

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

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

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	$[\frac{1}{2}, \frac{1}{4}, z]$	$[3, 16]$
4	$[\frac{1}{2}, \frac{3}{4}, z]$	$[4, 15]$
5	$[0, \frac{3}{4}, z + \frac{1}{2}]$	$[5, 10]$
6	$[0, \frac{1}{4}, z + \frac{1}{2}]$	$[6, 9]$
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:  $m \dots$ 

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

Table 4: Wyckoff site: 16d, site symmetry: 1

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