

Table 1: Wyckoff site: 2a, site symmetry: $-4m21'$

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: $-4m21'$

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: 2c, site symmetry: $-4m21'$

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

Table 4: Wyckoff site: 2d, site symmetry: $-4m21'$

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

Table 5: Wyckoff site: 4e, site symmetry: $2mm.1'$

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

Table 6: Wyckoff site: 4f, site symmetry: $2mm.1'$

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

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

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

Table 8: Wyckoff site: 8h, site symmetry: $. . 21'$

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

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

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

continued ...

Table 9

No.	position	mapping
8	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[12, 13, 28, 29]

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

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