

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

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

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

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

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

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

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

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

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

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

Table 6: Wyckoff site:  $16f$ , site symmetry:  $1$ 

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