

Table 1: Wyckoff site: 2a, site symmetry:  $m.mm1'$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 6, 7, 8, 9, 14, 15, 16, 17, 22, 23, 24, 25, 30, 31, 32]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[2, 3, 4, 5, 10, 11, 12, 13, 18, 19, 20, 21, 26, 27, 28, 29]$

Table 2: Wyckoff site: 2b, site symmetry:  $m.mm1'$

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	$[1, 6, 7, 8, 9, 14, 15, 16, 17, 22, 23, 24, 25, 30, 31, 32]$
2	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[2, 3, 4, 5, 10, 11, 12, 13, 18, 19, 20, 21, 26, 27, 28, 29]$

Table 3: Wyckoff site: 4c, site symmetry:  $2/m..1'$

No.	position	mapping
1	$[0, \frac{1}{2}, 0]$	$[1, 6, 9, 14, 17, 22, 25, 30]$
2	$[0, \frac{1}{2}, \frac{1}{2}]$	$[2, 3, 10, 11, 18, 19, 26, 27]$
3	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[4, 5, 12, 13, 20, 21, 28, 29]$
4	$[\frac{1}{2}, 0, 0]$	$[7, 8, 15, 16, 23, 24, 31, 32]$

Table 4: Wyckoff site: 4d, site symmetry:  $-4..1'$

No.	position	mapping
1	$[0, \frac{1}{2}, \frac{1}{4}]$	$[1, 6, 10, 11, 17, 22, 26, 27]$
2	$[0, \frac{1}{2}, \frac{3}{4}]$	$[2, 3, 9, 14, 18, 19, 25, 30]$
3	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[4, 5, 15, 16, 20, 21, 31, 32]$
4	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[7, 8, 12, 13, 23, 24, 28, 29]$

Table 5: Wyckoff site: 4e, site symmetry:  $2.mm1'$

No.	position	mapping
1	$[0, 0, z]$	$[1, 6, 15, 16, 17, 22, 31, 32]$
2	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[2, 3, 12, 13, 18, 19, 28, 29]$
3	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	$[4, 5, 10, 11, 20, 21, 26, 27]$
4	$[0, 0, -z]$	$[7, 8, 9, 14, 23, 24, 25, 30]$

Table 6: Wyckoff site: 4f, site symmetry:  $m.2m1'$ 

No.	position	mapping
1	$[x, x, 0]$	$[1, 7, 14, 16, 17, 23, 30, 32]$
2	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}]$	$[2, 5, 11, 12, 18, 21, 27, 28]$
3	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	$[3, 4, 10, 13, 19, 20, 26, 29]$
4	$[-x, -x, 0]$	$[6, 8, 9, 15, 22, 24, 25, 31]$

Table 7: Wyckoff site: 4g, site symmetry:  $m.m21'$ 

No.	position	mapping
1	$[x, -x, 0]$	$[1, 8, 14, 15, 17, 24, 30, 31]$
2	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	$[2, 4, 11, 13, 18, 20, 27, 29]$
3	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$	$[3, 5, 10, 12, 19, 21, 26, 28]$
4	$[-x, x, 0]$	$[6, 7, 9, 16, 22, 23, 25, 32]$

Table 8: Wyckoff site: 8h, site symmetry:  $2..1'$ 

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	$[1, 6, 17, 22]$
2	$[0, \frac{1}{2}, z + \frac{1}{2}]$	$[2, 3, 18, 19]$
3	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	$[4, 5, 20, 21]$
4	$[\frac{1}{2}, 0, -z]$	$[7, 8, 23, 24]$
5	$[0, \frac{1}{2}, -z]$	$[9, 14, 25, 30]$
6	$[0, \frac{1}{2}, \frac{1}{2} - z]$	$[10, 11, 26, 27]$
7	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	$[12, 13, 28, 29]$
8	$[\frac{1}{2}, 0, z]$	$[15, 16, 31, 32]$

Table 9: Wyckoff site: 8i, site symmetry:  $m..1'$ 

No.	position	mapping
1	$[x, y, 0]$	$[1, 14, 17, 30]$
2	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2}]$	$[2, 11, 18, 27]$
3	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	$[3, 10, 19, 26]$
4	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	$[4, 13, 20, 29]$
5	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2}]$	$[5, 12, 21, 28]$
6	$[-x, -y, 0]$	$[6, 9, 22, 25]$
7	$[y, x, 0]$	$[7, 16, 23, 32]$
8	$[-y, -x, 0]$	$[8, 15, 24, 31]$

Table 10: Wyckoff site: 8j, site symmetry:  $\cdot\cdot m1'$ 

No.	position	mapping
1	$[x, x, z]$	[1, 16, 17, 32]
2	$[\frac{1}{2} - x, x + \frac{1}{2}, z + \frac{1}{2}]$	[2, 12, 18, 28]
3	$[x + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[3, 13, 19, 29]
4	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[4, 10, 20, 26]
5	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - z]$	[5, 11, 21, 27]
6	$[-x, -x, z]$	[6, 15, 22, 31]
7	$[x, x, -z]$	[7, 14, 23, 30]
8	$[-x, -x, -z]$	[8, 9, 24, 25]

Table 11: Wyckoff site: 16k, site symmetry:  $11'$ 

No.	position	mapping
1	$[x, y, z]$	[1, 17]
2	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[2, 18]
3	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[3, 19]
4	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[4, 20]
5	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[5, 21]
6	$[-x, -y, z]$	[6, 22]
7	$[y, x, -z]$	[7, 23]
8	$[-y, -x, -z]$	[8, 24]
9	$[-x, -y, -z]$	[9, 25]
10	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[10, 26]
11	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[11, 27]
12	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[12, 28]
13	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[13, 29]
14	$[x, y, -z]$	[14, 30]
15	$[-y, -x, z]$	[15, 31]
16	$[y, x, z]$	[16, 32]