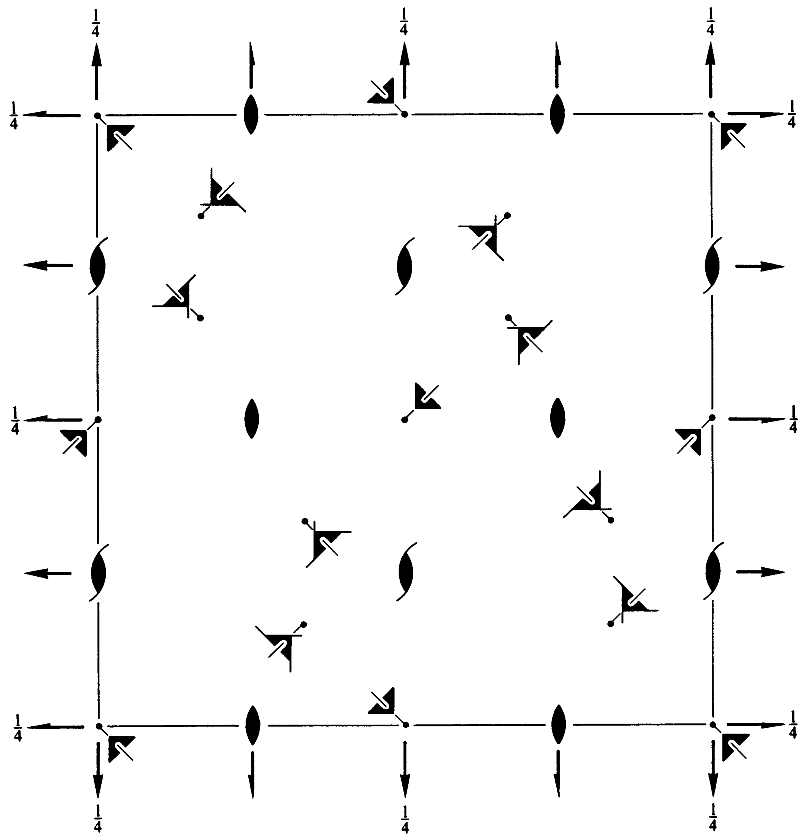
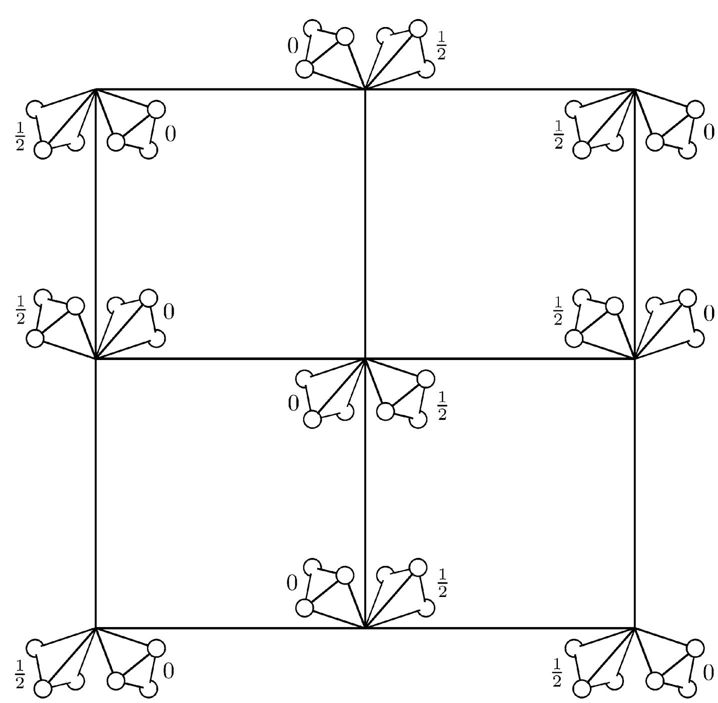
$I2_13$ T^5 23 Cubic

No. 199 $I2_13$ Patterson symmetry $Im\bar{3}$





Origin on 3[111] at midpoint of three non-intersecting pairs of parallel 2 axes and of three non-intersecting pairs of parallel 2_1 axes

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $z \le \min(x, y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $3^{+}\ x,x,x$	(6) $3^{+}\ \bar{x}+\frac{1}{2},x,\bar{x}$	(7) $3^{+}\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) $3^{+}\ \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^{-}\ x,x,x$	(10) $3^{-}(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^{-}(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^{-}(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2\quad 0,\frac{1}{4},z$	(3) $2\quad \frac{1}{4},y,0$	(4) $2\quad x,0,\frac{1}{4}$
(5) $3^{+}(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,x$	(6) $3^{+}(\frac{1}{6},-\frac{1}{6},\frac{1}{6})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$	(7) $3^{+}(-\frac{1}{6},\frac{1}{6},\frac{1}{6})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(8) $3^{+}(\frac{1}{6},\frac{1}{6},-\frac{1}{6})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(9) $3^{-}(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,x$	(10) $3^{-}(\frac{1}{6},-\frac{1}{6},-\frac{1}{6})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^{-}(-\frac{1}{6},-\frac{1}{6},\frac{1}{6})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^{-}(-\frac{1}{6},\frac{1}{6},-\frac{1}{6})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+\quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				h,k,l cyclically permutable General:
24	*c*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	hkl: $h+k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	$0kl$: $k+l=2n$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	hhl: $l=2n$ $h00$: $h=2n$
							Special: no extra conditions
12	*b*	2 . .	$x,0,\frac{1}{4}$ $\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\frac{1}{4},x,0$ $\frac{3}{4},\bar{x}+\frac{1}{2},0$	$0,\frac{1}{4},x$	$0,\frac{3}{4},\bar{x}+\frac{1}{2}$	
8	*a*	. 3 .	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$	

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}\qquad \mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},0,z$

Along [111] $p3$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})\qquad \mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})\qquad \mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x+\frac{1}{4},0$