

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	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[5, 6]$
4	$[\frac{1}{2}, \frac{1}{2}, z]$	$[7, 8]$
5	$[\frac{1}{2}, 0, z]$	$[9, 10]$
6	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	$[11, 12]$
7	$[0, \frac{1}{2}, z + \frac{1}{2}]$	$[13, 14]$
8	$[0, \frac{1}{2}, z]$	$[15, 16]$

Table 2: Wyckoff site: **8b**, 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	$[\frac{3}{4}, \frac{1}{2}, z + \frac{1}{2}]$	$[5, 14]$
6	$[\frac{1}{4}, \frac{1}{2}, z + \frac{1}{2}]$	$[6, 13]$
7	$[\frac{1}{4}, \frac{1}{2}, z]$	$[7, 16]$
8	$[\frac{3}{4}, \frac{1}{2}, z]$	$[8, 15]$

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

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

Table 4: Wyckoff site: 16d, 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	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[5]
6	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[6]
7	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[7]
8	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[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	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[13]
14	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	[14]
15	$[-x, y + \frac{1}{2}, z]$	[15]
16	$[x, \frac{1}{2} - y, z]$	[16]