

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

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

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

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

Table 3: Wyckoff site: 8c, site symmetry: $2..$

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

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

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

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

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

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