

Table 1: Wyckoff site: 1o, site symmetry: $-4'2'm$

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	$[0, 0, z]$	$[1, 2, 3, 4]$
2	$[0, 0, -z]$	$[5, 6, 7, 8]$

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

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

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

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

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

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

continued ...

Table 5

No.	position	mapping
8	$[y, x, z]$	[3]