



Communication

C–H activation in bithiazole ring with thallium(III) ion

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ABSTRACT

Two novel organometallic complex of 2,2'-dimethyl-4,4'-bithiazole (dm4bt) ligand (**L**) with formula $[\text{Tl}(\text{dm4bt})_2(\text{NO}_3)(\text{H}_2\text{O})]$ (**1**) and $[\text{Tl}(\text{dm4bt})_2(\text{NO}_3)(\text{DMSO})]$ (**2**) have been synthesized and structurally characterized by elemental analysis, FT-IR, ^1H NMR spectra and X-ray crystallography. These complexes also display the first transoid conformation in bithiazole ligands in which C–H bond activation in bithiazole ring is observed with Tl(III) ion.

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1. Introduction

Thallium organometallics have been found importance due to structural versatility, metal–metal interaction, relevance in environmental chemistry and organic synthesis as arylating agent [1]. However a few Tl^{3+} organometallic compounds have been studied by X-ray diffraction. A new type of cyclometallation, so called roll-over metallation [2] or transoid orientation [3] (Scheme 1), is observed for bipyridine derivatives for metals such as Pt, Pd, Ir and Rh [4]. There is no report for transoid coordination for thallium which enables cleavage of a C–H bond of a pyridine [4]. Coordination modes of bithiazole derivatives are similar with bipyridine on the manner that bithiazoles are coordinated to metals from two nitrogens lone pairs of the thiazole rings (Scheme 1).

Here we report first examples of Tl^{3+} bithiazole which used transoid orientation of thiazole rings, in which coordination is performed from one nitrogen of one thiazole ring and the carbon atom from the other thiazole ring (Scheme 2).

2. Results and discussion

2.1. Preparation of complexes 1–2

Treatment of thallium (III) nitrate with 2,2'-dimethyl-4,4'-bithiazole in methanol result in colorless precipitate of **1** after a few days. Suitable crystals were obtained by slow evaporation of a mixed methanol/acetonitrile solution of **1** in 72% yields.

Dissolution of compound **1** in DMSO converts **1** to compound **2** in which the water molecule is replaced by a DMSO molecule, accompanied by isomerization of the complex (Scheme 2).

2.2. Spectroscopic characterization

Compounds **1** and **2** were fully characterized by ^1H NMR, IR spectroscopy, elemental analysis and X-ray crystallography studies.

2.2.1. NMR investigation

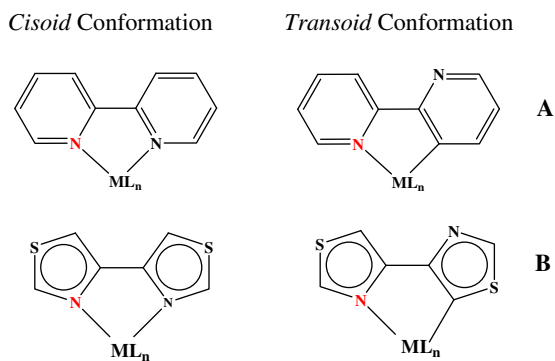
^1H NMR of **1** in DMSO shows two signals for CH_3 in 2.82 (3H) and 2.09 (3H) ppm and a signal for residual aromatic proton at 7.83 (1H) ppm. This is in accord to the structure of **2** and shows that exchange of H_2O with DMSO is fast. The ^1H NMR spectra of free ligand (**L**) and complex **1** in $\text{dmsO-}d_6$ which convert fastly to **2** are shown in Fig. 1. Compounds **1** and **2** are stable in solid states for weeks but in the solution spectrum of free ligand is build up gradually during hours (Fig. 1), so we were unable to observe desirable ^{13}C NMR spectra of these compounds in DMSO.

2.2.2. IR spectroscopy

The infrared spectra for dm4bt and complexes are presented in detail in experimental section. Compounds **1** and **2** have shown several bands in the range $3400\text{--}800\text{ cm}^{-1}$ which are corresponding to skeletal vibrations of the aromatic heterocycle [5]. These bands related to vibrational mode of C–H, C=C, C=N, C–C, C–N, S–C moiety and were observed at similar frequencies in coordination compounds **1** and **2** and the reason is the same anti orientation in free ligand [6] and coordination compounds **1** and **2**. The contrary trend was observed previously for dm4bt [6,7] and bipyridine

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Scheme 1. *Cisoid* and *Transoid* conformation in coordination compounds of bipyridine (A) and bithiazole ligands (B).

