

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	[0, 0, 0]	[1,9]
2	$[\frac{1}{2}, 0, \frac{1}{2}]$	[2,10]

*continued ...*

Table 5

No.	position	mapping
3	$[0, \frac{1}{2}, \frac{1}{2}]$	[3,11]
4	$[0, \frac{1}{2}, 0]$	[4,12]
5	$[\frac{1}{2}, 0, 0]$	[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 6: Wyckoff site: **8f**, site symmetry:  $2..$ 

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

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

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

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

No.	position	mapping
1	$[x, \frac{1}{4}, 0]$	[1,4]
2	$[\frac{1}{4}, x, \frac{1}{2}]$	[2,7]
3	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{2}]$	[3,8]
4	$[\frac{1}{2} - x, \frac{1}{4}, 0]$	[5,6]
5	$[-x, \frac{3}{4}, 0]$	[9,12]

*continued ...*

Table 8

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

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

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

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

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

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

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

continued ...

Table 11

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