

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]