

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

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

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	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[9, 10, 11, 12, 13, 14, 15, 16]$

Table 3: Wyckoff site: 2c, site symmetry: 4'22'

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

Table 4: Wyckoff site: 2d, site symmetry: 4'22'

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

Table 5: Wyckoff site: 4e, site symmetry: 2.22

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

Table 6: Wyckoff site: 4f, site symmetry: 2.22

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

Table 7: Wyckoff site: 4g, site symmetry: 4. .

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

Table 8: Wyckoff site: 4h, site symmetry: 4' . .

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

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

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

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

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

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

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

Table 12: Wyckoff site: $8l$, 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	$[x + \frac{1}{2}, x + \frac{1}{2}, 0]$	$[9, 15]$
6	$[\frac{1}{2} - x, x + \frac{1}{2}, 0]$	$[10, 13]$
7	$[x + \frac{1}{2}, \frac{1}{2} - x, 0]$	$[11, 12]$
8	$[\frac{1}{2} - x, \frac{1}{2} - x, 0]$	$[14, 16]$

Table 13: Wyckoff site: $8m$, site symmetry: $. . 2'$

No.	position	mapping
1	$[x, x + \frac{1}{2}, \frac{1}{2}]$	$[1, 15]$
2	$[\frac{1}{2} - x, x, \frac{1}{2}]$	$[2, 13]$
3	$[x + \frac{1}{2}, -x, \frac{1}{2}]$	$[3, 12]$

continued ...

Table 13

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

Table 14: Wyckoff site: 8n, site symmetry: $\cdot \cdot 2$

No.	position	mapping
1	$[x, x, \frac{1}{2}]$	[1,7]
2	$[-x, x, \frac{1}{2}]$	[2,5]
3	$[x, -x, \frac{1}{2}]$	[3,4]
4	$[-x, -x, \frac{1}{2}]$	[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 15: Wyckoff site: 8o, site symmetry: $\cdot \cdot 2'$

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

Table 16: Wyckoff site: 16p, 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]

continued ...

Table 16

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