

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

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

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

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

Table 3: Wyckoff site: 8c, site symmetry:  $-1'$

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

Table 4: Wyckoff site: 8d, site symmetry:  $-1$

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{2}, z]$	[1, 4]
2	$[\frac{1}{4}, 0, \frac{1}{2} - z]$	[2, 3]
3	$[\frac{3}{4}, \frac{1}{2}, -z]$	[5, 8]

*continued ...*

Table 8

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

Table 9: Wyckoff site: **16i**, site symmetry: **1**

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