Zhuang-yu Li, E Liu, Xiao-jing Liu and Fang-fang Jian*

Crystal structure of bis(2,3-diphenyltetrazolidine-5-thione- κ^1S)-(nitrate- κ^1O)-(nitrate- κ^2O,O') lead(II), $C_{26}H_{20}N_{10}O_6S_2Pb$

$\gamma = 102.75(3)^\circ$, $V = 1539.8(7) \text{ \AA}^3$, $Z = 2$, $R_{\text{gt}}(F) = 0.0336$, $wR_{\text{ref}}(F^2) = 0.0874$, $T = 293.0 \text{ K}$.

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The complex title structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Red block
Size:	$0.40 \times 0.24 \times 0.15 \text{ mm}$
Wavelength:	Mo $K\alpha$ radiation ($0.71073 \text{ \AA}$)
μ :	5.67 mm^{-1}
Diffractometer, scan mode:	Enraf-Nonius CAD-4, ω
θ_{max} , completeness:	27.0° , 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	7057, 6644, 0.025
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 5294
$N(\text{param})_{\text{refined}}$:	405
Programs:	CAD-4 [1, 2], Olex2 [3]

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Abstract

$C_{26}H_{20}N_{10}O_6S_2Pb$, triclinic, $P\bar{1}$ (no. 2), $a = 9.3480(19) \text{ \AA}$, $b = 12.985(3) \text{ \AA}$, $c = 14.278(3) \text{ \AA}$, $\alpha = 113.14(3)^\circ$, $\beta = 92.05(3)^\circ$,

Source of material

A mixture of (*E*)-1,5-diphenylthiocarbazone (8 mmol) was mixed in acetone (100 mL) and 30% hydrogen peroxide (1 mL), heated and refluxed for 5 h. Then add lead nitrate (2 mmol), heat and stir under reflux for 2 h. The mixture was filtered, washed with distilled water, and finally we get the title compound from the ethanol solution.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

Tetrazole is an important aromatic heterocyclic ring, which has a wide application prospect in many fields [4, 5]. Tetrazolium thioketone derivatives are a kind of tetrazolium compounds with unique structure. Because it has C, N, S atoms and other reaction points at the same time, it has strong

*Corresponding author: Fang-fang Jian, School of Chemical Engineering and Pharmaceuticals, Henan University of Science and Technology, Luoyang Hekeda Recycling Energy Co.LTD., Luoyang, Henan 471003, P.R. China, e-mail: Fangfjian@126.com

Zhuang-yu Li and Xiao-jing Liu: School of Chemical Engineering and Pharmaceuticals, Henan University of Science and Technology, Luoyang, Henan 471003, P.R. China. <https://orcid.org/0000-0003-4445-1455> (Z.-y. Li)

E Liu: School of Chemical Engineering and Pharmaceuticals, Henan University of Science and Technology, Luoyang Hekeda Recycling Energy Co.LTD., Luoyang, Henan 471003, P.R. China

