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catena-Poly[[methanoltrinitratothallium(III)]-μ-4,4′-bipyridine *N*,*N*′-dioxide]

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Key indicators

Single-crystal X-ray study
T = 203 K
Mean σ(C–C) = 0.009 Å
Disorder in main residue
R factor = 0.038
wR factor = 0.113
Data-to-parameter ratio = 12.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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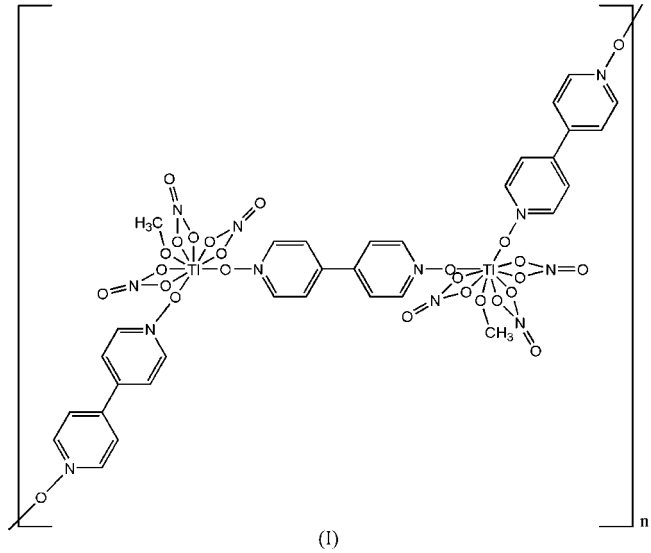
The title compound, $[Tl(NO_3)_3(C_{10}H_8N_2O_2)(CH_4O)]_n$, has a one-dimensional zigzag chain with nitrate and methanol ligands disordered over two positions.

Comment

The construction of a thallium(III) coordination polymer using 4,4′-bipyridine *N*,*N*′-dioxide (bpdo) as bridging ligand results in a crystal structure analogous to the terbium(III) compound reported by Long *et al.* (2002). We report here the structure of the title coordination polymer, (I); the asymmetric unit is labeled in Fig. 1.



(I)

Compound (I) is a one-dimensional zigzag coordination polymer (Fig. 2) in which the Tl^{III} is coordinated by one bpdo, one methanol and three nitrate ligands. The C_2 symmetry of the molecule causes one of the nitrate ligands and the methanol to be disordered over two positions with site-occupancy factors of 0.5. Zigzag polymeric chains run parallel to [101] (Fig. 3). These chains are linked by weak hydrogen bonding through (methanol)C—H···O(nitrate) and C_{ar}—H···O(nitrate). The hydrogen-bonding details are given in Table 1. All nitrate ligands are bidentate, giving nine-coordinate Tl.

Experimental

Compound (I) was prepared by layering a methanol solution of 4,4′-bipyridine *N*,*N*′-dioxide (0.10 mmol) on top of a layer of $CHCl_3$ in which 0.05 mmol of $Tl(NO_3)_3$ had been placed (but not fully dissolved). The layers mixed over several days at ambient temperature and crystals grew at the interface.

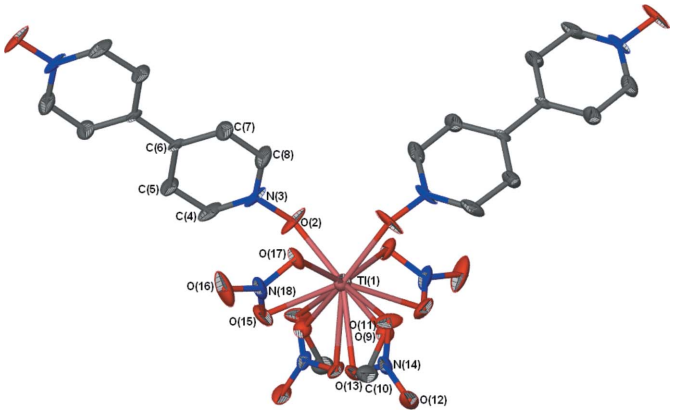


Figure 1
Part of the polymeric chain structure of (I) showing the atom labeling. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity. Atoms of the asymmetric unit are labeled.

