

Table 1: Wyckoff site: 4a, site symmetry:  $.321'$ 

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

Table 2: Wyckoff site: 4b, site symmetry:  $.321'$ 

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

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

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

Table 4: Wyckoff site: 12d, site symmetry:  $..21'$ 

No.	position	mapping
1	$[\frac{1}{8}, y, \frac{1}{4} - y]$	[1, 14, 25, 38]
2	$[\frac{7}{8}, y + \frac{1}{2}, y + \frac{1}{4}]$	[2, 9, 26, 33]
3	$[\frac{3}{8}, -y, \frac{3}{4} - y]$	[3, 10, 27, 34]
4	$[\frac{1}{2} - y, y + \frac{3}{4}, \frac{5}{8}]$	[4, 21, 28, 45]
5	$[y + \frac{1}{2}, y + \frac{1}{4}, \frac{7}{8}]$	[5, 23, 29, 47]
6	$[\frac{3}{4} - y, \frac{3}{8}, -y]$	[6, 22, 30, 46]
7	$[y + \frac{3}{4}, \frac{5}{8}, \frac{1}{2} - y]$	[7, 24, 31, 48]
8	$[\frac{5}{8}, \frac{1}{2} - y, y + \frac{3}{4}]$	[8, 13, 32, 37]
9	$[y + \frac{1}{4}, \frac{7}{8}, y + \frac{1}{2}]$	[11, 20, 35, 44]

*continued ...*

Table 4

No.	position	mapping
10	$[\frac{1}{4} - y, \frac{1}{8}, y]$	[12, 17, 36, 41]
11	$[-y, \frac{3}{4} - y, \frac{3}{8}]$	[15, 19, 39, 43]
12	$[y, \frac{1}{4} - y, \frac{1}{8}]$	[16, 18, 40, 42]

Table 5: Wyckoff site: **24e**, site symmetry:  $11'$ 

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