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Pb1	−0.01253(2)	0.326147(17)	0.430355(16)	0.04009(8)
S1	0.11310(16)	0.15207(12)	0.43936(11)	0.0466(3)
S2	0.25732(15)	0.46339(15)	0.42217(12)	0.0551(4)
O4	−0.1892(5)	0.1555(5)	0.2602(4)	0.0797(15)
O5	0.0331(4)	0.2365(4)	0.2505(3)	0.0549(10)
N1	−0.1399(5)	0.1214(4)	0.5245(3)	0.0402(10)
N2	−0.1735(4)	0.1297(3)	0.6148(3)	0.0356(9)
N3	−0.0498(4)	0.1547(3)	0.6790(3)	0.0352(9)
N4	0.0665(4)	0.1623(4)	0.6301(3)	0.0364(9)
N5	0.3587(5)	0.4374(4)	0.5908(3)	0.0456(10)
N6	0.4173(5)	0.5088(4)	0.6853(3)	0.0424(10)
N7	0.4325(5)	0.6182(4)	0.6993(4)	0.0434(10)
N8	0.3860(5)	0.6231(4)	0.6135(4)	0.0443(10)
C1	−0.4145(6)	0.1636(6)	0.6064(5)	0.0588(16)
H1	−0.3802(6)	0.2120(6)	0.5739(5)	0.071(2)*
C2	−0.5631(7)	0.1399(7)	0.6251(6)	0.076(2)
H2	−0.6292(7)	0.1735(7)	0.6046(6)	0.091(3)*
C3	−0.6108(7)	0.0685(7)	0.6729(6)	0.076(2)
H3	−0.7092(7)	0.0542(7)	0.6841(6)	0.092(3)*
C4	−0.5173(7)	0.0174(7)	0.7046(6)	0.072(2)
H4	−0.5514(7)	−0.0309(7)	0.7373(6)	0.087(2)*
C5	−0.3687(6)	0.0392(5)	0.6870(5)	0.0558(15)
H5	−0.3027(6)	0.0055(5)	0.7075(5)	0.0670(18)*
C6	−0.3239(5)	0.1107(5)	0.6393(4)	0.0434(12)
C7	−0.0769(7)	0.2877(5)	0.8486(5)	0.0508(14)
H7	−0.1118(7)	0.3312(5)	0.8190(5)	0.0610(16)*
C8	−0.0597(8)	0.3221(5)	0.9546(5)	0.0581(15)
H8	−0.0835(8)	0.3896(5)	0.9973(5)	0.0697(18)*
C9	−0.0072(7)	0.2557(6)	0.9959(5)	0.0578(15)
H9	0.0052(7)	0.2793(6)	1.0668(5)	0.0694(19)*
C10	0.0272(8)	0.1550(6)	0.9339(5)	0.0630(17)
H10	0.0607(8)	0.1106(6)	0.9632(5)	0.076(2)*
C11	0.0122(6)	0.1194(5)	0.8287(5)	0.0508(14)
H11	0.0369(6)	0.0522(5)	0.7863(5)	0.0610(17)*
C12	−0.0404(5)	0.1865(4)	0.7887(4)	0.0359(10)
C13	0.0100(5)	0.1431(4)	0.5349(4)	0.0352(11)
C14	0.3501(8)	0.3996(5)	0.7889(5)	0.0622(17)
H14	0.2516(8)	0.3801(5)	0.7605(5)	0.075(2)*
C15	0.3918(10)	0.3586(6)	0.8595(6)	0.077(2)
H15	0.3210(10)	0.3107(6)	0.8786(6)	0.093(3)*
C16	0.5360(11)	0.3886(7)	0.9004(6)	0.079(2)
H16	0.5632(11)	0.3596(7)	0.9466(6)	0.095(3)*
C17	0.6433(8)	0.4615(6)	0.8748(5)	0.0660(18)
H17	0.7411(8)	0.4825(6)	0.9050(5)	0.079(2)*
C18	0.6055(7)	0.5029(6)	0.8045(5)	0.0561(15)
H18	0.6768(7)	0.5515(6)	0.7863(5)	0.0673(18)*
C19	0.4596(6)	0.4705(5)	0.7622(4)	0.0444(12)
C20	0.6245(6)	0.7894(5)	0.8104(5)	0.0589(16)
H20	0.6819(6)	0.7778(5)	0.7571(5)	0.0707(19)*
C21	0.6757(8)	0.8802(6)	0.9063(6)	0.0696(19)
H21	0.7685(8)	0.9307(6)	0.9177(6)	0.084(2)*
C22	0.5890(9)	0.8956(6)	0.9848(6)	0.073(2)
H22	0.6247(9)	0.9557(6)	1.0492(6)	0.088(2)*
C23	0.4503(9)	0.8227(6)	0.9682(6)	0.0707(19)
H23	0.3929(9)	0.8342(6)	1.0215(6)	0.085(2)*

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C24	0.3948(7)	0.7320(5)	0.8725(5)	0.0539(14)
H24	0.3003(7)	0.6834(5)	0.8601(5)	0.0647(17)*
C25	0.4856(6)	0.7170(5)	0.7966(5)	0.0466(13)
C26	0.3386(5)	0.5097(5)	0.5465(4)	0.0462(13)
N10	−0.0874(6)	0.1596(4)	0.2068(4)	0.0501(12)
O6	−0.0987(7)	0.0942(4)	0.1173(4)	0.0848(16)
N9	0.0149(5)	0.4737(4)	0.6998(4)	0.0480(11)
O1	0.0883(5)	0.5263(5)	0.6522(5)	0.0810(16)
O2	0.0076(8)	0.5225(5)	0.7900(4)	0.106(2)
O3	−0.0484(7)	0.3706(4)	0.6529(4)	0.0917(18)

coordination ability, which has caused widespread use [6, 7]. In medicine and pharmacy, tetrazolium thioketones have activities such as hypotensive, anti-radiation drugs and anti-convulsion [8, 9]. In materials science, tetrazolium thioke-tone derivatives can be used as optical materials and bleaching agents [10].

The molecular structure of the title compound is shown in the figure, bond lengths and angles are within normal ranges [11]. In the complex, the S1–Pb1 bond length is 2.810 Å and the S2–Pb1 bond length is 2.784 Å. The S1–C13 bond length is 1.724 Å and the S2–C26 bond length is 1.718 Å. A tetra-zole ring formed by N1, N2, N3, N4, and C13, where the N1–N2 bond length is 1.307 Å, the N2–N3 bond length is 1.344 Å, and the N3–N4 bond length is 1.320 Å, all of which are between their single and double bond lengths, indicating the existence of conjugation between atoms in the ring.

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