

Table 1: Wyckoff site: 2a, site symmetry:  $-42m1'$

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

Table 2: Wyckoff site: 2b, site symmetry:  $-42m1'$

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

Table 3: Wyckoff site: 4c, site symmetry:  $222.1'$

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

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

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

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

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

Table 6: Wyckoff site:  $8f$ , site symmetry:  $.2.1'$ 

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

Table 7: Wyckoff site:  $8g$ , site symmetry:  $.2.1'$ 

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

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

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

Table 9: Wyckoff site:  $8i$ , site symmetry:  $..m1'$ 

No.	position	mapping
1	$[x, x, z]$	$[1, 8, 17, 24]$
2	$[x, -x, -z]$	$[2, 5, 18, 21]$
3	$[-x, x, -z]$	$[3, 6, 19, 22]$

*continued ...*

Table 9

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

Table 10: Wyckoff site: 16j, site symmetry: 11'

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