

Table 1: Wyckoff site: 4a, site symmetry: $22'2'$

No.	position	mapping
1	$[\frac{3}{4}, \frac{3}{4}, 0]$	[1,2,11,12]
2	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$	[3,4,9,10]
3	$[\frac{1}{4}, \frac{1}{4}, 0]$	[5,6,15,16]
4	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$	[7,8,13,14]

Table 2: Wyckoff site: 4b, site symmetry: $22'2'$

No.	position	mapping
1	$[\frac{1}{4}, \frac{3}{4}, 0]$	[1,2,11,12]
2	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	[3,4,9,10]
3	$[\frac{3}{4}, \frac{1}{4}, 0]$	[5,6,15,16]
4	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$	[7,8,13,14]

Table 3: Wyckoff site: 4c, site symmetry: $. . 2'/m$

No.	position	mapping
1	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[1,8,12,13]
2	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[2,7,11,14]
3	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[3,6,10,15]
4	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[4,5,9,16]

Table 4: Wyckoff site: 4d, site symmetry: $. . 2'/m$

No.	position	mapping
1	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[1,8,12,13]
2	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[2,7,11,14]
3	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[3,6,10,15]
4	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[4,5,9,16]

Table 5: Wyckoff site: 8e, site symmetry: -1

No.	position	mapping
1	[0, 0, 0]	[1,5]
2	$[0, \frac{1}{2}, 0]$	[2,6]

continued ...

Table 5

No.	position	mapping
3	$[0, \frac{1}{2}, \frac{1}{2}]$	[3,7]
4	$[0, 0, \frac{1}{2}]$	[4,8]
5	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[9,13]
6	$[\frac{1}{2}, 0, \frac{1}{2}]$	[10,14]
7	$[\frac{1}{2}, 0, 0]$	[11,15]
8	$[\frac{1}{2}, \frac{1}{2}, 0]$	[12,16]

Table 6: Wyckoff site: 8f, site symmetry: 2.

No.	position	mapping
1	$[x, \frac{3}{4}, 0]$	[1,2]
2	$[-x, \frac{1}{4}, \frac{1}{2}]$	[3,4]
3	$[-x, \frac{1}{4}, 0]$	[5,6]
4	$[x, \frac{3}{4}, \frac{1}{2}]$	[7,8]
5	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{2}]$	[9,10]
6	$[\frac{1}{2} - x, \frac{3}{4}, 0]$	[11,12]
7	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{2}]$	[13,14]
8	$[x + \frac{1}{2}, \frac{1}{4}, 0]$	[15,16]

Table 7: Wyckoff site: 8g, site symmetry: .2'

No.	position	mapping
1	$[\frac{3}{4}, y, 0]$	[1,11]
2	$[\frac{3}{4}, \frac{1}{2} - y, 0]$	[2,12]
3	$[\frac{1}{4}, y + \frac{1}{2}, \frac{1}{2}]$	[3,9]
4	$[\frac{1}{4}, -y, \frac{1}{2}]$	[4,10]
5	$[\frac{1}{4}, -y, 0]$	[5,15]
6	$[\frac{1}{4}, y + \frac{1}{2}, 0]$	[6,16]
7	$[\frac{3}{4}, \frac{1}{2} - y, \frac{1}{2}]$	[7,13]
8	$[\frac{3}{4}, y, \frac{1}{2}]$	[8,14]

Table 8: Wyckoff site: 8h, site symmetry: ..2'

No.	position	mapping
1	$[\frac{3}{4}, \frac{3}{4}, z]$	[1,12]
2	$[\frac{3}{4}, \frac{3}{4}, -z]$	[2,11]
3	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[3,10]
4	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[4,9]
5	$[\frac{1}{4}, \frac{1}{4}, -z]$	[5,16]

continued ...

Table 8

No.	position	mapping
6	$[\frac{1}{4}, \frac{1}{4}, z]$	[6,15]
7	$[\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[7,14]
8	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[8,13]

Table 9: Wyckoff site: 8i, site symmetry: $\dots 2'$

No.	position	mapping
1	$[\frac{3}{4}, \frac{1}{4}, z]$	[1,12]
2	$[\frac{3}{4}, \frac{1}{4}, -z]$	[2,11]
3	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[3,10]
4	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[4,9]
5	$[\frac{1}{4}, \frac{3}{4}, -z]$	[5,16]
6	$[\frac{1}{4}, \frac{3}{4}, z]$	[6,15]
7	$[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[7,14]
8	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[8,13]

Table 10: Wyckoff site: 8j, site symmetry: $\dots m$

No.	position	mapping
1	$[x, y, \frac{3}{4}]$	[1,8]
2	$[x, \frac{1}{2} - y, \frac{1}{4}]$	[2,7]
3	$[-x, y + \frac{1}{2}, \frac{3}{4}]$	[3,6]
4	$[-x, -y, \frac{1}{4}]$	[4,5]
5	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{4}]$	[9,16]
6	$[x + \frac{1}{2}, -y, \frac{3}{4}]$	[10,15]
7	$[\frac{1}{2} - x, y, \frac{1}{4}]$	[11,14]
8	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{3}{4}]$	[12,13]

Table 11: Wyckoff site: 16k, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x, \frac{1}{2} - y, -z]$	[2]
3	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[3]
4	$[-x, -y, z + \frac{1}{2}]$	[4]
5	$[-x, -y, -z]$	[5]
6	$[-x, y + \frac{1}{2}, z]$	[6]
7	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[7]
8	$[x, y, \frac{1}{2} - z]$	[8]

continued ...

Table 11

No.	position	mapping
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9]
10	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	[10]
11	$[\frac{1}{2} - x, y, -z]$	[11]
12	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[12]
13	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[13]
14	$[\frac{1}{2} - x, y, z + \frac{1}{2}]$	[14]
15	$[x + \frac{1}{2}, -y, z]$	[15]
16	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[16]