

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]