

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

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4, 17, 18, 19, 20]$
2	$[0, 0, z + \frac{1}{2}]$	$[5, 6, 7, 8, 21, 22, 23, 24]$
3	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[9, 10, 11, 12, 25, 26, 27, 28]$
4	$[\frac{1}{2}, \frac{1}{2}, z]$	$[13, 14, 15, 16, 29, 30, 31, 32]$

Table 2: Wyckoff site: 4b, site symmetry:  $2.mm1'$ 

No.	position	mapping
1	$[\frac{1}{2}, 0, z]$	$[1, 4, 15, 16, 17, 20, 31, 32]$
2	$[0, \frac{1}{2}, z]$	$[2, 3, 13, 14, 18, 19, 29, 30]$
3	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	$[5, 6, 10, 11, 21, 22, 26, 27]$
4	$[0, \frac{1}{2}, z + \frac{1}{2}]$	$[7, 8, 9, 12, 23, 24, 25, 28]$

Table 3: Wyckoff site: 8c, site symmetry:  $..m1'$ 

No.	position	mapping
1	$[x, x + \frac{1}{2}, z]$	$[1, 16, 17, 32]$
2	$[\frac{1}{2} - x, x, z]$	$[2, 13, 18, 29]$
3	$[x + \frac{1}{2}, -x, z]$	$[3, 14, 19, 30]$
4	$[-x, \frac{1}{2} - x, z]$	$[4, 15, 20, 31]$
5	$[-x, x + \frac{1}{2}, z + \frac{1}{2}]$	$[5, 10, 21, 26]$
6	$[x, \frac{1}{2} - x, z + \frac{1}{2}]$	$[6, 11, 22, 27]$
7	$[\frac{1}{2} - x, -x, z + \frac{1}{2}]$	$[7, 12, 23, 28]$
8	$[x + \frac{1}{2}, x, z + \frac{1}{2}]$	$[8, 9, 24, 25]$

Table 4: Wyckoff site: 16d, site symmetry:  $11'$ 

No.	position	mapping
1	$[x, y, z]$	$[1, 17]$
2	$[-y, x, z]$	$[2, 18]$
3	$[y, -x, z]$	$[3, 19]$
4	$[-x, -y, z]$	$[4, 20]$
5	$[-x, y, z + \frac{1}{2}]$	$[5, 21]$
6	$[x, -y, z + \frac{1}{2}]$	$[6, 22]$
7	$[-y, -x, z + \frac{1}{2}]$	$[7, 23]$
8	$[y, x, z + \frac{1}{2}]$	$[8, 24]$
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	$[9, 25]$

*continued ...*

Table 4

No.	position	mapping
10	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[10,26]
11	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[11,27]
12	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[12,28]
13	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[13,29]
14	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[14,30]
15	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[15,31]
16	$[y + \frac{1}{2}, x + \frac{1}{2}, z]$	[16,32]