APPLIED ORGANOMETALLIC CHEMISTRY
Appl. Organometal. Chem. 2005; **19**: 184–185
Published online in Wiley InterScience (www.interscience.wiley.com). DOI:10.1002/aoc.750

Crystallographic report

Hydro[tris(3-phenyl-2-thioimidazol-1-yl)]boratobismuth dinitrate

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Received 8 July 2004; Revised 13 July 2004; Accepted 14 July 2004

$Bi[HB(tim^{Ph})_3](NO_3)_2$ features a distorted pentagonal pyramidal geometry defined by a sulfur-rich tripodal ligand and three oxygen atoms, derived from mono- and bi-dentate nitrate ligands. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; tripodal ligand; bismuth

COMMENT

Tripodal S_3 ligands of the tris(mercaptoimidazolyl)borate type have attracted much attention for their coordination to main group[1,2] and transition metal ions.[3–5] $Bi[HB(tim^{Ph})_3](NO_3)_2$ (Fig. 1) is a neutral compound with a BiS_3O_3 coordination core that forms a distorted pentagonal pyramidal environment.

EXPERIMENTAL

The complex was prepared in 60% yield by adding an equivalent amount of potassium hydro[tris(3-phenyl-2-thioimidazol-1-yl)]borate in methanol solution to a methanol suspension of $Bi(NO_3)_3{\cdot}5H_2O$. Crystals suitable for X-ray structural analysis were obtained from the slow evaporation of a methanol solution of the complex. Anal. Found: C, 37.10; H, 2.64; N, 12.77; S, 11.36. Calc. for $C_{27}H_{22}BBiN_8O_6S_3$: C, 37.25; H, 2.55; N, 12.87; S 11.05%. IR data (KBr pellet, cm^{-1}): 2431 (s, B–H). Intensity data were collected at 293(2) K on a Bruker Smart Apex CCD diffractometer for a crystal $0.14 \times 0.18 \times 0.21$ mm^3. $C_{27}H_{22}BBiN_8O_6S_3$, $M = 870.50$, triclinic, space group $P\bar{1}$ with $a = 10.9914(11)$, $b = 11.4411(11)$, $c = 14.0557(14)$Å, $\alpha = 68.896(2)$, $\beta = 74.811(2)$, $\gamma = 85.454(2)°$, $Z = 2$, $V = 1591.2(3)$Å^3, 7055 unique data ($\theta_{max} = 28.3°$), $R = 0.053$ (5139 data with $I \geq 2\sigma(I)$), $wR = 0.114$ (all 9746 data), $\rho = 3.29$ e$^-$ Å^{-3} (0.98 Å from bismuth). Programs used: SHELXL 97 and ORTEP. CCDC deposition number: 238996.

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Contract/grant sponsor: Scientific Research Foundation for Returned Overseas Chinese Scholars, State Education Ministry, China.
Contract/grant sponsor: PRP programme of Shanghai Jiao Tong University, China.

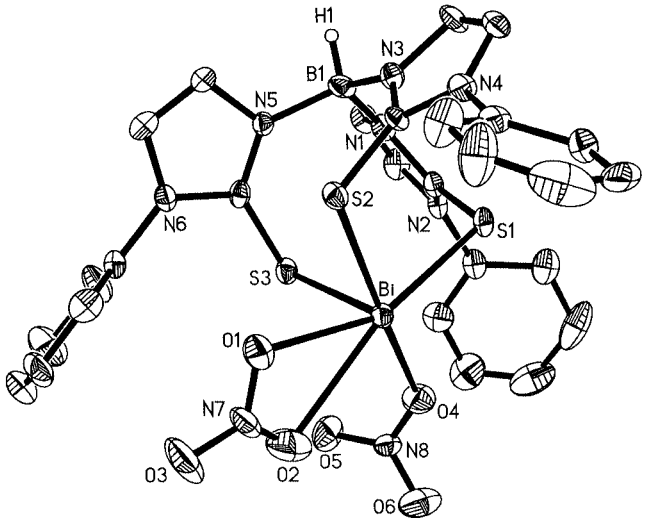

Figure 1. The molecular structure of $Bi[HB(tim^{Ph})_3](NO_3)_2$; hydrogen atoms have been omitted for clarity. Key geometric parameters: Bi–S1 2.696(2), Bi–S2 2.644(2), Bi–S3 2.672(2), Bi–O1 2.572(7), Bi–O2 2.732(9), Bi–O4 2.574(7) Å; S1–Bi–S2 89.75(7), S1–Bi–S3 86.42(7), S2–Bi–S3 90.81(7), O1–Bi–O2 48.5(3), S2–Bi–O1 66.66(16), S2–Bi–O2 115.0(2), S2–Bi–O4 166.39(16)°.

Acknowledgements

We acknowledge financial support by the Scientific Research Foundation for Returned Overseas Chinese Scholars, State Education Ministry, China, and the PRP programme of Shanghai Jiao Tong University, China.

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