

Table 1: Wyckoff site: $1o$, site symmetry: $m'mm'$

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

Table 2: Wyckoff site: $2a$, site symmetry: $2'mm'$

No.	position	mapping
1	$[x, 0, 0]$	$[1, 4, 5, 8]$
2	$[-x, 0, 0]$	$[2, 3, 6, 7]$

Table 3: Wyckoff site: $2b$, site symmetry: $m'2m'$

No.	position	mapping
1	$[0, y, 0]$	$[1, 4, 6, 7]$
2	$[0, -y, 0]$	$[2, 3, 5, 8]$

Table 4: Wyckoff site: $2c$, site symmetry: $m'2m'$

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

Table 5: Wyckoff site: $4d$, site symmetry: $m'..$

No.	position	mapping
1	$[0, y, z]$	$[1, 7]$
2	$[0, -y, z]$	$[2, 8]$
3	$[0, y, -z]$	$[4, 6]$
4	$[0, -y, -z]$	$[3, 5]$

Table 6: Wyckoff site: $4e$, site symmetry: $.m.$

No.	position	mapping
1	$[x, 0, z]$	$[1, 8]$

continued ...

Table 6

No.	position	mapping
2	$[-x, 0, z]$	$[2, 7]$
3	$[-x, 0, -z]$	$[3, 6]$
4	$[x, 0, -z]$	$[4, 5]$

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

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

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

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