

Table 1: Wyckoff site: 2a, site symmetry: $2'22'$

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

Table 2: Wyckoff site: 2b, site symmetry: $2'22'$

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

Table 3: Wyckoff site: 2c, site symmetry: $2'22'$

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

Table 4: Wyckoff site: 2d, site symmetry: $2'22'$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 12: Wyckoff site: $4\mathbf{l}$, site symmetry: $\cdot\cdot 2'$

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

Table 13: Wyckoff site: $8\mathbf{m}$, site symmetry: 1

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