

Table 1: Wyckoff site: 4a, site symmetry: 222

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

Table 2: Wyckoff site: 4b, site symmetry: 222

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

Table 3: Wyckoff site: 4c, site symmetry: 2/m' . .

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

Table 4: Wyckoff site: 4d, site symmetry: 2/m' . .

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

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

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, 0]$	[1,3,13,15]
2	$[\frac{1}{4}, \frac{3}{4}, 0]$	[2,4,14,16]

continued ...

Table 5

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

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

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

Table 7: Wyckoff site: 4g, site symmetry: $m'm'2$

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

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

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

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

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	[1, 2]
2	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	[3, 4]
3	$[-x, 0, \frac{1}{2}]$	[5, 6]

continued ...

Table 9

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

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

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

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

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

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

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

continued ...

Table 12

No.	position	mapping
7	$[\frac{1}{4}, \frac{1}{2}, -z]$	[13,16]
8	$[\frac{1}{4}, \frac{1}{2}, z]$	[14,15]

Table 13: Wyckoff site: $8\mathbf{m}$, site symmetry: \mathbf{m}' . .

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

Table 14: Wyckoff site: $8\mathbf{n}$, site symmetry: $\mathbf{.m}'$.

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

Table 15: Wyckoff site: $16\mathbf{o}$, site symmetry: $\mathbf{1}$

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x, -y, -z]$	[2]
3	$[\frac{1}{2} - x, y, -z]$	[3]
4	$[\frac{1}{2} - x, -y, z]$	[4]
5	$[-x, -y, -z]$	[5]
6	$[-x, y, z]$	[6]
7	$[x + \frac{1}{2}, -y, z]$	[7]
8	$[x + \frac{1}{2}, y, -z]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[9]

continued ...

Table 15

No.	position	mapping
10	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[10]
11	$[-x, y + \frac{1}{2}, -z]$	[11]
12	$[-x, \frac{1}{2} - y, z]$	[12]
13	$[\frac{1}{2} - x, \frac{1}{2} - y, -z]$	[13]
14	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[14]
15	$[x, \frac{1}{2} - y, z]$	[15]
16	$[x, y + \frac{1}{2}, -z]$	[16]