

Table 1: Wyckoff site: **4a**, site symmetry:  $4..$ 

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

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

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

Table 3: Wyckoff site: **8c**, site symmetry:  $..m'$ 

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

Table 4: Wyckoff site: **16d**, site symmetry:  $1$ 

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-y, x, z]$	$[2]$
3	$[y, -x, z]$	$[3]$
4	$[-x, -y, z]$	$[4]$
5	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	$[5]$
6	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	$[6]$
7	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	$[7]$
8	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	$[8]$
9	$[x, y, z + \frac{1}{2}]$	$[9]$

*continued ...*

Table 4

No.	position	mapping
10	$[-y, x, z + \frac{1}{2}]$	[10]
11	$[y, -x, z + \frac{1}{2}]$	[11]
12	$[-x, -y, z + \frac{1}{2}]$	[12]
13	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[13]
14	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[14]
15	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[15]
16	$[y + \frac{1}{2}, x + \frac{1}{2}, z]$	[16]