

Table 1: Wyckoff site: 4a, site symmetry:  $\dots 21'$

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

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

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

Table 3: Wyckoff site: 8c, site symmetry:  $11'$

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