

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

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

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	$[x, \frac{1}{2}, z + \frac{1}{2}]$	[5,16]
6	$[-x, \frac{1}{2}, z + \frac{1}{2}]$	[6,15]
7	$[\frac{1}{2} - x, \frac{1}{2}, z + \frac{1}{2}]$	[7,14]
8	$[x + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[8,13]

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

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

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	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	$[5]$
6	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	$[6]$
7	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	$[7]$
8	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	$[8]$
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	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	$[13]$
14	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	$[14]$
15	$[-x, y + \frac{1}{2}, z + \frac{1}{2}]$	$[15]$
16	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	$[16]$