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

continued ...

Table 4

No.	position	mapping
8	$\left[\frac{1}{2},\ \frac{1}{4},\ z+\frac{1}{4}\right]$	`[15,16]`

Table 5: Wyckoff site: `16e`, site symmetry: `.2.`

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

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

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

Table 7: Wyckoff site: `32g`, 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]`
4	$\left[y+\frac{1}{4},\ \frac{1}{4}-x,\ z+\frac{3}{4}\right]$	`[4]`
5	$\left[\frac{1}{2}-x,\ y,\ -z\right]$	`[5]`
6	$\left[x,\ -y,\ \frac{1}{2}-z\right]$	`[6]`
7	$\left[y+\frac{1}{4},\ x+\frac{3}{4},\ \frac{3}{4}-z\right]$	`[7]`
8	$\left[\frac{1}{4}-y,\ \frac{1}{4}-x,\ \frac{1}{4}-z\right]$	`[8]`
9	$[-x,\ -y,\ -z]$	`[9]`
10	$\left[x+\frac{1}{2},\ y,\ \frac{1}{2}-z\right]$	`[10]`

continued ...

Table 7

No.	position	mapping
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	$\left[x+\frac{1}{2},\ -y,\ z\right]$	[13]
14	$\left[-x,\ y,\ z+\frac{1}{2}\right]$	[14]
15	$\left[\frac{3}{4}-y,\ \frac{1}{4}-x,\ z+\frac{1}{4}\right]$	[15]
16	$\left[y+\frac{3}{4},\ x+\frac{3}{4},\ z+\frac{3}{4}\right]$	[16]