

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

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry:  $2.2'2'$

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

Table 5: Wyckoff site: 4e, site symmetry:  $4..$

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

Table 6: Wyckoff site: **8f**, site symmetry:  $2..$ 

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

Table 7: Wyckoff site: **8g**, site symmetry:  $..2'$ 

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

Table 8: Wyckoff site: **8h**, site symmetry:  $m..$ 

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

Table 9: Wyckoff site: **16i**, site symmetry:  $1$ 

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x, z]$	[2]
3	$[y, -x, z]$	[3]

*continued ...*

Table 9

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