

Table 1: Wyckoff site: 8a, site symmetry: $2..$

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

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

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

Table 3: Wyckoff site: 8c, site symmetry: $.2.$

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

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

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

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

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