

Table 1: Wyckoff site: 2a, site symmetry:  $42'2'$

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

Table 2: Wyckoff site: 2b, site symmetry:  $42'2'$

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry:  $4..$

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

Table 6: Wyckoff site:  $8f$ , site symmetry:  $-1'$ 

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

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

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

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

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

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

No.	position	mapping
1	$[x, \frac{1}{4}, \frac{1}{4}]$	$[1, 9]$
2	$[\frac{1}{4}, x, \frac{1}{4}]$	$[2, 11]$
3	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}]$	$[3, 12]$

*continued ...*

Table 9

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

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

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

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

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