

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

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

Table 2: Wyckoff site: 4b, site symmetry: $\dots 21'$

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

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

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

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

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