

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: **8e**, site symmetry: **m**.

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

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	$[x + \frac{1}{2}, y, z]$	[9]
10	$[\frac{1}{2} - x, -y, z]$	[10]
11	$[-x, y, z]$	[11]
12	$[x, -y, z]$	[12]
13	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[13]
14	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	[14]
15	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[15]
16	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[16]