

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

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: $4'2'2$

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: $-42'm'$

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

Table 4: Wyckoff site: 2d, site symmetry: $-42'm'$

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

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

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

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

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

Table 7: Wyckoff site: **4g**, site symmetry: $4' \dots$

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

Table 8: Wyckoff site: **4h**, site symmetry: $2.m'm'$

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

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

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

Table 10: Wyckoff site: 8j, site symmetry: $\dots 2$

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	$[x + \frac{1}{2}, -x, \frac{1}{2}]$	[5,8]
4	$[-x, x + \frac{1}{2}, \frac{1}{2}]$	[6,7]
5	$[\frac{1}{2} - x, x, \frac{1}{2}]$	[9,12]
6	$[x, \frac{1}{2} - x, \frac{1}{2}]$	[10,11]
7	$[-x, -x, \frac{1}{2}]$	[13,15]
8	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[14,16]

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

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

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

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

Table 13: Wyckoff site: 8m, site symmetry: $\dots m'$

No.	position	mapping
1	$[x, -x, z]$	[1,15]
2	$[\frac{1}{2} - x, x + \frac{1}{2}, z]$	[2,16]
3	$[-x, x, -z]$	[3,13]

continued ...

Table 13

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

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