

Table 1: Wyckoff site: 2a, site symmetry:  $-42m$

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

Table 2: Wyckoff site: 2b, site symmetry:  $-42m$

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

Table 3: Wyckoff site: 4c, site symmetry:  $222$ .

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

Table 4: Wyckoff site: 4d, site symmetry:  $2.2'2'$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*continued ...*

Table 13

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

Table 14: Wyckoff site: 16n, site symmetry: 1

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