

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, \frac{1}{4}, 0]$	[1,8,10,15]
2	$[x + \frac{1}{2}, \frac{1}{4}, 0]$	[2,7,9,16]

continued ...

Table 5

No.	position	mapping
3	$[\frac{1}{2} - x, \frac{3}{4}, 0]$	[3, 6, 12, 13]
4	$[-x, \frac{3}{4}, 0]$	[4, 5, 11, 14]

Table 6: Wyckoff site: $4\mathbf{f}$, site symmetry: $2'm'm$

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

Table 7: Wyckoff site: $8\mathbf{g}$, site symmetry: $..2'$

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

Table 8: Wyckoff site: $8\mathbf{h}$, site symmetry: $..2$

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

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

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

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

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

Table 11: Wyckoff site: 8k, site symmetry: $\dots m'$

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

Table 12: Wyckoff site: 16l, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[2]
3	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[3]

continued ...

Table 12

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