

Table 1: Wyckoff site: 4a, site symmetry:  $.-3'.1'$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 5, 6, 13, 17, 18, 25, 29, 30, 37, 41, 42]$
2	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[2, 10, 11, 14, 22, 23, 26, 34, 35, 38, 46, 47]$
3	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, 7, 12, 15, 19, 24, 27, 31, 36, 39, 43, 48]$
4	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[4, 8, 9, 16, 20, 21, 28, 32, 33, 40, 44, 45]$

Table 2: Wyckoff site: 4b, site symmetry:  $.-3'.1'$

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, 5, 6, 13, 17, 18, 25, 29, 30, 37, 41, 42]$
2	$[0, 0, \frac{1}{2}]$	$[2, 10, 11, 14, 22, 23, 26, 34, 35, 38, 46, 47]$
3	$[\frac{1}{2}, 0, 0]$	$[3, 7, 12, 15, 19, 24, 27, 31, 36, 39, 43, 48]$
4	$[0, \frac{1}{2}, 0]$	$[4, 8, 9, 16, 20, 21, 28, 32, 33, 40, 44, 45]$

Table 3: Wyckoff site: 8c, site symmetry:  $.3.1'$

No.	position	mapping
1	$[x, x, x]$	$[1, 5, 6, 25, 29, 30]$
2	$[x + \frac{1}{2}, \frac{1}{2} - x, -x]$	$[2, 10, 11, 26, 34, 35]$
3	$[-x, x + \frac{1}{2}, \frac{1}{2} - x]$	$[3, 7, 12, 27, 31, 36]$
4	$[\frac{1}{2} - x, -x, x + \frac{1}{2}]$	$[4, 8, 9, 28, 32, 33]$
5	$[-x, -x, -x]$	$[13, 17, 18, 37, 41, 42]$
6	$[\frac{1}{2} - x, x + \frac{1}{2}, x]$	$[14, 22, 23, 38, 46, 47]$
7	$[x, \frac{1}{2} - x, x + \frac{1}{2}]$	$[15, 19, 24, 39, 43, 48]$
8	$[x + \frac{1}{2}, x, \frac{1}{2} - x]$	$[16, 20, 21, 40, 44, 45]$

Table 4: Wyckoff site: 24d, site symmetry:  $11'$

No.	position	mapping
1	$[x, y, z]$	$[1, 25]$
2	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	$[2, 26]$
3	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	$[3, 27]$
4	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	$[4, 28]$
5	$[z, x, y]$	$[5, 29]$
6	$[y, z, x]$	$[6, 30]$
7	$[-y, z + \frac{1}{2}, \frac{1}{2} - x]$	$[7, 31]$
8	$[\frac{1}{2} - z, -x, y + \frac{1}{2}]$	$[8, 32]$
9	$[\frac{1}{2} - y, -z, x + \frac{1}{2}]$	$[9, 33]$

*continued ...*

Table 4

No.	position	mapping
10	$[z + \frac{1}{2}, \frac{1}{2} - x, -y]$	[10,34]
11	$[y + \frac{1}{2}, \frac{1}{2} - z, -x]$	[11,35]
12	$[-z, x + \frac{1}{2}, \frac{1}{2} - y]$	[12,36]
13	$[-x, -y, -z]$	[13,37]
14	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[14,38]
15	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[15,39]
16	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[16,40]
17	$[-z, -x, -y]$	[17,41]
18	$[-y, -z, -x]$	[18,42]
19	$[y, \frac{1}{2} - z, x + \frac{1}{2}]$	[19,43]
20	$[z + \frac{1}{2}, x, \frac{1}{2} - y]$	[20,44]
21	$[y + \frac{1}{2}, z, \frac{1}{2} - x]$	[21,45]
22	$[\frac{1}{2} - z, x + \frac{1}{2}, y]$	[22,46]
23	$[\frac{1}{2} - y, z + \frac{1}{2}, x]$	[23,47]
24	$[z, \frac{1}{2} - x, y + \frac{1}{2}]$	[24,48]