

Table 1: Wyckoff site: 2a, site symmetry: $-4'm2'$

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

Table 2: Wyckoff site: 2b, site symmetry: $-4'm2'$

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $..2'/m'$

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

Table 6: Wyckoff site: 4f, site symmetry: 2mm.

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

Table 7: Wyckoff site: 8g, site symmetry: $\dots 2'$

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

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

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

Table 9: Wyckoff site: 8i, site symmetry: $\dots m$.

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

continued ...

Table 9

No.	position	mapping
8	$[-y, \frac{3}{4}, -z]$	[12,14]

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

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

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	$[-x, y + \frac{1}{2}, -z]$	[3]
4	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[4]
5	$[-x, -y, -z]$	[5]
6	$[\frac{1}{2} - x, y, z]$	[6]
7	$[x, \frac{1}{2} - y, z]$	[7]
8	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[8]
9	$[\frac{1}{2} - y, x, z]$	[9]
10	$[y, \frac{1}{2} - x, z]$	[10]
11	$[y + \frac{1}{2}, x + \frac{1}{2}, -z]$	[11]
12	$[-y, -x, -z]$	[12]
13	$[y + \frac{1}{2}, -x, -z]$	[13]
14	$[-y, x + \frac{1}{2}, -z]$	[14]
15	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[15]
16	$[y, x, z]$	[16]