

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:  $..2$

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]