

Table 1: Wyckoff site: $1o$, site symmetry: $mmm1'$

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: $2a$, site symmetry: $2mm$

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

Table 3: Wyckoff site: $2b$, site symmetry: $m2m$

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

Table 4: Wyckoff site: $2c$, site symmetry: $mm2$

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

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

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

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

No.	position	mapping
1	$[x, 0, z]$	$[1, 7, 9, 15]$

continued ...

Table 6

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

Table 7: Wyckoff site: $4f$, site symmetry: $\dots m$

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

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

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