

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, y, 0]$	$[1, 6]$
2	$[-x, -y, 0]$	$[2, 5]$
3	$[y, x, 0]$	$[3, 8]$

*continued ...*

Table 14

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

Table 15: Wyckoff site: 8o, site symmetry:  $\bar{3}m$ 

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

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

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