

Table 1: Wyckoff site: 4a, site symmetry:  $22'2'$ .

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

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

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

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

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

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

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

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

No.	position	mapping
1	[0, 0, 0]	[1,13]
2	$[\frac{1}{2}, \frac{1}{2}, 0]$	[2,14]

*continued ...*

Table 5

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

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

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

*continued ...*

Table 8

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

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

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

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

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

*continued ...*

Table 11

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