

Table 1: Wyckoff site: $1o$, site symmetry: $-42m1'$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]$

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

No.	position	mapping
1	$[0, 0, z]$	$[1, 4, 5, 8, 9, 12, 13, 16]$
2	$[0, 0, -z]$	$[2, 3, 6, 7, 10, 11, 14, 15]$

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

No.	position	mapping
1	$[x, 0, 0]$	$[1, 2, 9, 10]$
2	$[-x, 0, 0]$	$[3, 4, 11, 12]$
3	$[0, -x, 0]$	$[6, 8, 14, 16]$
4	$[0, x, 0]$	$[5, 7, 13, 15]$

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

No.	position	mapping
1	$[x, x, z]$	$[1, 5, 9, 13]$
2	$[-x, -x, z]$	$[4, 8, 12, 16]$
3	$[x, -x, -z]$	$[2, 6, 10, 14]$
4	$[-x, x, -z]$	$[3, 7, 11, 15]$

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

No.	position	mapping
1	$[x, y, z]$	$[1, 9]$
2	$[-x, -y, z]$	$[4, 12]$
3	$[y, -x, -z]$	$[6, 14]$
4	$[-y, x, -z]$	$[7, 15]$
5	$[-x, y, -z]$	$[3, 11]$
6	$[x, -y, -z]$	$[2, 10]$
7	$[-y, -x, z]$	$[8, 16]$

continued ...

Table 5

No.	position	mapping
8	$[y, x, z]$	$[5, 13]$