

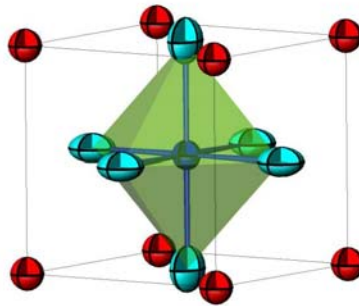
SrTiO₃ (strontium titanate)

a=3.9 Å, cubic, Pm3m (No.221), Z=1

Sr 1a 0,0,0

Ti 1b 1/2, 1/2, 1/2

O 3c 0, 1/2, 1/2



$\lambda=1.4 \text{ \AA}$, $b = 0.1$, $Z_0=8$ (for O), $Z_0=22$ (for Ti), $Z_0=38$ (for Sr)

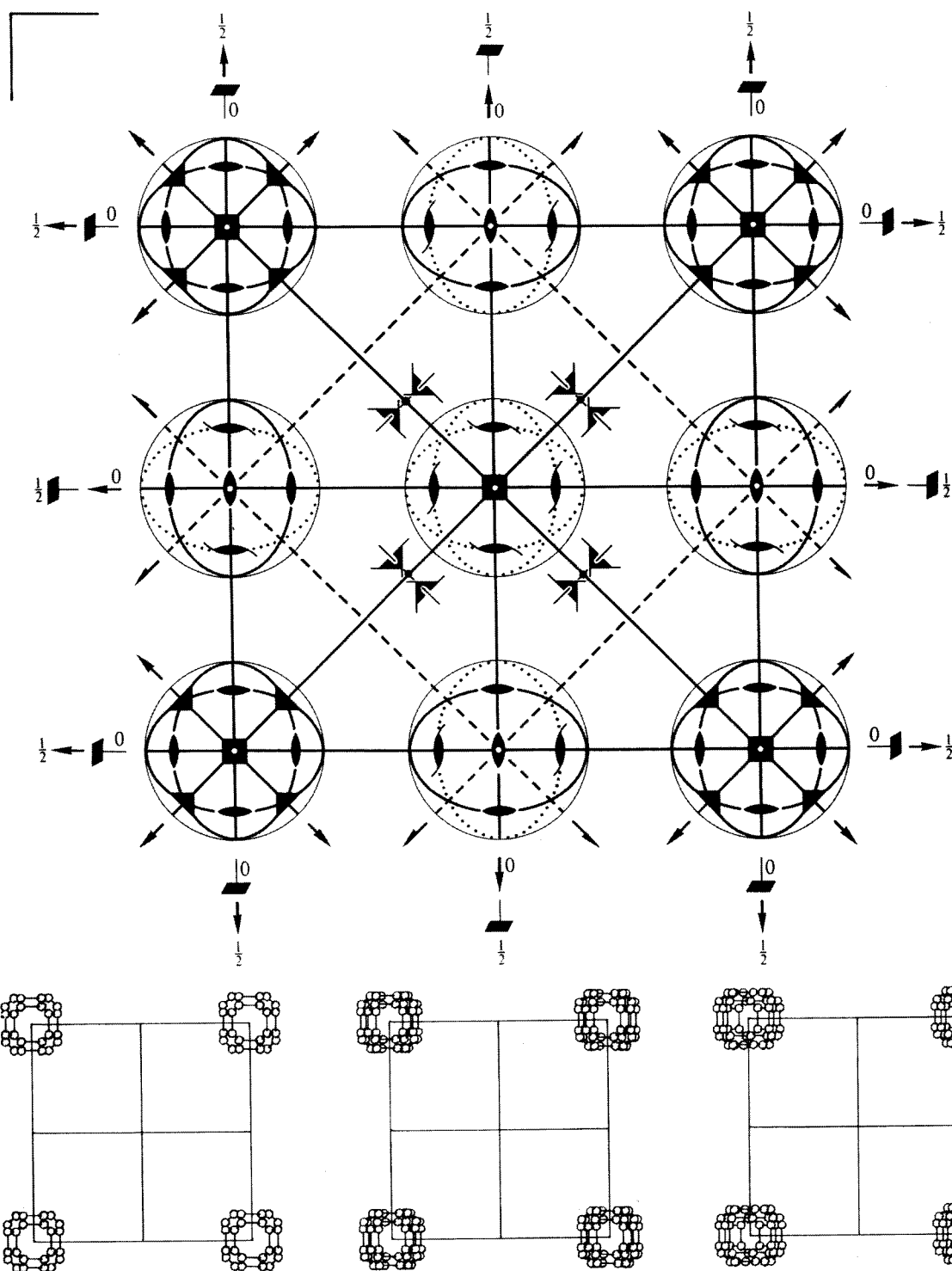
$$f_{\text{ATOM}}(\sin \theta / \lambda) = Z_0 \exp \{-4\pi^2 b (\sin \theta / \lambda)^2\}$$

