

SG No. 123 D_{4h}^1 $P4/mmm$ [tetragonal]

* plus set: $+ [0, 0, 0]$

Table 1: Wyckoff site: 1a, 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: 1b, site symmetry: $4/mmm$

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

Table 3: Wyckoff site: 1c, site symmetry: $4/mmm$

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

Table 4: Wyckoff site: 1d, site symmetry: $4/mmm$

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

Table 5: Wyckoff site: 2e, site symmetry: mmm .

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

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

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

Table 7: Wyckoff site: $2g$, 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 8: Wyckoff site: $2h$, site symmetry: $4mm$

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

Table 9: Wyckoff site: $4i$, site symmetry: $2mm$.

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

Table 10: Wyckoff site: $4j$, 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 11: Wyckoff site: $4k$, site symmetry: $m.2m$

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

Table 12: Wyckoff site: 4i, 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 13: Wyckoff site: 4m, site symmetry: m2m.

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

Table 14: Wyckoff site: 4n, site symmetry: m2m.

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

Table 15: Wyckoff site: 4o, site symmetry: m2m.

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

Table 16: Wyckoff site: 8p, 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	$[y, -x, 0]$	$[4, 11]$

continued ...

Table 16

No.	position	mapping
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 17: Wyckoff site: $8q$, site symmetry: $m..$

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

Table 18: Wyckoff site: $8r$, 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 19: Wyckoff site: $8s$, site symmetry: $.m.$

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

continued ...

Table 19

No.	position	mapping
8	$[0, -x, -z]$	$[8, 11]$

Table 20: Wyckoff site: $8t$, site symmetry: $.m$.

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

Table 21: Wyckoff site: $16u$, 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	$[y, x, z]$	$[16]$