

Table 1: Wyckoff site: 2a, site symmetry:  $42'2'$

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

Table 2: Wyckoff site: 2b, site symmetry:  $42'2'$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*continued ...*

Table 13

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