

Table 1: Wyckoff site: $1o$, site symmetry: $-4m2$

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

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

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

Table 3: Wyckoff site: $4b$, site symmetry: $. . 2$

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

Table 4: Wyckoff site: $4c$, site symmetry: $.m.$

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

Table 5: Wyckoff site: $8d$, site symmetry: 1

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

continued ...

Table 5

No.	position	mapping
8	$[-y, -x, -z]$	[5]