

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

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

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

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

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

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

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

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

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

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

Table 6: Wyckoff site: **4f**, site symmetry:  $\bar{3}2$ 

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

Table 7: Wyckoff site: **4g**, site symmetry:  $\bar{3}m'$ 

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

Table 8: Wyckoff site: **4h**, site symmetry:  $\bar{3}m'$ 

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

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

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