

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, \frac{3}{4}, z]$	$[1, 12]$
2	$[-x, \frac{1}{4}, z + \frac{1}{2}]$	$[2, 11]$
3	$[-x, \frac{3}{4}, z]$	$[3, 10]$
4	$[x, \frac{1}{4}, z + \frac{1}{2}]$	$[4, 9]$
5	$[x + \frac{1}{2}, \frac{1}{4}, z]$	$[5, 16]$

continued ...

Table 4

No.	position	mapping
6	$[\frac{1}{2} - x, \frac{3}{4}, z + \frac{1}{2}]$	[6, 15]
7	$[\frac{1}{2} - x, \frac{1}{4}, z]$	[7, 14]
8	$[x + \frac{1}{2}, \frac{3}{4}, z + \frac{1}{2}]$	[8, 13]

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

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