

Table 1: Wyckoff site: 1a, site symmetry: $-4m21'$

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

Table 2: Wyckoff site: 1b, site symmetry: $-4m21'$

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

Table 3: Wyckoff site: 1c, site symmetry: $-4m21'$

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

Table 4: Wyckoff site: 1d, site symmetry: $-4m21'$

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

Table 5: Wyckoff site: 2e, site symmetry: $2mm.1'$

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

Table 6: Wyckoff site: 2f, site symmetry: $2mm.1'$

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

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

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

Table 8: Wyckoff site: $4h$, site symmetry: $. . 21'$

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

Table 9: Wyckoff site: $4i$, site symmetry: $. . 21'$

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

Table 10: Wyckoff site: $4j$, site symmetry: $.m.1'$

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

Table 11: Wyckoff site: $4k$, site symmetry: $.m.1'$

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

Table 12: Wyckoff site: 81 , site symmetry: $11'$

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