

Table 1: Wyckoff site: 2a, site symmetry: 422

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

Table 2: Wyckoff site: 2b, site symmetry: 422

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

Table 3: Wyckoff site: 4c, site symmetry: 222.

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $4..$

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

Table 6: Wyckoff site: **8f**, site symmetry: -1

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

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

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

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

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

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

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

continued ...

Table 9

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

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

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

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

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