

SG No. 132 D_{4h}^{10} $P4_2/mcm$ [tetragonal]

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

Table 1: Wyckoff site: 2a, site symmetry: m.m̄m

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

Table 2: Wyckoff site: 2b, site symmetry: -42m̄

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

Table 3: Wyckoff site: 2c, site symmetry: m.m̄m

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

Table 4: Wyckoff site: 2d, site symmetry: -42m̄

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

Table 5: Wyckoff site: 4e, site symmetry: 222.

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

Table 6: Wyckoff site: 4f, site symmetry: 2/m..

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

Table 7: Wyckoff site: 4g, site symmetry: 2.mm

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

Table 8: Wyckoff site: 4h, site symmetry: 2.mm

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

Table 9: Wyckoff site: 4i, 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, $\frac{1}{2}$]	[3,5,12,14]
4	[x, -x, $\frac{1}{2}$]	[4,6,11,13]

Table 10: Wyckoff site: 4j, 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, 0]	[3,5,12,14]
4	[x, -x, 0]	[4,6,11,13]

Table 11: Wyckoff site: 8k, site symmetry: 2..

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

Table 12: Wyckoff site: 8l, site symmetry: .2.

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

Table 13: Wyckoff site: 8m, site symmetry: .2.

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

Table 14: Wyckoff site: 8n, site symmetry: m..

No.	position	mapping
1	$[x, y, 0]$	[1,10]
2	$[-x, -y, 0]$	[2,9]
3	$[-y, x, \frac{1}{2}]$	[3,12]

continued ...

Table 14

No.	position	mapping
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	$[y, x, 0]$	[7,16]
8	$[-y, -x, 0]$	[8,15]

Table 15: Wyckoff site: 8o, site symmetry: . . m

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

Table 16: Wyckoff site: 16p, site symmetry: 1

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