

Table 1: Wyckoff site: 4a, site symmetry:  $mm21'$

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

Table 2: Wyckoff site: 8b, site symmetry:  $. . 21'$

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

Table 3: Wyckoff site: 8c, site symmetry:  $m . . 1'$

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

Table 4: Wyckoff site: 8d, site symmetry:  $.m . 1'$

No.	position	mapping
1	$[x, 0, z]$	$[1, 4, 17, 20]$
2	$[-x, 0, z]$	$[2, 3, 18, 19]$
3	$[x, \frac{1}{2}, z + \frac{1}{2}]$	$[5, 8, 21, 24]$
4	$[-x, \frac{1}{2}, z + \frac{1}{2}]$	$[6, 7, 22, 23]$
5	$[x + \frac{1}{2}, 0, z + \frac{1}{2}]$	$[9, 12, 25, 28]$

*continued ...*

Table 4

No.	position	mapping
6	$[\frac{1}{2} - x, 0, z + \frac{1}{2}]$	[10, 11, 26, 27]
7	$[x + \frac{1}{2}, \frac{1}{2}, z]$	[13, 16, 29, 32]
8	$[\frac{1}{2} - x, \frac{1}{2}, z]$	[14, 15, 30, 31]

Table 5: Wyckoff site: 16e, site symmetry: 11'

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