

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry:  $22'2'$ .

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

Table 4: Wyckoff site: 4d, site symmetry:  $2.22$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*continued ...*

Table 13

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

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

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