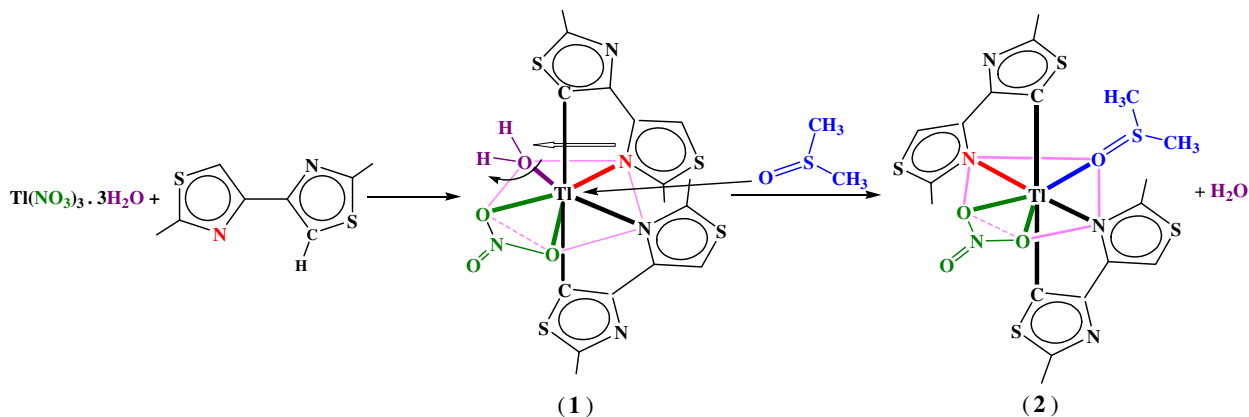
in coordination to metal centers [8] and can be due to conformation change from anti in free ligands to syn in complexes. As shown by X-ray diffraction study of compounds **1** and **2**, the nitrate groups act as a chelating bidentate ligand. So nitrate group should have three vibrational frequencies [9]. These observed frequencies are related to chelating bidentate [$\nu_a(\text{NO}_2)$, $\nu(\text{N}=\text{O})$, and $\nu_s(\text{NO}_2)$]

which are appeared at 1286, 1450, 1026 cm^{-1} and 1299, 1433, 1064 cm^{-1} for **1** and **2**, respectively. Compounds **1** and **2** also show vibration frequencies for $\text{Ti}-\text{N}_{\text{thiazole}}$, respectively in 325 and 329 cm^{-1} [9,10]. In addition, these complexes show $\nu(\text{Ti}-\text{C}_{\text{thiazole}})$ in 459 and 456 cm^{-1} for **1** and **2**, respectively [9,10]. As described in the literature $\nu(\text{S}=\text{O})$ must appear in 1025–985 cm^{-1} and we observed that in 986 cm^{-1} for compound **2** [9].

2.3. Description of the molecular structures of **1** and **2**

The structure of compounds **1** and **2** were determined by X-ray crystallography and their molecular structures and selected bond distances and angles are shown in Fig. 2 and 3.

Compound **1** is the best described as pentagonal bipyramid with carbons (C1 and C9) as apical ligands ($\text{C1}-\text{Ti}-\text{C9} = 169.22^\circ$). This structure is severely distorted due to bite angles of chelating bithiazole rings and different ligands coordinated to thallium. Two bithiazole rings are oriented in *cis* fashion and are almost perpendicular to each other with the angle between two bithiazole rings around 83° (Fig. 2). As can be seen from the packing diagram of complex **1** (Fig. 4), There is some $\text{O}(\text{water})-\text{H}\cdots\text{O}(\text{nitrate})$ [$\text{H4A}\cdots\text{O1}^i = 2.19(8)$, $\text{O4}\cdots\text{O1}^i = 2.858(11)$ Å and $\text{O4}-\text{H4A}\cdots\text{O1}^i = 158.0(8)^\circ$, symmetry codes: (i) $-X, -Y, 1-Z$] and $\text{O}(\text{water})-\text{H}\cdots\text{N}(\text{thiazole})$ [$\text{H4B}\cdots\text{N2}^{ii} = 1.98(10)$, $\text{O4}\cdots\text{N2}^{ii} = 2.907(10)$ Å and



Scheme 2. The synthesis route for **1** and **2** showing also isomerization from *cis* in **1** to *trans* in **2**.

