

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

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[1,2,3,4,13,14,15,16]
2	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[5,6,7,8,9,10,11,12]

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

No.	position	mapping
1	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[1,2,3,4,13,14,15,16]
2	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[5,6,7,8,9,10,11,12]

Table 3: Wyckoff site: 2c, site symmetry: $m'm'm'$

No.	position	mapping
1	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[1,2,3,4,13,14,15,16]
2	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[5,6,7,8,9,10,11,12]

Table 4: Wyckoff site: 2d, site symmetry: $m'm'm'$

No.	position	mapping
1	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[1,2,3,4,13,14,15,16]
2	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[5,6,7,8,9,10,11,12]

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

No.	position	mapping
1	$[x, \frac{1}{4}, \frac{1}{4}]$	[1,2,15,16]
2	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[3,4,13,14]
3	$[-x, \frac{3}{4}, \frac{3}{4}]$	[5,6,11,12]
4	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[7,8,9,10]

Table 6: Wyckoff site: $4\mathbf{f}$, site symmetry: $2\mathbf{m}'\mathbf{m}'$

No.	position	mapping
1	$[x, \frac{3}{4}, \frac{1}{4}]$	$[1, 2, 15, 16]$
2	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}]$	$[3, 4, 13, 14]$
3	$[-x, \frac{1}{4}, \frac{3}{4}]$	$[5, 6, 11, 12]$
4	$[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	$[7, 8, 9, 10]$

Table 7: Wyckoff site: $4\mathbf{g}$, site symmetry: $\mathbf{m}'2\mathbf{m}'$

No.	position	mapping
1	$[\frac{1}{4}, y, \frac{1}{4}]$	$[1, 3, 14, 16]$
2	$[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{4}]$	$[2, 4, 13, 15]$
3	$[\frac{3}{4}, -y, \frac{3}{4}]$	$[5, 7, 10, 12]$
4	$[\frac{3}{4}, y + \frac{1}{2}, \frac{3}{4}]$	$[6, 8, 9, 11]$

Table 8: Wyckoff site: $4\mathbf{h}$, site symmetry: $\mathbf{m}'2\mathbf{m}'$

No.	position	mapping
1	$[\frac{1}{4}, y, \frac{3}{4}]$	$[1, 3, 14, 16]$
2	$[\frac{1}{4}, \frac{1}{2} - y, \frac{3}{4}]$	$[2, 4, 13, 15]$
3	$[\frac{3}{4}, -y, \frac{1}{4}]$	$[5, 7, 10, 12]$
4	$[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{4}]$	$[6, 8, 9, 11]$

Table 9: Wyckoff site: $4\mathbf{i}$, site symmetry: $\mathbf{m}'\mathbf{m}'2$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, z]$	$[1, 4, 14, 15]$
2	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - z]$	$[2, 3, 13, 16]$
3	$[\frac{3}{4}, \frac{3}{4}, -z]$	$[5, 8, 10, 11]$
4	$[\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}]$	$[6, 7, 9, 12]$

Table 10: Wyckoff site: $4\mathbf{j}$, site symmetry: $\mathbf{m}'\mathbf{m}'2$

No.	position	mapping
1	$[\frac{3}{4}, \frac{1}{4}, z]$	$[1, 4, 14, 15]$
2	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	$[2, 3, 13, 16]$
3	$[\frac{1}{4}, \frac{3}{4}, -z]$	$[5, 8, 10, 11]$
4	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	$[6, 7, 9, 12]$

Table 11: Wyckoff site: $8k$, site symmetry: -1

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, 5]$
2	$[\frac{1}{2}, 0, 0]$	$[2, 6]$
3	$[0, \frac{1}{2}, 0]$	$[3, 7]$
4	$[0, 0, \frac{1}{2}]$	$[4, 8]$
5	$[0, 0, 0]$	$[9, 13]$
6	$[0, \frac{1}{2}, \frac{1}{2}]$	$[10, 14]$
7	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[11, 15]$
8	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[12, 16]$

Table 12: Wyckoff site: $8l$, site symmetry: $m'..$

No.	position	mapping
1	$[\frac{1}{4}, y, z]$	$[1, 14]$
2	$[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{2} - z]$	$[2, 13]$
3	$[\frac{1}{4}, y, \frac{1}{2} - z]$	$[3, 16]$
4	$[\frac{1}{4}, \frac{1}{2} - y, z]$	$[4, 15]$
5	$[\frac{3}{4}, -y, -z]$	$[5, 10]$
6	$[\frac{3}{4}, y + \frac{1}{2}, z + \frac{1}{2}]$	$[6, 9]$
7	$[\frac{3}{4}, -y, z + \frac{1}{2}]$	$[7, 12]$
8	$[\frac{3}{4}, y + \frac{1}{2}, -z]$	$[8, 11]$

Table 13: Wyckoff site: $8m$, site symmetry: $.m'$.

No.	position	mapping
1	$[x, \frac{1}{4}, z]$	$[1, 15]$
2	$[x, \frac{1}{4}, \frac{1}{2} - z]$	$[2, 16]$
3	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{2} - z]$	$[3, 13]$
4	$[\frac{1}{2} - x, \frac{1}{4}, z]$	$[4, 14]$
5	$[-x, \frac{3}{4}, -z]$	$[5, 11]$
6	$[-x, \frac{3}{4}, z + \frac{1}{2}]$	$[6, 12]$
7	$[x + \frac{1}{2}, \frac{3}{4}, z + \frac{1}{2}]$	$[7, 9]$
8	$[x + \frac{1}{2}, \frac{3}{4}, -z]$	$[8, 10]$

Table 14: Wyckoff site: $8n$, site symmetry: $..m'$

No.	position	mapping
1	$[x, y, \frac{1}{4}]$	$[1, 16]$
2	$[x, \frac{1}{2} - y, \frac{1}{4}]$	$[2, 15]$
3	$[\frac{1}{2} - x, y, \frac{1}{4}]$	$[3, 14]$

continued ...

Table 14

No.	position	mapping
4	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{4}]$	[4,13]
5	$[-x, -y, \frac{3}{4}]$	[5,12]
6	$[-x, y + \frac{1}{2}, \frac{3}{4}]$	[6,11]
7	$[x + \frac{1}{2}, -y, \frac{3}{4}]$	[7,10]
8	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}]$	[8,9]

Table 15: Wyckoff site: **16o**, site symmetry: **1**

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x, \frac{1}{2} - y, \frac{1}{2} - z]$	[2]
3	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[3]
4	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[4]
5	$[-x, -y, -z]$	[5]
6	$[-x, y + \frac{1}{2}, z + \frac{1}{2}]$	[6]
7	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	[7]
8	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9]
10	$[x + \frac{1}{2}, -y, -z]$	[10]
11	$[-x, y + \frac{1}{2}, -z]$	[11]
12	$[-x, -y, z + \frac{1}{2}]$	[12]
13	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[13]
14	$[\frac{1}{2} - x, y, z]$	[14]
15	$[x, \frac{1}{2} - y, z]$	[15]
16	$[x, y, \frac{1}{2} - z]$	[16]