

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: **4e**, site symmetry: $2..$

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

Table 6: Wyckoff site: **4f**, site symmetry: $2..$

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

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

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

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

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

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

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

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

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

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

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