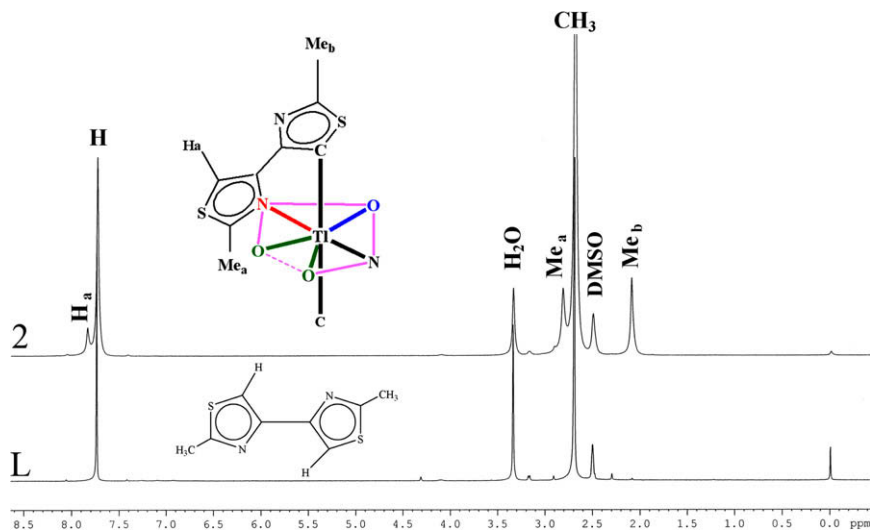


Fig. 1. ^1H NMR Spectra of 2,2'-dimethyl-4,4'-bithiazole (L) and complex **1** in $\text{dms0}-d_6$ which results in formation of complex **2**.

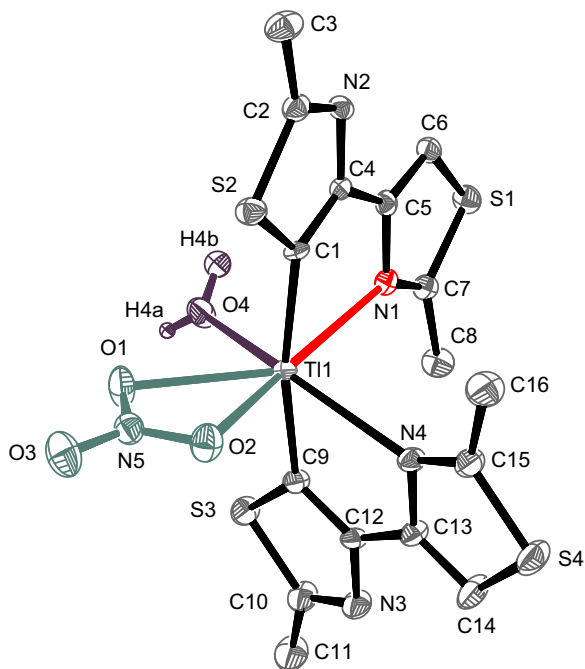


Fig. 2. The labeled diagram of **1**. Thermal ellipsoids are at 30% probability level. Selected bond lengths (Å) and bond angles ($^{\circ}$): C(1)–Ti(1) 2.118(7), C(9)–Ti(1) 2.094(8), N(1)–Ti(1) 2.623(7), N(4)–Ti(1) 2.675(7), O(1)–Ti(1) 2.649(7), O(2)–Ti(1) 2.651(7), O(4)–Ti(1) 2.608(7), C(1)–Ti(1)–C(9) 169.2(3), C(9)–Ti(1)–O(4) 89.5(3), C(1)–Ti(1)–O(4) 94.1(3), C(9)–Ti(1)–N(1) 99.1(3), C(1)–Ti(1)–N(1) 72.2(2), O(4)–Ti(1)–N(1) 74.4(2), C(9)–Ti(1)–O(1) 97.7(3), C(1)–Ti(1)–O(1) 93.1(3), C(1)–Ti(1)–O(2) 94.6(3), C(1)–Ti(1)–O(2) 92.2(3), N(1)–Ti(1)–O(2) 159.1(2), O(1)–Ti(1)–O(2) 47.9(2), C(9)–Ti(1)–N(4) 72.5(3), C(1)–Ti(1)–N(4) 101.0(2), N(1)–Ti(1)–N(4) 92.4(2), C(1)–C(4)–C(5)–N(1) 3.2(10), N(2)–C(4)–C(5)–C(6) 1.7(12), C(9)–C(12)–C(13)–N(4) 1.7(13), N(3)–C(12)–C(13)–C(14) 4.9(15).

