

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

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

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

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

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

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

Table 4: Wyckoff site: 8d, site symmetry:  $\dots m'$ 

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

Table 5: Wyckoff site: 16e, site symmetry: 1

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