$$F(hkl) = \sum_{j=1}^{\text{cell}} f_{\text{ATOM}} \exp \{2\pi i (hx_j + ky_j + lz_j)\}$$

$Pm\bar{3}m$ O_h^1 $m\bar{3}m$

Cubic

No. 221

 $P 4/m \bar{3} 2/m$ Patterson symmetry $Pm\bar{3}m$ **Origin** at centre ($m\bar{3}m$)**Asymmetric unit** $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{2}; y \leq x; z \leq y$ Vertices $0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{2},\frac{1}{2},0 \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$ **Symmetry operations**

(given on page 674)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)**Positions**

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
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 h, k, l permutable

General:

no conditions

Special: no extra conditions

48	n	1	(1) x, y, z	(2) $\bar{x}, \bar{y}, z$	(3) $\bar{x}, y, \bar{z}$	(4) $x, \bar{y}, \bar{z}$
			(5) z, x, y	(6) $z, \bar{x}, \bar{y}$	(7) $\bar{z}, \bar{x}, y$	(8) $\bar{z}, x, \bar{y}$
			(9) y, z, x	(10) $\bar{y}, z, \bar{x}$	(11) $y, \bar{z}, \bar{x}$	(12) $\bar{y}, \bar{z}, x$
			(13) $y, x, \bar{z}$	(14) $\bar{y}, \bar{x}, \bar{z}$	(15) $y, \bar{x}, z$	(16) $\bar{y}, x, z$
			(17) $x, z, \bar{y}$	(18) $\bar{x}, z, y$	(19) $\bar{x}, \bar{z}, \bar{y}$	(20) $x, \bar{z}, y$
			(21) $z, y, \bar{x}$	(22) $z, \bar{y}, x$	(23) $\bar{z}, y, x$	(24) $\bar{z}, \bar{y}, \bar{x}$
			(25) $\bar{x}, \bar{y}, \bar{z}$	(26) $x, y, \bar{z}$	(27) $x, \bar{y}, z$	(28) $\bar{x}, y, z$
			(29) $\bar{z}, \bar{x}, \bar{y}$	(30) $\bar{z}, x, y$	(31) $z, x, \bar{y}$	(32) $z, \bar{x}, y$
			(33) $\bar{y}, \bar{z}, \bar{x}$	(34) $y, \bar{z}, x$	(35) $\bar{y}, z, x$	(36) $y, z, \bar{x}$
			(37) $\bar{y}, \bar{x}, z$	(38) y, x, z	(39) $\bar{y}, x, \bar{z}$	(40) $y, \bar{x}, \bar{z}$
			(41) $\bar{x}, \bar{z}, y$	(42) $x, \bar{z}, \bar{y}$	(43) x, z, y	(44) $\bar{x}, z, \bar{y}$
			(45) $\bar{z}, \bar{y}, x$	(46) $\bar{z}, y, \bar{x}$	(47) $z, \bar{y}, \bar{x}$	(48) z, y, x
24	m	$\dots m$	x, x, z	$\bar{x}, \bar{x}, z$	$\bar{x}, x, \bar{z}$	$x, \bar{x}, \bar{z}$
			$\bar{z}, \bar{x}, x$	$\bar{z}, x, \bar{x}$	x, z, x	$\bar{x}, z, \bar{x}$
			$x, x, \bar{z}$	$\bar{x}, \bar{x}, \bar{z}$	$\bar{x}, x, z$	$x, \bar{x}, z$
			$\bar{x}, \bar{z}, \bar{x}$	$x, \bar{z}, x$	$z, x, \bar{x}$	$\bar{z}, x, \bar{x}$