O4–H4B...N2ⁱⁱ = 173.0(10) $^{\circ}$, symmetry code: (ii) 1–X, –Y, 1–Z] hydrogen bonds that it seems to be effective in the stabilization of the crystal packing. The NO₃[–] plane and water molecule are almost perpendicular to the basal coordination axis and the angles are 89.63(2) $^{\circ}$ and 88.84(2) $^{\circ}$, respectively. There is also some weak π , π -stacking between adjacent thiazoline rings [(C1–C2–N2–C4–S2)/(C5–C6–N1–C7–S1) = 3.681(5) Å and (C9–C10–N3–C12–S3)/(C13–C14–N4–C15–S4) = 3.996(6) Å] affected the lattice structure of this complex.

Compound **2** can be viewed as octahedral in which one axial position is occupied with bidentate nitrate ion (Fig. 3). In this structure two bithiazole are arranged in the equatorial plane therefore considerable isomerization took place over exchange of water with DMSO. It seems DMSO is coordinated from opposite site of H₂O and H₂O is left and reorientation of the complex was occurred (Scheme 2). Some weak π , π -stacking between adjacent thiazoline rings [(C1–C2–N2–C4–S2)/(C5–C6–N1–C7–S1) = 3.835(5) Å and (C9–C10–N3–C12–S3)/(C13–C14–N4–C15–S4) = 3.975(7) Å] affected the stabilization of the lattice structure.

In both structures thallium–carbon bonds are trans to each other C–Ti–C equal to 169.22 $^{\circ}$ in **1** and 176.30 in **2** and their bond distances are considerably shorter than the Ti–N and Ti–O bonds, indicates that considerable π -back donation is present from full d-orbitals of thallium to the p-orbital of the carbon. The multiple bond character in Ti–C makes it short and strong and result in stability of **1** and **2** in aerobic condition. Organo thallium compounds with Ti–C(phenyl) bond is known to have bond distances between 2.14 and 2.25 Å in complexes with lower coordination number [1,3,11–13] so compound **2** has lower bond distances for Ti–C. Although coordination number of thallium is seven which confirms considerable back donation in **1** and **2**.

