

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: 41, site symmetry: $\text{m}2\text{m}$.

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: $\text{m}2\text{m}$.

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: $\text{m}2\text{m}$.

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: $\text{m}2\text{m}$.

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: $\text{m}\cdot$.

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]