

Table 1: Wyckoff site: 2a, site symmetry:  $mm21'$

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

Table 2: Wyckoff site: 2b, site symmetry:  $mm21'$

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

Table 3: Wyckoff site: 4c, site symmetry:  $.m.1'$

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

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

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

Table 5: Wyckoff site: 4e, site symmetry:  $m..1'$

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

Table 6: Wyckoff site:  $8f$ , site symmetry:  $11'$ 

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