

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: -1

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

Table 6: Wyckoff site: $4f$, site symmetry: -1

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

Table 7: Wyckoff site: $4g$, site symmetry: $2'..$

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

Table 8: Wyckoff site: $4h$, site symmetry: $2'..$

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

Table 9: Wyckoff site: $4i$, site symmetry: $.2'$

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

Table 10: Wyckoff site: $4j$, site symmetry: $.2'$

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

Table 11: Wyckoff site: $4k$, site symmetry: $\dots 2$

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

Table 12: Wyckoff site: $4l$, site symmetry: $\dots 2$

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

Table 13: Wyckoff site: $8m$, site symmetry: 1

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