

Table 1: Wyckoff site: 4a, site symmetry: 2.22

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

Table 2: Wyckoff site: 4b, site symmetry: 2.22

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

Table 3: Wyckoff site: 8c, site symmetry: 2'..

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

Table 4: Wyckoff site: 8d, site symmetry: ..2

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

Table 5: Wyckoff site: **8e**, site symmetry: $. . 2'$

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

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

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

Table 7: Wyckoff site: **16g**, site symmetry: 1

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