

MSG No. 91.107 $P4_1'2'2$ [Type III, tetragonal]

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

No.	position	mapping
1	$[0, y, 0]$	$[1, 8]$
2	$[0, -y, \frac{1}{2}]$	$[2, 7]$
3	$[y, 0, \frac{3}{4}]$	$[3, 6]$
4	$[-y, 0, \frac{1}{4}]$	$[4, 5]$

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

No.	position	mapping
1	$[\frac{1}{2}, y, 0]$	$[1, 8]$
2	$[\frac{1}{2}, -y, \frac{1}{2}]$	$[2, 7]$
3	$[y, \frac{1}{2}, \frac{3}{4}]$	$[3, 6]$
4	$[-y, \frac{1}{2}, \frac{1}{4}]$	$[4, 5]$

Table 3: Wyckoff site: 4c, site symmetry: $.2$

No.	position	mapping
1	$[x, x, \frac{3}{8}]$	$[1, 3]$
2	$[-x, -x, \frac{7}{8}]$	$[2, 4]$
3	$[-x, x, \frac{5}{8}]$	$[5, 8]$
4	$[x, -x, \frac{1}{8}]$	$[6, 7]$

Table 4: Wyckoff site: 8d, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-x, -y, z + \frac{1}{2}]$	$[2]$
3	$[y, x, \frac{3}{4} - z]$	$[3]$
4	$[-y, -x, \frac{1}{4} - z]$	$[4]$
5	$[-y, x, z + \frac{1}{4}]$	$[5]$
6	$[y, -x, z + \frac{3}{4}]$	$[6]$
7	$[x, -y, \frac{1}{2} - z]$	$[7]$
8	$[-x, y, -z]$	$[8]$