

Table 1: Wyckoff site: 4a, site symmetry: $m'm2'$

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

Table 2: Wyckoff site: 8b, site symmetry: $. . 2'$

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

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

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

Table 4: Wyckoff site: 8d, site symmetry: $.m.$

No.	position	mapping
1	$[x, 0, z]$	$[1, 2]$
2	$[-x, 0, z]$	$[3, 4]$
3	$[x, \frac{1}{2}, z + \frac{1}{2}]$	$[5, 6]$
4	$[-x, \frac{1}{2}, z + \frac{1}{2}]$	$[7, 8]$
5	$[x + \frac{1}{2}, 0, z + \frac{1}{2}]$	$[9, 10]$

continued ...

Table 4

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

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

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