

Table 1: Wyckoff site: 4a, site symmetry: $mm'2'$

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

Table 2: Wyckoff site: 4b, site symmetry: $mm'2'$

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

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

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

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

No.	position	mapping
1	$[\frac{3}{4}, y, z]$	[1,3]
2	$[\frac{1}{4}, -y, z]$	[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	$[\frac{3}{4}, y, z + \frac{1}{2}]$	[9,11]
6	$[\frac{1}{4}, -y, z + \frac{1}{2}]$	[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 5: Wyckoff site: **8e**, site symmetry: $.m'$.

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

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