

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: $2mm$

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: $m'2'm$

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: $m'm2'$

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: $\dots m$

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]