

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[\frac{3}{4}, 0, \frac{1}{4}]$	[1,4,10,11]
2	$[\frac{1}{4}, 0, \frac{1}{4}]$	[2,3,9,12]

continued ...

Table 5

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

Table 6: Wyckoff site: 4f, site symmetry: 2'22'

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

Table 7: Wyckoff site: 4g, site symmetry: 2'2'2

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

Table 8: Wyckoff site: 4h, site symmetry: 2'22'

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

Table 9: Wyckoff site: 8i, site symmetry: 2'..

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

continued ...

Table 9

No.	position	mapping
8	$[x + \frac{1}{2}, 0, \frac{3}{4}]$	[8,15]

Table 10: Wyckoff site: 8j, site symmetry: $2'..$

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

Table 11: Wyckoff site: 8k, site symmetry: $.2'$

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

Table 12: Wyckoff site: 8l, site symmetry: $.2$

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

Table 13: Wyckoff site: $8m$, site symmetry: $\dots 2$

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

Table 14: Wyckoff site: $8n$, site symmetry: $\dots 2'$

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

Table 15: Wyckoff site: $8o$, site symmetry: $\dots 2$

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

Table 16: Wyckoff site: $8p$, site symmetry: $\dots 2'$

No.	position	mapping
1	$[0, 0, z]$	[1,12]
2	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[2,11]
3	$[0, 0, \frac{1}{2} - z]$	[3,10]

continued ...

Table 16

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

Table 17: Wyckoff site: 8q, site symmetry: $. . m'$

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

Table 18: Wyckoff site: 16r, site symmetry: 1

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