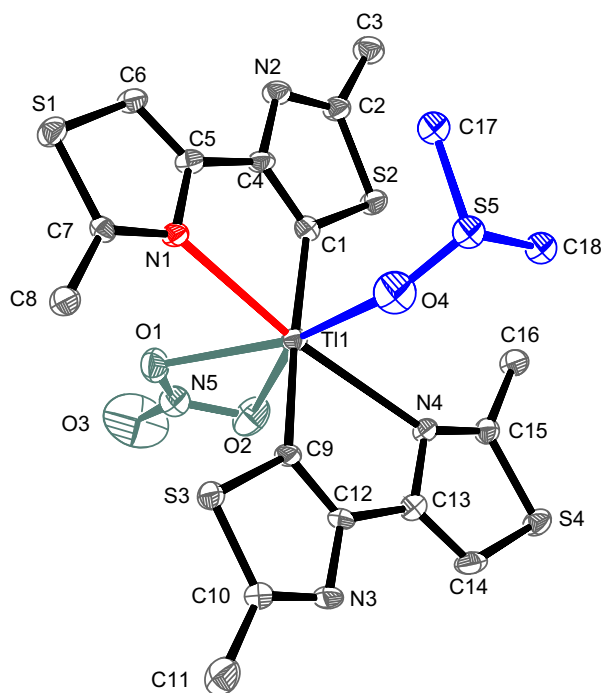


Fig. 3. The labeled diagram of **2**. Thermal ellipsoids are at 30% probability level. Selected bond lengths (Å) and bond angles ($^{\circ}$): C(1)–Ti(1) 2.083(7), C(9)–Ti(1) 2.091(6), N(1)–Ti(1) 2.723(5), N(4)–Ti(1) 2.754(6), O(1)–Ti(1) 2.640(7), O(2)–Ti(1) 2.685(9), O(4)–Ti(1) 2.644(7), C(1)–Ti(1)–C(9) 176.3(3), C(9)–Ti(1)–O(4) 84.3(3), C(1)–Ti(1)–O(4) 92.4(3), C(9)–Ti(1)–N(1) 109.2(2), C(1)–Ti(1)–N(1) 72.2(2), O(4)–Ti(1)–N(1) 87.0(2), C(9)–Ti(1)–O(1) 92.0(3), C(1)–Ti(1)–O(1) 91.7(3), C(1)–Ti(1)–O(2) 94.9(3), N(1)–Ti(1)–O(2) 114.3(2), O(1)–Ti(1)–O(2) 46.8(3), C(9)–Ti(1)–N(4) 72.1(2), C(1)–Ti(1)–N(4) 106.0(2), N(1)–Ti(1)–N(4) 171.85(19), C(1)–C(4)–C(5)–N(1) 6.0(12), N(2)–C(4)–C(5)–C(6) 6.7(13), C(9)–C(12)–C(13)–N(4) 4.3(12), N(3)–C(12)–C(13)–C(14) 1.9(13).

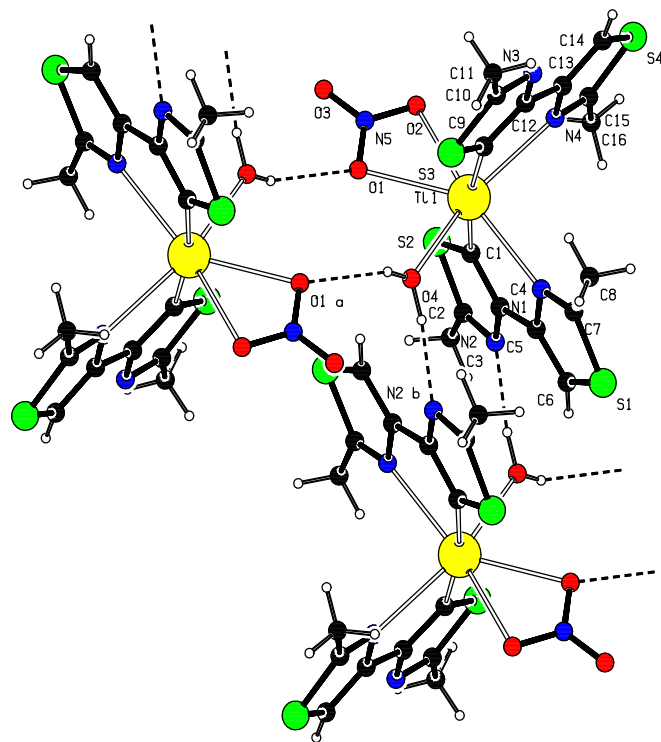


Fig. 4. Crystal packing diagram for compound **1** showing hydrogen bonding.

3. Experimental

3.1. Materials and instruments

All reagents and solvents were purchased from chemical sources and were used directly without further purification. UV–Vis spectra were recorded on a Shimadzu 2100 spectrometer using a 1 cm path length cell. ¹H NMR spectra were acquired on a Bruker AC-300 MHz spectrometer at ambient temperature in dmsd-*d*₆. Infrared spectra (4000–250 cm⁻¹) of solid samples were taken as a 1% dispersion in KBr or CsI pellets using a Shimadzu-470 spectrometer. Elemental analysis was performed using a Heraeus CHN–O Rapid analyzer. Melting points are uncorrected and were obtained by a Kofler Heizbank Rechart type 7841 melting point apparatus.

Caution: Thallium containing material is toxic.

