

Table 1: Wyckoff site: 4a, site symmetry: $2/m'..$

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

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

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

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

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

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

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

Table 5: Wyckoff site: $8e$, 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	$[x + \frac{1}{2}, \frac{1}{4}, 0]$	[9,10]
6	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{2}]$	[11,12]
7	$[\frac{1}{2} - x, \frac{3}{4}, 0]$	[13,14]
8	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{2}]$	[15,16]

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

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

Table 7: Wyckoff site: $8g$, site symmetry: $..m$

No.	position	mapping
1	$[x, y, \frac{1}{4}]$	[1,8]
2	$[x, \frac{1}{2} - y, \frac{3}{4}]$	[2,7]
3	$[-x, y + \frac{1}{2}, \frac{1}{4}]$	[3,6]
4	$[-x, -y, \frac{3}{4}]$	[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 8: Wyckoff site: $16h$, 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]

continued ...

Table 8

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