

Table 1: Wyckoff site: 2a, site symmetry:  $2.mm$

No.	position	mapping
1	$[0, 0, z]$	$[1, 4, 7, 8]$
2	$[0, 0, z + \frac{1}{2}]$	$[2, 3, 5, 6]$

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

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, z]$	$[1, 4, 7, 8]$
2	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[2, 3, 5, 6]$

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

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	$[1, 4]$
2	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	$[2, 3]$
3	$[0, \frac{1}{2}, z + \frac{1}{2}]$	$[5, 6]$
4	$[\frac{1}{2}, 0, z]$	$[7, 8]$

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

No.	position	mapping
1	$[x, x, z]$	$[1, 8]$
2	$[-x, x, z + \frac{1}{2}]$	$[2, 5]$
3	$[x, -x, z + \frac{1}{2}]$	$[3, 6]$
4	$[-x, -x, z]$	$[4, 7]$

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

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-y, x, z + \frac{1}{2}]$	$[2]$
3	$[y, -x, z + \frac{1}{2}]$	$[3]$
4	$[-x, -y, z]$	$[4]$
5	$[-x, y, z + \frac{1}{2}]$	$[5]$
6	$[x, -y, z + \frac{1}{2}]$	$[6]$

*continued ...*

Table 5

No.	position	mapping
7	$[-y, -x, z]$	[7]
8	$[y, x, z]$	[8]