

Table 1: Wyckoff site: 2a, site symmetry:  $m' .mm$

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

Table 2: Wyckoff site: 2b, site symmetry:  $-4'2'm$

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

Table 3: Wyckoff site: 2c, site symmetry:  $m' .mm$

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

Table 4: Wyckoff site: 2d, site symmetry:  $-4'2'm$

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

Table 5: Wyckoff site: 4e, site symmetry:  $22'2'$ .

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, y, 0]$	[1,16]
2	$[-y, x, \frac{1}{2}]$	[2,15]
3	$[y, -x, \frac{1}{2}]$	[3,14]

*continued ...*

Table 14

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

Table 15: Wyckoff site: 8o, site symmetry:  $\cdot \cdot m$ 

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

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

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