

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

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: 2.22

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	$[1, 4]$
2	$[0, x, \frac{1}{2}]$	$[2, 7]$
3	$[0, -x, \frac{1}{2}]$	$[3, 8]$

continued ...

Table 9

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

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

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

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

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