Crystal data

$[Tl(NO_3)_3(C_{10}H_8N_2O_2)(CH_4O)]$	D_x = 2.251 Mg m^{-3}
M_r = 609.62	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 12558 reflections
a = 15.337 (3) Å	θ = 1.0–27.5°
b = 8.3370 (17) Å	μ = 9.06 mm^{-1}
c = 14.091 (3) Å	T = 203 (2) K
β = 93.40 (3)°	Block, colorless
V = 1798.6 (6) Å^3	0.10 × 0.10 × 0.09 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	1795 reflections with $I > 2\sigma(I)$
ω and φ scans	R_{int} = 0.049
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)	θ_{max} = 27.1°
T_{min} = 0.405, T_{max} = 0.445	$h = -19 \rightarrow 19$
12558 measured reflections	$k = -10 \rightarrow 10$
1975 independent reflections	$l = -17 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0603P)^2 + 12.8828P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.038	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.113	$\Delta\rho_{max}$ = 0.97 e Å^{-3}
S = 1.21	$\Delta\rho_{min}$ = −2.18 e Å^{-3}
1975 reflections	
155 parameters	
H-atom parameters constrained	

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O12^{i}	0.94	2.36	3.286 (10)	169
C10—H10A···O16^{ii}	0.97	2.40	2.90 (2)	112

Symmetry codes: (i) $x, -y, z-\frac{1}{2}$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

Methanol and one nitrate group are disordered over two positions, with symmetry-defined site-occupancy factors of 0.50. H atoms were placed in geometrically calculated positions and refined using a riding model, with C—H = 0.94 (aromatic) and 0.97 Å (methanol), with U_{iso}(H) = 1.2U_{eq}(aromatic C) and 1.5U_{eq}(methanol C). All non-H atoms were refined anisotropically, except for O9 of the disordered methanol. The deepest residual electron-density hole is 0.87 Å from the Tl atom.

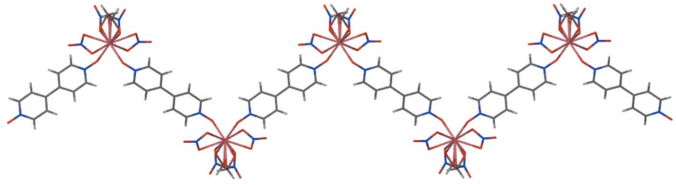


Figure 2
The zigzag polymeric chain in (I).

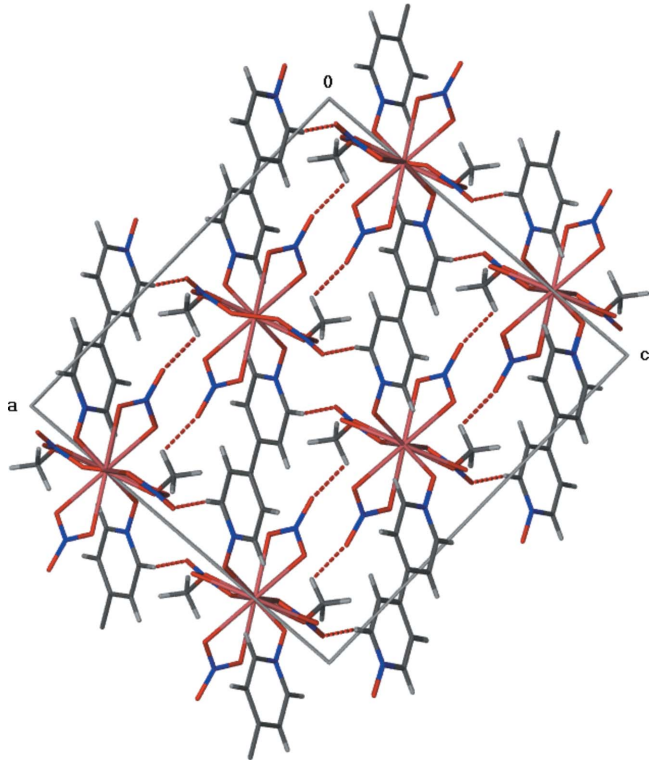


Figure 3
Packing of compound (I), viewed along [010], showing hydrogen bonds (dashed lines) and polymeric chains running parallel to [101].

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001) and *POV-RAY* (Persistence of Vision, 1999); software used to prepare material for publication: *SHELXL97*.

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