

Table 1: Wyckoff site: 4a, site symmetry: $2.2'2'$

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $4..$

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

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

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

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

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

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

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

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

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