

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

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

Table 2: Wyckoff site: 2a, site symmetry: 2m'm'

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: m2'm'

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: mm'2'

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	$[-x, y, z]$	$[7]$