

Table 1: Wyckoff site: 8a, site symmetry:  $\dots 2$

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

Table 2: Wyckoff site: 8b, site symmetry:  $\dots 2'$

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

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

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

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

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

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

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