

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

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

Table 2: Wyckoff site: 4b, site symmetry:  $.2.1'$

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

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

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

Table 4: Wyckoff site: 8d, site symmetry:  $11'$

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