

Table 1: Wyckoff site: 2a, site symmetry: 222 .

No.	position	mapping
1	$[0, 0, 0]$	$[1, 4, 5, 6]$
2	$[0, 0, \frac{1}{2}]$	$[2, 3, 7, 8]$

Table 2: Wyckoff site: 2b, site symmetry: 222 .

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[1, 4, 5, 6]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[2, 3, 7, 8]$

Table 3: Wyckoff site: 2c, site symmetry: 222 .

No.	position	mapping
1	$[0, \frac{1}{2}, 0]$	$[1, 4, 5, 6]$
2	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[2, 3, 7, 8]$

Table 4: Wyckoff site: 2d, site symmetry: 222 .

No.	position	mapping
1	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, 4, 5, 6]$
2	$[\frac{1}{2}, 0, 0]$	$[2, 3, 7, 8]$

Table 5: Wyckoff site: 2e, site symmetry: 2.22

No.	position	mapping
1	$[0, 0, \frac{1}{4}]$	$[1, 6, 7, 8]$
2	$[0, 0, \frac{3}{4}]$	$[2, 3, 4, 5]$

Table 6: Wyckoff site: 2f, site symmetry: 2.22

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	$[1, 6, 7, 8]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	$[2, 3, 4, 5]$

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

No.	position	mapping
1	$[0, 0, z]$	$[1, 6]$
2	$[0, 0, z + \frac{1}{2}]$	$[2, 3]$
3	$[0, 0, -z]$	$[4, 5]$
4	$[0, 0, \frac{1}{2} - z]$	$[7, 8]$

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

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, z]$	$[1, 6]$
2	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[2, 3]$
3	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[4, 5]$
4	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	$[7, 8]$

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

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	$[1, 6]$
2	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	$[2, 3]$
3	$[0, \frac{1}{2}, -z]$	$[4, 5]$
4	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	$[7, 8]$

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

No.	position	mapping
1	$[x, 0, 0]$	$[1, 4]$
2	$[0, x, \frac{1}{2}]$	$[2, 7]$
3	$[0, -x, \frac{1}{2}]$	$[3, 8]$
4	$[-x, 0, 0]$	$[5, 6]$

Table 11: Wyckoff site: $4\mathbf{k}$, site symmetry: $.2.$

No.	position	mapping
1	$[x, \frac{1}{2}, \frac{1}{2}]$	$[1, 4]$
2	$[\frac{1}{2}, x, 0]$	$[2, 7]$
3	$[\frac{1}{2}, -x, 0]$	$[3, 8]$
4	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[5, 6]$

Table 12: Wyckoff site: $4\bar{1}$, site symmetry: $\cdot 2$.

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	$[1, 4]$
2	$[0, x, 0]$	$[2, 7]$
3	$[0, -x, 0]$	$[3, 8]$
4	$[-x, 0, \frac{1}{2}]$	$[5, 6]$

Table 13: Wyckoff site: $4\bar{\mathbf{m}}$, site symmetry: $\cdot 2$.

No.	position	mapping
1	$[x, \frac{1}{2}, 0]$	$[1, 4]$
2	$[\frac{1}{2}, x, \frac{1}{2}]$	$[2, 7]$
3	$[\frac{1}{2}, -x, \frac{1}{2}]$	$[3, 8]$
4	$[-x, \frac{1}{2}, 0]$	$[5, 6]$

Table 14: Wyckoff site: $4\bar{\mathbf{n}}$, site symmetry: $\cdot \cdot 2$

No.	position	mapping
1	$[x, x, \frac{1}{4}]$	$[1, 7]$
2	$[-x, x, \frac{3}{4}]$	$[2, 5]$
3	$[x, -x, \frac{3}{4}]$	$[3, 4]$
4	$[-x, -x, \frac{1}{4}]$	$[6, 8]$

Table 15: Wyckoff site: $4\bar{\mathbf{o}}$, site symmetry: $\cdot \cdot 2$

No.	position	mapping
1	$[x, x, \frac{3}{4}]$	$[1, 7]$
2	$[-x, x, \frac{1}{4}]$	$[2, 5]$
3	$[x, -x, \frac{1}{4}]$	$[3, 4]$
4	$[-x, -x, \frac{3}{4}]$	$[6, 8]$

Table 16: Wyckoff site: $8\bar{\mathbf{p}}$, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-y, x, z + \frac{1}{2}]$	$[2]$
3	$[y, -x, z + \frac{1}{2}]$	$[3]$
4	$[x, -y, -z]$	$[4]$

continued ...

Table 16

No.	position	mapping
5	$[-x, y, -z]$	[5]
6	$[-x, -y, z]$	[6]
7	$[y, x, \frac{1}{2} - z]$	[7]
8	$[-y, -x, \frac{1}{2} - z]$	[8]