

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

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

Table 2: Wyckoff site: 2b, site symmetry:  $m.mm$

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

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

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

Table 4: Wyckoff site: 4d, site symmetry:  $-4..$

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

Table 5: Wyckoff site: 4e, site symmetry:  $2.mm$

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

Table 6: Wyckoff site: **4f**, site symmetry: **m.2m**

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

Table 7: Wyckoff site: **4g**, site symmetry: **m.m2**

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

Table 8: Wyckoff site: **8h**, site symmetry: **2. .**

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

Table 9: Wyckoff site: **8i**, site symmetry: **m. .**

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

Table 10: Wyckoff site: **8j**, site symmetry:  $\bar{3}m$ 

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

Table 11: Wyckoff site: **16k**, site symmetry:  $\bar{1}$ 

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