

Table 1: Wyckoff site: 8a, site symmetry: -1

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

Table 2: Wyckoff site: 8b, site symmetry: $-1'$

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

Table 3: Wyckoff site: 8c, site symmetry: $\dots 2$

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

Table 4: Wyckoff site: **8d**, site symmetry: $2'..$

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

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

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

Table 6: Wyckoff site: **16f**, 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	$[x, y, z + \frac{1}{2}]$	[9]
10	$[x, \frac{1}{2} - y, -z]$	[10]
11	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[11]
12	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[12]
13	$[-x, -y, \frac{1}{2} - z]$	[13]
14	$[-x, y + \frac{1}{2}, z]$	[14]
15	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[15]
16	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[16]