

Table 1: Wyckoff site: 2a, site symmetry: $\dots 2/m1'$

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

Table 2: Wyckoff site: 2b, site symmetry: $\dots 2/m1'$

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

Table 3: Wyckoff site: 2c, site symmetry: $\dots 2/m1'$

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

Table 4: Wyckoff site: 2d, site symmetry: $\dots 2/m1'$

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

Table 5: Wyckoff site: 4e, site symmetry: $\dots 21'$

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

Table 6: Wyckoff site: $4\mathbf{f}$, site symmetry: $..21'$

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

Table 7: Wyckoff site: $4\mathbf{g}$, site symmetry: $..m1'$

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

Table 8: Wyckoff site: $4\mathbf{h}$, site symmetry: $..m1'$

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

Table 9: Wyckoff site: $8\mathbf{i}$, site symmetry: $11'$

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