

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

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

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

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

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

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

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

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

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

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

Table 6: Wyckoff site:  $4\mathbf{f}$ , site symmetry:  $2'm'm$ 

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

Table 7: Wyckoff site:  $4\mathbf{g}$ , site symmetry:  $m'2'm$ 

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

Table 8: Wyckoff site:  $4\mathbf{h}$ , site symmetry:  $m'2'm$ 

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

Table 9: Wyckoff site:  $4\mathbf{i}$ , site symmetry:  $m'm'2$ 

No.	position	mapping
1	$[0, 0, z]$	[1,2,7,8]
2	$[0, 0, -z]$	[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 10: Wyckoff site:  $4\mathbf{j}$ , site symmetry:  $m'm'2$ 

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

Table 11: Wyckoff site:  $8k$ , site symmetry:  $-1$ 

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

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

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

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

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

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

No.	position	mapping
1	$[x, y, 0]$	[1, 4]
2	$[-x, -y, 0]$	[2, 3]
3	$[x, -y, 0]$	[5, 8]

*continued ...*

Table 14

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

Table 15: Wyckoff site: 16o, 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]
5	$[x, -y, -z]$	[5]
6	$[-x, y, -z]$	[6]
7	$[-x, y, z]$	[7]
8	$[x, -y, z]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9]
10	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[10]
11	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[11]
12	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[12]
13	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[13]
14	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[14]
15	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[15]
16	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[16]