3.2. Synthesis of 2,2'-dimethyl-4,4'-bithiazole (*dm4bt*) (**L**)

2,2'-Dimethyl-4,4'-bithiazole was prepared according to the procedure described previously [6]. 1.00 g (4.10 mmol) of 1,4-dibromo-2,3-butandione and 0.62 g (8.20 mmol) of thioacetamide was dissolved in 20 ml of dry methanol. The reaction mixture was refluxed for 3 h. The resulting solution was added to 20 ml water. Neutralization (pH 7) with Na₂CO₃ solution produces bright brown solid which was characterized as 2,2'-dimethyl-4,4'-bithiazole (yield 0.48 g, 60%, mp. 171–173 °C). ¹H NMR δ_H (CDCl₃): 7.61 (s, 1H, Ar) and 2.78 (s, 3H, CH₃). ¹³C NMR δ_C (CDCl₃): 166.46, 150.08, 114.52 (Ar) and 19.45 (CH₃). IR (KBr, cm⁻¹) selected bands: 879 (ν_{S–C}), 1184 (ν_{C–N}), 1419 (ν_{C–C}), 1496 (ν_{C=N}), 1558 (ν_{C=C}), 3103 (ν_{C–H}, Me) and 3434 (ν_{C–H}, cycle). UV–Vis (CH₃OH): λ_{max}: 3.76 × 10⁴ cm⁻¹. Anal. Calc. for C₈H₈N₂S₂ (%). C, 48.90; H, 4.07; N, 14.26. Found: C, 48.71; H, 3.96; N, 14.12%.

3.3. Synthesis of [Tl(dm4bt)₂(NO₃)(H₂O)] (**1**)

Tl(NO₃)₃ · 3H₂O (0.0225 g, 0.0506 mmol) was dissolved in methanol (5 ml) and mixed with 2,2'-dimethyl-4,4'-bithiazole (0.03 g, 0.152 mmol) in (10 ml) methanol without stirring. The colorless precipitates were formed after several days and suitable crystals of **1** were obtained by slow evaporation of a methanol/acetonitrile solution of **1** in room temperature. In the ¹H NMR, complex **1** converts fastly to complex **2**. IR (CsI, cm⁻¹) selected bands: 860 (ν_{S–C}), 1186 (ν_{C–N}), 1417 (ν_{C–C}), 1491 (ν_{C=N}), 1657 (ν_{C=C}), 3143 (ν_{C–H}, Me), 3400 (ν_{C–H}, cycle), 325 (ν_{Tl–N}), 459 (ν_{Tl–C}), 1286 (ν_{a(NO₂)}), 1450 (ν_(NO)), 1026 (ν_{s(NO₂)}). Anal. Calc. for C₁₆H₁₆N₅O₄S₄ Tl₁(%): C, 28.47; H, 2.38; N, 10.37. Found: C, 28.20; H, 2.24; N, 10.21%.

3.4. Synthesis of [Tl(dm4bt)₂(NO₃)(DMSO)] (**2**)

Recrystallization of compound [Tl(dm4bt)₂(NO₃)(H₂O)] (**1**) in DMSO converts **1** to compound [Tl(dm4bt)₂(NO₃)(DMSO)] (**2**) in which the water molecule is replaced by a DMSO molecule. Single crystals of **2** suitable for X-ray diffraction were grown by slow evaporation of **1** in DMSO-*d*₆. ¹H NMR δ_H (dmsd-*d*₆): 7.83 (s, 1H, Ar), 2.82 (s, 3H, CH₃), 2.09 (s, 3H, CH₃). IR (CsI, cm⁻¹) selected bands: 879 (ν_{S–C}), 1184 (ν_{C–N}), 1419 (ν_{C–C}), 1496 (ν_{C=N}), 1557 (ν_{C=C}), 3105 (ν_{C–H}, Me), 3500 (ν_{C–H}, cycle), 329 (ν_{Tl–N}), 456 (ν_{Tl–C}), 1299 (ν_{a(NO₂)}), 1433 (ν_(NO)), 1064 (ν_{s(NO₂)}), 986 (ν_{S=O}). UV–Vis (DMSO): λ_{max}: 3.69 × 10⁴ cm⁻¹. Anal. Calc. for C₁₈H₂₀N₅O₄S₅ Tl₁(%): C, 29.41; H, 2.74; N, 9.52. Found: C, 29.08; H, 2.44; N, 9.31%.

3.5. Crystal structure determination and refinement

The X-ray diffraction measurements were made on a STOE IPDS-II diffractometer with graphite monochromated Mo Kα radiation.

