

Table 1: Wyckoff site:  $1o$ , site symmetry:  $-4m21'$ 

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:  $2mm$ .

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

Table 3: Wyckoff site:  $4b$ , site symmetry:  $\dots 2$ 

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

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

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

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	$[-y, -x, -z]$	<b>[5,13]</b>