

Table 1: Wyckoff site: 4a, site symmetry:  $\dots 2/m$

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

Table 2: Wyckoff site: 4b, site symmetry:  $\dots 2/m$

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

Table 3: Wyckoff site: 8c, site symmetry:  $-1'$

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

Table 4: Wyckoff site: 8d, site symmetry:  $\dots 2$

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

Table 5: Wyckoff site: **8e**, site symmetry:  $.2'$ .

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

Table 6: Wyckoff site: **8f**, site symmetry:  $.m$ 

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

Table 7: Wyckoff site: **16g**, site symmetry:  $1$ 

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