Table 1

Crystallographic and structure refinement data for compounds **1** and **2**

	Compound 1	Compound 2
Empirical formula	C ₁₆ H ₁₆ N ₅ O ₄ S ₄ Tl ₁	C ₁₈ H ₁₄ D ₆ N ₅ O ₄ S ₅ Tl ₁
Formula weight	675.00	741.16
Temperature (K)	293(2)	293(2)
Wavelength λ (Å)	0.71073	0.71073
Crystal system	Orthorhombic	Monoclinic
Space group	<i>P</i> _{bcu}	<i>P</i> _{21/c}
Crystal size (mm)	0.40 × 0.10 × 0.02	0.20 × 0.15 × 0.15
<i>a</i> (Å)	9.9149(5)	9.0704(5)
<i>b</i> (Å)	18.2872(12)	29.0493(16)
<i>c</i> (Å)	24.8870(15)	9.4753(5)
β (°)	90	99.460(4)
Volume (Å ³)	4512.4(5)	2462.7(2)
<i>Z</i>	8	4
<i>D</i> _{calc} (g cm ⁻³)	1.987	1.986
θ ranges for data collection	2.37–29.22	2.28–29.26
<i>F</i> (000)	2592	1424.0
Absorption coefficient	7.561	7.018
Index ranges	–13 ≤ <i>h</i> ≤ 12 –25 ≤ <i>k</i> ≤ 20 –22 ≤ <i>l</i> ≤ 34	–12 ≤ <i>h</i> ≤ 12 –34 ≤ <i>k</i> ≤ 39 –9 ≤ <i>l</i> ≤ 13
Data collected	15808	17990
Unique data (<i>R</i> _{int})	6064, (0.0734)	6621, (0.0887)
Parameters, restraints	281, 0	300, 0
Final <i>R</i> ₁ , <i>wR</i> ₂ ^a (Obs. data)	0.0606, 0.1300	0.0572, 0.1391
Final <i>R</i> ₁ , <i>wR</i> ₂ ^a (All data)	0.0863, 0.1409	0.0707, 0.1467
Goodness of fit on <i>F</i> ² (<i>S</i>)	1.159	1.137
Largest diff peak and hole (e Å ⁻³)	2.304, –2.469	2.640, –3.063

$$^a R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|, wR_2 = [\sum (w(F_o^2 - F_c^2))^2 / \sum w(F_o^2)^2]^{1/2}.$$

For [Tl(dm4bt)₂(NO₃)(H₂O)] (**1**) colorless plate shape and [Tl(dm4bt)₂(NO₃)(DMSO)] (**2**) colorless block shape crystals with a dimension of 0.40 × 0.10 × 0.02 mm and 0.20 × 0.15 × 0.15 mm, respectively were chosen under a polarizing microscope and were mounted on a glass fiber and used for data collection. Cell constants and an orientation matrix for data collection were obtained by least-squares refinement of diffraction data from 6064 unique reflections for **1**, and 6621 for **2**. Data were collected at a temperature of 293(2) K to a maximum 2θ value of 29.22° for **1** and 29.26° for **2**, in a series of ω scans in 1° oscillations and integrated using the Stoe X-Area [14] software package. The numerical absorption coefficient, μ, for Mo Kα radiation is 7.561 mm⁻¹ for **1**, and 7.018 mm⁻¹ for **2**. A numerical absorption correction was applied using X-RED [15] and X-SHAPE [16] software. The data were corrected for Lorentz and Polarizing effects. The structures were solved by direct methods [17] and subsequent difference Fourier maps and then refined on *F*² by a full-matrix least-squares procedure using anisotropic displacement parameters [18]. All hydrogen atoms were located in a difference Fourier map and then refined isotropically. Subsequent refinement then converged with *R* factors and parameters errors significantly better than for all attempts to model the solvent disorder. Atomic factors are from International Tables for X-ray Crystallography [19]. All refinements were performed using the X-STEP32 crystallographic software package [20]. A summary of the crystal data, experimental details and refinement results are given in Table 1.

4. Conclusion

In conclusion, two rare new cyclometalated Tl(III) with relatively short Tl–C bonds are prepared and characterized. To the best of our knowledge there are just a few examples for organometallic compound of substituted bithiazole ligands [21–23] but there is not any report on the transoid mode of coordination for them [4]. These compounds show important C–H bond activation in the presence of thallium salt.

Acknowledgment

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Appendix A. Supplementary material

CCDC 693446 and 693447 contain the supplementary crystallographic data for **1** and **2**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.jorganchem.2008.08.027.

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