

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

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

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

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

Table 3: Wyckoff site: 8c, site symmetry: -1

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

Table 4: Wyckoff site: 8d, site symmetry: -1

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

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

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

Table 6: Wyckoff site: $16f$, site symmetry: 1

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