

Table 1: Wyckoff site: 1o, site symmetry: mmm'

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, 2, 3, 4]
2	[$-x$, 0, 0]	[5, 6, 7, 8]

Table 3: Wyckoff site: 2b, site symmetry: $m2'm'$

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

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

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

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

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

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

No.	position	mapping
1	[x , 0, z]	[1, 3]

continued ...

Table 6

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

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

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

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

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