

Table 1: Wyckoff site: 8a, site symmetry: $.3.1'$

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

Table 2: Wyckoff site: 12b, site symmetry: $2..1'$

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

Table 3: Wyckoff site: 24c, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	[1, 25]
2	$[x, -y, \frac{1}{2} - z]$	[2, 26]
3	$[\frac{1}{2} - x, y, -z]$	[3, 27]
4	$[-x, \frac{1}{2} - y, z]$	[4, 28]
5	$[z, x, y]$	[5, 29]
6	$[y, z, x]$	[6, 30]
7	$[\frac{1}{2} - y, z, -x]$	[7, 31]
8	$[-z, \frac{1}{2} - x, y]$	[8, 32]
9	$[-y, \frac{1}{2} - z, x]$	[9, 33]
10	$[z, -x, \frac{1}{2} - y]$	[10, 34]
11	$[y, -z, \frac{1}{2} - x]$	[11, 35]

continued ...

Table 3

No.	position	mapping
12	$[\frac{1}{2} - z, x, -y]$	[12, 36]
13	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[13, 37]
14	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[14, 38]
15	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[15, 39]
16	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[16, 40]
17	$[z + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}]$	[17, 41]
18	$[y + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}]$	[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]