

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: 222

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, 0]$	[1,2,3,4]
2	$[\frac{3}{4}, \frac{3}{4}, 0]$	[5,6,7,8]

continued ...

Table 5

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

Table 6: Wyckoff site: $4\mathbf{f}$, site symmetry: $22'2'$

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

Table 7: Wyckoff site: $4\mathbf{g}$, site symmetry: 222

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

Table 8: Wyckoff site: $4\mathbf{h}$, site symmetry: $22'2'$

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

Table 9: Wyckoff site: $8\mathbf{i}$, site symmetry: $2. .$

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

continued ...

Table 9

No.	position	mapping
8	$[x, \frac{3}{4}, 0]$	[15, 16]

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

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

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

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

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

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

Table 13: Wyckoff site: $8\mathbf{m}$, site symmetry: $.2$.

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

Table 14: Wyckoff site: $8\mathbf{n}$, site symmetry: $.2'$.

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

Table 15: Wyckoff site: $8\mathbf{o}$, site symmetry: $.2$.

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

Table 16: Wyckoff site: $8\mathbf{p}$, site symmetry: $.2'$.

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

continued ...

Table 16

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

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

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

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

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