

Table 1: Wyckoff site: 2a, site symmetry: $mm2$

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

Table 2: Wyckoff site: 2b, site symmetry: $mm2$

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

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

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

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

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

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

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

Table 6: Wyckoff site: $4f$, site symmetry: $\bar{4}2m$.

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

Table 7: Wyckoff site: $8g$, site symmetry: 1

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