

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

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

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

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

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

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

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

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

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

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

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	$[x + \frac{1}{2}, -y, z]$	[3]
4	$[x, y + \frac{1}{2}, -z]$	[4]
5	$[\frac{1}{2} - x, y, -z]$	[5]
6	$[-x, \frac{1}{2} - y, z]$	[6]
7	$[-x, -y, -z]$	[7]
8	$[-x, y, z + \frac{1}{2}]$	[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	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[11]
12	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[12]
13	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[13]
14	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[14]
15	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[15]
16	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[16]