

Table 1: Wyckoff site: 2a, site symmetry: $-4..$

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

Table 2: Wyckoff site: 2b, site symmetry: $-4..$

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

Table 3: Wyckoff site: 2c, site symmetry: 2.22

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

Table 4: Wyckoff site: 2d, site symmetry: 2.22

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

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

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

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

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

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

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

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

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

Table 9: Wyckoff site: **8i**, site symmetry: 1

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