

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

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

Table 2: Wyckoff site: 4b, site symmetry:  $-4..1'$ 

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

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	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[2, 3, 10, 11, 18, 19, 26, 27]$
3	$[\frac{1}{2}, 0, 0]$	$[4, 5, 12, 13, 20, 21, 28, 29]$
4	$[0, \frac{1}{2}, \frac{1}{2}]$	$[7, 8, 15, 16, 23, 24, 31, 32]$

Table 4: Wyckoff site: 4d, site symmetry:  $2.221'$ 

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

Table 5: Wyckoff site: 8e, site symmetry:  $2..1'$ 

No.	position	mapping
1	$[0, 0, z]$	$[1, 6, 17, 22]$
2	$[0, 0, z + \frac{1}{2}]$	$[2, 3, 18, 19]$

*continued ...*

Table 5

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

Table 6: Wyckoff site: **8f**, site symmetry:  $2..1'$ 

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

Table 7: Wyckoff site: **8g**, site symmetry:  $..21'$ 

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

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

No.	position	mapping
1	$[x, y, 0]$	[1, 14, 17, 30]
2	$[-y, x, \frac{1}{2}]$	[2, 11, 18, 27]
3	$[y, -x, \frac{1}{2}]$	[3, 10, 19, 26]
4	$[x + \frac{1}{2}, \frac{1}{2} - y, 0]$	[4, 13, 20, 29]
5	$[\frac{1}{2} - x, y + \frac{1}{2}, 0]$	[5, 12, 21, 28]

*continued ...*

Table 8

No.	position	mapping
6	$[-x, -y, 0]$	$[6, 9, 22, 25]$
7	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	$[7, 16, 23, 32]$
8	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2}]$	$[8, 15, 24, 31]$

Table 9: Wyckoff site: 16i, site symmetry:  $11'$ 

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