

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $\dots 2/m$

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

Table 4: Wyckoff site: 4d, site symmetry: $\dots 2/m$

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

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

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[1, 8, 12, 13]$
2	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	$[2, 7, 11, 14]$

continued ...

Table 5

No.	position	mapping
3	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$	[3,6,10,15]
4	$[\frac{3}{4}, \frac{3}{4}, 0]$	[4,5,9,16]

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

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

Table 7: Wyckoff site: 8g, site symmetry: $2' \dots$

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, y, 0]$	$[1, 8]$
2	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	$[2, 7]$
3	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2}]$	$[3, 6]$

continued ...

Table 12

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

Table 13: Wyckoff site: **16m**, site symmetry: **1**

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