

Table 1: Wyckoff site: 4a, site symmetry: $-11'$

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

Table 2: Wyckoff site: 4b, site symmetry: $-11'$

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

Table 3: Wyckoff site: 4c, site symmetry: $..21'$

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

Table 4: Wyckoff site: 4d, site symmetry: $..21'$

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

Table 5: Wyckoff site: 8e, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	$[1, 9]$
2	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	$[2, 10]$

continued ...

Table 5

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