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Hexakis(dimethyl sulfoxide-κO)-thallium(III) trinitrate

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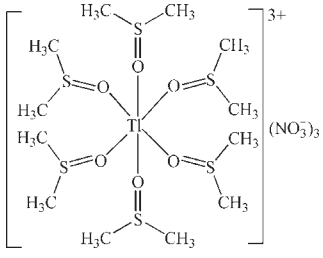
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(S–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.022; wR factor = 0.058; data-to-parameter ratio = 25.1.

The title compound, $[Tl(C_2H_6OS)_6](NO_3)_3$, consists of six dimethyl sulfoxide (DMSO) molecules coordinated to a Tl^{III} atom, which lies on a $\overline{3}$ axis, and three nitrate anions (3. symmetry) to neutralize the charge. The coordination polyhedron around the Tl^{III} atom is octahedral, defined by six O atoms of the DMSO molecules. In the crystal structure, C—H···O hydrogen bonds are observed. One of the nitrate groups exhibits half-occupation.

Related literature

For general background to thallium(III) chemistry, see: Tóth & Gyõri (1994). For related structures, see: Aghabozorg, Ghadermazi *et al.* (2006); Aghabozorg, Ramezanipour *et al.* (2006); Ma *et al.* (2002); Notash *et al.* (2008).



Experimental

Crystal data

$[Tl(C_2H_6OS)_6](NO_3)_3$
M_r = 859.17
Trigonal, $R\overline{3}$
a = 11.7207 (9) Å
c = 19.209 (3) Å
V = 2285.3 (4) Å^3
Z = 3
Mo $K\alpha$ radiation
μ = 5.78 mm^{-1}
T = 100 K
0.23 × 0.12 × 0.04 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.442, T_{max} = 0.786
9649 measured reflections
1480 independent reflections
1480 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.058
S = 0.99
1480 reflections
59 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.97 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1B···O1	0.96	2.42	3.311 (4)	154
C1—H1C···O2^{i}	0.96	2.54	3.448 (11)	158
C2—H2A···O1^{ii}	0.96	2.55	3.380 (6)	145
C2—H2B···O2	0.96	1.99	2.915 (10)	161
C2—H2C···O1	0.96	2.55	3.423 (6)	152

Symmetry codes: (i) $y-\frac{1}{3}, -x+y+\frac{1}{3}, -z+\frac{1}{3}$; (ii) $x-y+\frac{2}{3}, x+\frac{1}{3}, -z+\frac{1}{3}$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2321).

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