

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

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry:  $2..1'$

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

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