

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

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:  $4'2'2$

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, 2, 11, 12]
2	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[3, 4, 9, 10]
3	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[5, 6, 15, 16]
4	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[7, 8, 13, 14]

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

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

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

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

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

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

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

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

Table 8: Wyckoff site:  $8h$ , 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	$[x + \frac{1}{2}, -x, \frac{3}{4}]$	$[5, 8]$
4	$[-x, x + \frac{1}{2}, \frac{3}{4}]$	$[6, 7]$
5	$[\frac{1}{2} - x, x, \frac{1}{4}]$	$[9, 12]$
6	$[x, \frac{1}{2} - x, \frac{1}{4}]$	$[10, 11]$
7	$[-x, -x, \frac{3}{4}]$	$[13, 15]$
8	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}]$	$[14, 16]$

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

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

*continued ...*

Table 9

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

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

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

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	$[y + \frac{1}{2}, -x, -z]$	[5]
6	$[-y, x + \frac{1}{2}, -z]$	[6]
7	$[-x, y + \frac{1}{2}, z + \frac{1}{2}]$	[7]
8	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	[8]
9	$[\frac{1}{2} - y, x, z]$	[9]
10	$[y, \frac{1}{2} - x, z]$	[10]
11	$[x, \frac{1}{2} - y, \frac{1}{2} - z]$	[11]
12	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[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]