

Table 1: Wyckoff site: 4a, site symmetry: $.2.1'$

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

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

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

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

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

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

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