

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: -4 .

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

Table 4: Wyckoff site: 4d, site symmetry: $-4'$.

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

Table 5: Wyckoff site: 8e, site symmetry: $.2$.

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

continued ...

Table 5

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

Table 6: Wyckoff site: **8f**, site symmetry: $.2.$

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

Table 7: Wyckoff site: **8g**, site symmetry: $2..$

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

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

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

continued ...

Table 8

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

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

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

Table 10: Wyckoff site: 16j, site symmetry: 1

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