

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

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

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

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

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

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	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[2, 3, 4, 5, 18, 19, 20, 21]$
3	$[0, \frac{1}{2}, \frac{3}{4}]$	$[9, 14, 15, 16, 25, 30, 31, 32]$
4	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[10, 11, 12, 13, 26, 27, 28, 29]$

Table 5: Wyckoff site: 4e, site symmetry: $4..1'$

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

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

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

continued ...

Table 9

No.	position	mapping
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	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[7,23]
8	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[8,24]
9	$[-x, -y, -z]$	[9,25]
10	$[y, -x, -z]$	[10,26]
11	$[-y, x, -z]$	[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	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[15,31]
16	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[16,32]