

Table 1: Wyckoff site: 2a, site symmetry: $2221'$

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

Table 2: Wyckoff site: 2b, site symmetry: $2221'$

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

Table 3: Wyckoff site: 2c, site symmetry: $2221'$

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

Table 4: Wyckoff site: 2d, site symmetry: $2221'$

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

Table 5: Wyckoff site: 4e, site symmetry: $-11'$

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

Table 6: Wyckoff site: 4f, site symmetry: $-11'$

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

Table 7: Wyckoff site: 4g, site symmetry: $2..1'$

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

Table 8: Wyckoff site: 4h, site symmetry: $2..1'$

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

Table 9: Wyckoff site: 4i, site symmetry: $.2.1'$

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

Table 10: Wyckoff site: 4j, site symmetry: $.2.1'$

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

Table 11: Wyckoff site: $4k$, site symmetry: $\dots 21'$

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

Table 12: Wyckoff site: $4l$, site symmetry: $\dots 21'$

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

Table 13: Wyckoff site: $8m$, site symmetry: $11'$

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