24	l	$m \dots$	$\frac{1}{2}, y, z$	$\frac{1}{2}, \bar{y}, z$	$\frac{1}{2}, y, \bar{z}$	$\frac{1}{2}, \bar{y}, \bar{z}$
			$\bar{z}, \frac{1}{2}, y$	$\bar{z}, \frac{1}{2}, \bar{y}$	$y, z, \frac{1}{2}$	$\bar{y}, z, \frac{1}{2}$
			$y, \frac{1}{2}, \bar{z}$	$\bar{y}, \frac{1}{2}, \bar{z}$	$y, \frac{1}{2}, z$	$\bar{y}, \frac{1}{2}, z$
			$\frac{1}{2}, \bar{z}, \bar{y}$	$\frac{1}{2}, \bar{z}, y$	$z, y, \frac{1}{2}$	$\bar{z}, y, \frac{1}{2}$
24	k	$m \dots$	$0, y, z$	$0, \bar{y}, z$	$0, y, \bar{z}$	$0, \bar{y}, \bar{z}$
			$\bar{z}, 0, y$	$\bar{z}, 0, \bar{y}$	$y, z, 0$	$\bar{y}, z, 0$
			$y, 0, \bar{z}$	$\bar{y}, 0, \bar{z}$	$y, 0, z$	$\bar{y}, 0, z$
			$0, \bar{z}, \bar{y}$	$0, \bar{z}, y$	$z, y, 0$	$\bar{z}, y, 0$
12	j	$m \dots m2$	$\frac{1}{2}, y, y$	$\frac{1}{2}, \bar{y}, y$	$\frac{1}{2}, y, \bar{y}$	$\frac{1}{2}, \bar{y}, \bar{y}$
			$\bar{y}, \frac{1}{2}, y$	$\bar{y}, \frac{1}{2}, \bar{y}$	$y, y, \frac{1}{2}$	$\bar{y}, y, \frac{1}{2}$
12	i	$m \dots m2$	$0, y, y$	$0, \bar{y}, y$	$0, y, \bar{y}$	$0, \bar{y}, \bar{y}$
			$\bar{y}, 0, y$	$\bar{y}, 0, \bar{y}$	$y, y, 0$	$\bar{y}, y, 0$
12	h	$m m 2 \dots$	$x, \frac{1}{2}, 0$	$\bar{x}, \frac{1}{2}, 0$	$0, x, \frac{1}{2}$	$0, \bar{x}, \frac{1}{2}$
			$\frac{1}{2}, x, 0$	$\frac{1}{2}, \bar{x}, 0$	$x, 0, \frac{1}{2}$	$\bar{x}, 0, \frac{1}{2}$
8	g	$\dots 3m$	x, x, x	$\bar{x}, \bar{x}, x$	$\bar{x}, x, \bar{x}$	$x, \bar{x}, \bar{x}$
			$x, x, \bar{x}$	$\bar{x}, \bar{x}, \bar{x}$	$x, \bar{x}, x$	$\bar{x}, x, \bar{x}$
6	f	$4m \dots m$	$x, \frac{1}{2}, \frac{1}{2}$	$\bar{x}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, x, \frac{1}{2}$	$\frac{1}{2}, \bar{x}, \frac{1}{2}$
6	e	$4m \dots m$	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$
3	d	$4/m m \dots m$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, 0$	$0, 0, \frac{1}{2}$	
3	c	$4/m m \dots m$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$	
1	b	$m\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			
1	a	$m\bar{3}m$	$0, 0, 0$			

Symmetry of special projectionsAlong [001] $p4mm$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ Origin at $0, 0, z$ Along [111] $p6mm$ $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$ Origin at x, x, x Along [110] $p2mm$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ Origin at $x, x, 0$