

Table 1: Wyckoff site: 2a, site symmetry: 222.

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4]$
2	$[0, 0, \frac{1}{2}]$	$[5, 6, 7, 8]$

Table 2: Wyckoff site: 2b, site symmetry: 222.

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[1, 2, 3, 4]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[5, 6, 7, 8]$

Table 3: Wyckoff site: 2c, site symmetry: 222.

No.	position	mapping
1	$[0, \frac{1}{2}, 0]$	$[1, 2, 3, 4]$
2	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, 6, 7, 8]$

Table 4: Wyckoff site: 2d, site symmetry: 222.

No.	position	mapping
1	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, 2, 3, 4]$
2	$[\frac{1}{2}, 0, 0]$	$[5, 6, 7, 8]$

Table 5: Wyckoff site: 2e, site symmetry: 2.2'2'

No.	position	mapping
1	$[0, 0, \frac{1}{4}]$	$[1, 4, 7, 8]$
2	$[0, 0, \frac{3}{4}]$	$[2, 3, 5, 6]$

Table 6: Wyckoff site: 2f, site symmetry: 2.2'2'

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	$[1, 4, 7, 8]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	$[2, 3, 5, 6]$

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

No.	position	mapping
1	$[0, 0, z]$	$[1, 4]$
2	$[0, 0, -z]$	$[2, 3]$
3	$[0, 0, z + \frac{1}{2}]$	$[5, 6]$
4	$[0, 0, \frac{1}{2} - z]$	$[7, 8]$

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

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, z]$	$[1, 4]$
2	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[2, 3]$
3	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[5, 6]$
4	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	$[7, 8]$

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

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	$[1, 4]$
2	$[0, \frac{1}{2}, -z]$	$[2, 3]$
3	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	$[5, 6]$
4	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	$[7, 8]$

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

No.	position	mapping
1	$[x, 0, 0]$	$[1, 2]$
2	$[-x, 0, 0]$	$[3, 4]$
3	$[0, x, \frac{1}{2}]$	$[5, 7]$
4	$[0, -x, \frac{1}{2}]$	$[6, 8]$

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

No.	position	mapping
1	$[x, \frac{1}{2}, \frac{1}{2}]$	$[1, 2]$
2	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[3, 4]$
3	$[\frac{1}{2}, x, 0]$	$[5, 7]$
4	$[\frac{1}{2}, -x, 0]$	$[6, 8]$

Table 12: Wyckoff site: 4l, site symmetry:  $.2$ .

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	[1,2]
2	$[-x, 0, \frac{1}{2}]$	[3,4]
3	$[0, x, 0]$	[5,7]
4	$[0, -x, 0]$	[6,8]

Table 13: Wyckoff site: 4m, site symmetry:  $.2$ .

No.	position	mapping
1	$[x, \frac{1}{2}, 0]$	[1,2]
2	$[-x, \frac{1}{2}, 0]$	[3,4]
3	$[\frac{1}{2}, x, \frac{1}{2}]$	[5,7]
4	$[\frac{1}{2}, -x, \frac{1}{2}]$	[6,8]

Table 14: Wyckoff site: 4n, site symmetry:  $.2'$ 

No.	position	mapping
1	$[x, x, \frac{1}{4}]$	[1,7]
2	$[x, -x, \frac{3}{4}]$	[2,6]
3	$[-x, x, \frac{3}{4}]$	[3,5]
4	$[-x, -x, \frac{1}{4}]$	[4,8]

Table 15: Wyckoff site: 4o, site symmetry:  $.2'$ 

No.	position	mapping
1	$[x, x, \frac{3}{4}]$	[1,7]
2	$[x, -x, \frac{1}{4}]$	[2,6]
3	$[-x, x, \frac{1}{4}]$	[3,5]
4	$[-x, -x, \frac{3}{4}]$	[4,8]

Table 16: Wyckoff site: 8p, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x, -y, -z]$	[2]
3	$[-x, y, -z]$	[3]
4	$[-x, -y, z]$	[4]

*continued ...*

Table 16

No.	position	mapping
5	$[-y, x, z + \frac{1}{2}]$	[5]
6	$[y, -x, z + \frac{1}{2}]$	[6]
7	$[y, x, \frac{1}{2} - z]$	[7]
8	$[-y, -x, \frac{1}{2} - z]$	[8]