

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: -1

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

continued ...

Table 5

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

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

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

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

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

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

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

continued ...

Table 8

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

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

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

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

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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

continued ...

Table 11

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