

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 8e, site symmetry:  $2'..$

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

*continued ...*

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$[\frac{3}{4}, y, \frac{1}{4}]$	[1,11]
2	$[\frac{3}{4}, -y, \frac{1}{4}]$	[2,16]
3	$[\frac{3}{4}, y, \frac{3}{4}]$	[3,9]
4	$[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{4}]$	[4,14]
5	$[\frac{1}{4}, y + \frac{1}{2}, \frac{3}{4}]$	[5,15]

*continued ...*

Table 8

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

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

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

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

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

Table 11: Wyckoff site: 8k, site symmetry:  $\dots 2$ 

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

Table 12: Wyckoff site: 161, site symmetry: 1

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