

Table 1: Wyckoff site: 4a, site symmetry:  $2'2'2$ .

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

Table 2: Wyckoff site: 4b, site symmetry:  $2'2'2$ .

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

Table 3: Wyckoff site: 4c, site symmetry:  $2'2'2$ .

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

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

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

Table 5: Wyckoff site: 4e, site symmetry:  $2.22$

No.	position	mapping
1	$[0, 0, \frac{1}{8}]$	$[1, 7, 14, 16]$
2	$[0, 0, \frac{7}{8}]$	$[2, 5, 11, 12]$

*continued ...*

Table 5

No.	position	mapping
3	$[0, 0, \frac{3}{8}]$	[3, 4, 10, 13]
4	$[0, 0, \frac{5}{8}]$	[6, 8, 9, 15]

Table 6: Wyckoff site: 4f, site symmetry: 2.22

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

Table 7: Wyckoff site: 8g, site symmetry: 2' . .

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

Table 8: Wyckoff site: 8h, site symmetry: 2' . .

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

Table 9: Wyckoff site: 8i, site symmetry:  $2'..$ 

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

Table 10: Wyckoff site: 8j, site symmetry:  $.2.$ 

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

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

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

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

No.	position	mapping
1	$[0, y, \frac{1}{4}]$	[1, 13]
2	$[-y, 0, 0]$	[2, 16]
3	$[y, 0, \frac{1}{2}]$	[3, 15]

*continued ...*

Table 12

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

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

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

Table 14: Wyckoff site: 8n, site symmetry: .2'

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

Table 15: Wyckoff site: 8o, site symmetry: .2

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

*continued ...*

Table 15

No.	position	mapping
7	$[-x, -x, \frac{1}{8}]$	[11,13]
8	$[-x, x, \frac{3}{8}]$	[14,15]

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

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