

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

No.	position	mapping
1	$[0, 0, z]$	$[1, 4, 5, 6, 17, 20, 21, 22]$
2	$[0, \frac{1}{2}, z + \frac{1}{4}]$	$[2, 3, 7, 8, 18, 19, 23, 24]$
3	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[9, 12, 13, 14, 25, 28, 29, 30]$
4	$[\frac{1}{2}, 0, z + \frac{3}{4}]$	$[10, 11, 15, 16, 26, 27, 31, 32]$

Table 2: Wyckoff site: 8b, site symmetry: $.m.1'$

No.	position	mapping
1	$[0, y, z]$	$[1, 5, 17, 21]$
2	$[-y, \frac{1}{2}, z + \frac{1}{4}]$	$[2, 7, 18, 23]$
3	$[y, \frac{1}{2}, z + \frac{1}{4}]$	$[3, 8, 19, 24]$
4	$[0, -y, z]$	$[4, 6, 20, 22]$
5	$[\frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	$[9, 13, 25, 29]$
6	$[\frac{1}{2} - y, 0, z + \frac{3}{4}]$	$[10, 15, 26, 31]$
7	$[y + \frac{1}{2}, 0, z + \frac{3}{4}]$	$[11, 16, 27, 32]$
8	$[\frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	$[12, 14, 28, 30]$

Table 3: Wyckoff site: 16c, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	$[1, 17]$
2	$[-y, x + \frac{1}{2}, z + \frac{1}{4}]$	$[2, 18]$
3	$[y, \frac{1}{2} - x, z + \frac{1}{4}]$	$[3, 19]$
4	$[-x, -y, z]$	$[4, 20]$
5	$[-x, y, z]$	$[5, 21]$
6	$[x, -y, z]$	$[6, 22]$
7	$[-y, \frac{1}{2} - x, z + \frac{1}{4}]$	$[7, 23]$
8	$[y, x + \frac{1}{2}, z + \frac{1}{4}]$	$[8, 24]$
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	$[9, 25]$
10	$[\frac{1}{2} - y, x, z + \frac{3}{4}]$	$[10, 26]$
11	$[y + \frac{1}{2}, -x, z + \frac{3}{4}]$	$[11, 27]$
12	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	$[12, 28]$
13	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	$[13, 29]$
14	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	$[14, 30]$
15	$[\frac{1}{2} - y, -x, z + \frac{3}{4}]$	$[15, 31]$
16	$[y + \frac{1}{2}, x, z + \frac{3}{4}]$	$[16, 32]$