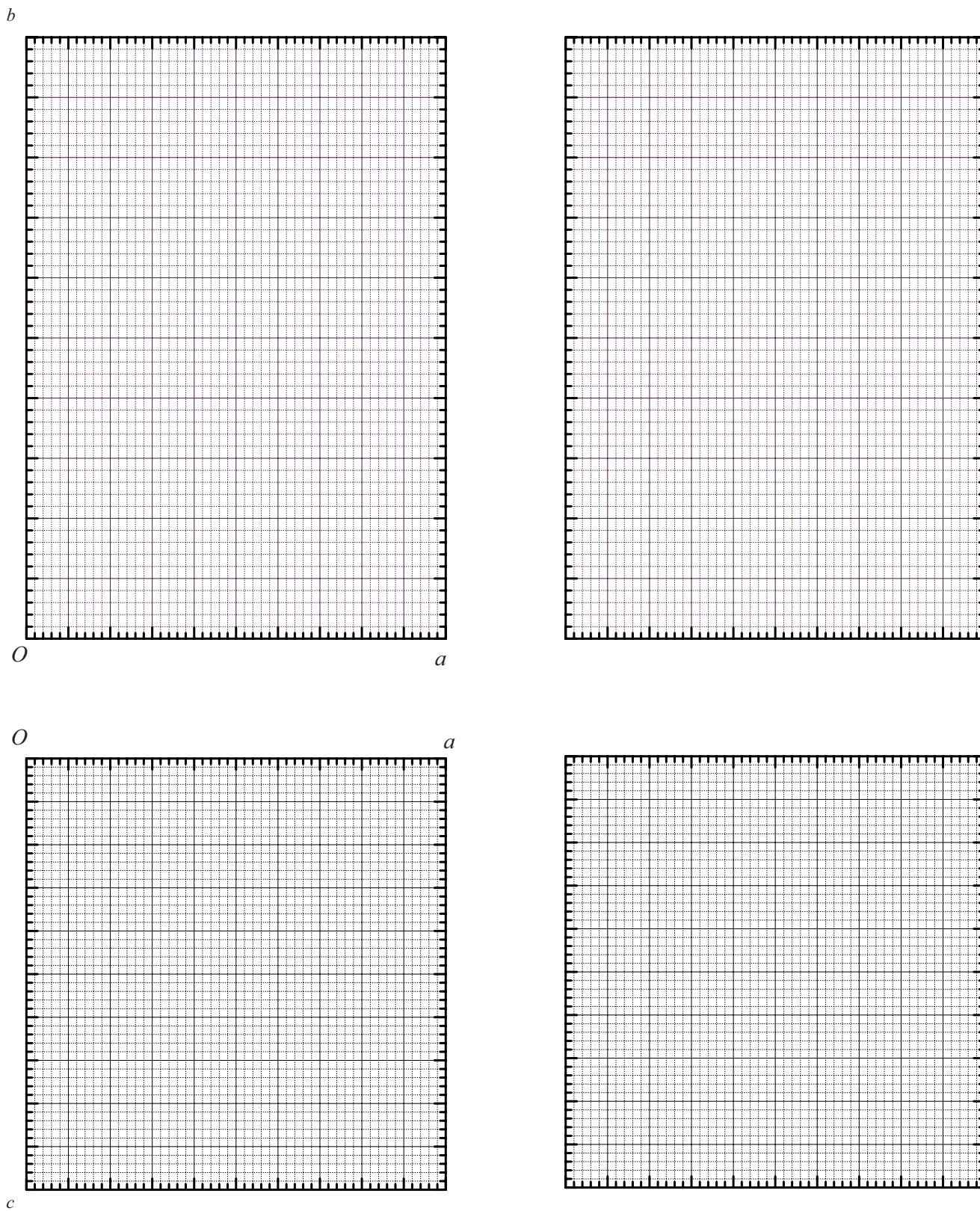




CaTiO₃の結晶学的データ

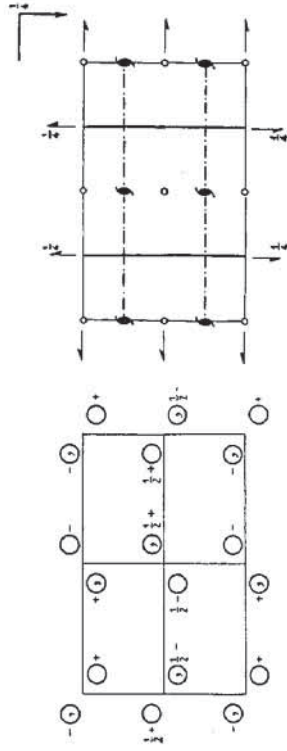
$a=5.38, b=7.64, c=5.44, \text{ Pnma}, Z=4$

Ca 4c (0, 1/4, 0.02); Ti 4b (0, 0, 1/2);

O1 4c (0.42, 1/4, 0.01); O2 8d (0.28, 0.04, 0.21)

$$Pnma \quad D_{2h}^{16}$$
 D_{2h}^{16}

No. 62

$$P_{2_1/n} 2_1/m 2_1/a$$
Orthorhombic $m m m$ 

Origin at $\bar{I}$

Co-ordinates of equivalent positions

Conditions limiting possible reflections

General:

hkl :	No conditions
$0kl$:	$k+l=2n$
$h0l$:	No conditions
$hk0$:	$h=2n$
$h00$:	$(h=2n)$
$0k0$:	$(k=2n)$
$00l$:	$(l=2n)$

**Special: as above, plus
no extra conditions**

$$\} hkl: h+l=2n; \quad k=2n$$

Symmetry of special projections

(100) *cmm*; $b' = b$, $c' = c$

$$(010) \text{ } pgg; \quad c' = c, \quad a' = a$$

(001) *pgm*; $a' = a/2$, $b' = b$

Number of positions,
Wyckoff notation,
and point symmetry

8	d	1	$x, y, z;$ $\bar{x}, \bar{y}, \bar{z};$
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4	c	m	$x, \frac{1}{4}, z;$
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4	b	$\bar{I}$	$0,0,\frac{1}{2};$
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4	α	$\bar{\Gamma}$	0,0,0;
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