

Table 1: Wyckoff site: 4a, site symmetry: 2.22

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

Table 2: Wyckoff site: 4b, site symmetry: 2.2'2'

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

Table 3: Wyckoff site: 4c, site symmetry: 2.22

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: 22'2'.

No.	position	mapping
1	$[0, 0, \frac{1}{4}]$	$[1, 6, 12, 13]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	$[2, 3, 15, 16]$

continued ...

Table 5

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

Table 6: Wyckoff site: 4f, site symmetry: $22'2'$.

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, x + \frac{1}{2}, \frac{1}{2}]$	[1,15]
2	$[-x, x + \frac{1}{2}, 0]$	[2,13]
3	$[x, \frac{1}{2} - x, 0]$	[3,12]
4	$[x + \frac{1}{2}, -x, 0]$	[4,11]
5	$[\frac{1}{2} - x, x, 0]$	[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 12: Wyckoff site: 8l, site symmetry: $..2$

No.	position	mapping
1	$[x, x, \frac{1}{2}]$	[1,7]
2	$[\frac{1}{2} - x, x + \frac{1}{2}, 0]$	[2,5]
3	$[x + \frac{1}{2}, \frac{1}{2} - x, 0]$	[3,4]

continued ...

Table 12

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

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

No.	position	mapping
1	$[x, x + \frac{1}{2}, 0]$	[1,15]
2	$[-x, x + \frac{1}{2}, \frac{1}{2}]$	[2,13]
3	$[x, \frac{1}{2} - x, \frac{1}{2}]$	[3,12]
4	$[x + \frac{1}{2}, -x, \frac{1}{2}]$	[4,11]
5	$[\frac{1}{2} - x, x, \frac{1}{2}]$	[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 14: Wyckoff site: 8n, site symmetry: $.2'$

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

Table 15: Wyckoff site: 8o, site symmetry: $.2'$

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

continued ...

Table 15

No.	position	mapping
7	$[y, 0, \frac{1}{4}]$	[7,11]
8	$[-y, 0, \frac{1}{4}]$	[8,10]

Table 16: Wyckoff site: 16p, site symmetry: 1

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