SG No. 140 D_{4h}^{18} $I4/mcm$ [tetragonal]

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

Table 1: Wyckoff site: `4a`, site symmetry: `422`

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

Table 2: Wyckoff site: `4b`, site symmetry: `-42m`

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

Table 3: Wyckoff site: `4c`, site symmetry: `4/m..`

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

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

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

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

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

Table 6: Wyckoff site: `8f`, site symmetry: `4..`

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

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

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

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

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

Table 9: Wyckoff site: `16i`, site symmetry: `..2`

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

Table 10: Wyckoff site: 16j, site symmetry: .2.

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

Table 11: Wyckoff site: 16k, 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	$\left[-x, y, \frac{1}{2}\right]$	[5,14]
6	$\left[x, -y, \frac{1}{2}\right]$	[6,13]
7	$\left[y, x, \frac{1}{2}\right]$	[7,16]
8	$\left[-y, -x, \frac{1}{2}\right]$	[8,15]

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

No.	position	mapping
1	$\left[x, x + \frac{1}{2}, z\right]$	[1,16]
2	$\left[-x, \frac{1}{2} - x, z\right]$	[2,15]
3	$\left[\frac{1}{2} - x, x, z\right]$	[3,14]
4	$\left[x + \frac{1}{2}, -x, z\right]$	[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	$\left[\frac{1}{2} - x, -x, \frac{1}{2} - z\right]$	[8,9]

Table 13: Wyckoff site: 32m, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-x, -y, z]$	[2]
3	$[-y, x, z]$	[3]

continued ...

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Table 13

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

$\left[y,\ x,\ \frac{1}{2}\right]$