

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]