

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

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

Table 2: Wyckoff site: 4b, site symmetry:  $-4..$

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

Table 3: Wyckoff site: 4c, site symmetry:  $2.m'm'$

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

Table 4: Wyckoff site: 8d, site symmetry:  $2..$

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

Table 5: Wyckoff site:  $8e$ , site symmetry:  $\bar{3}m'$ 

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

Table 6: Wyckoff site:  $16f$ , site symmetry:  $1$ 

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