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Crystal structure of hexadecyltrimethylammonium bis(1,3-dithiole-2-thione-4,5-dithiolato)aurate(III), $[C_{16}H_{33}(CH_3)_3N][Au(C_3S_5)_2]$

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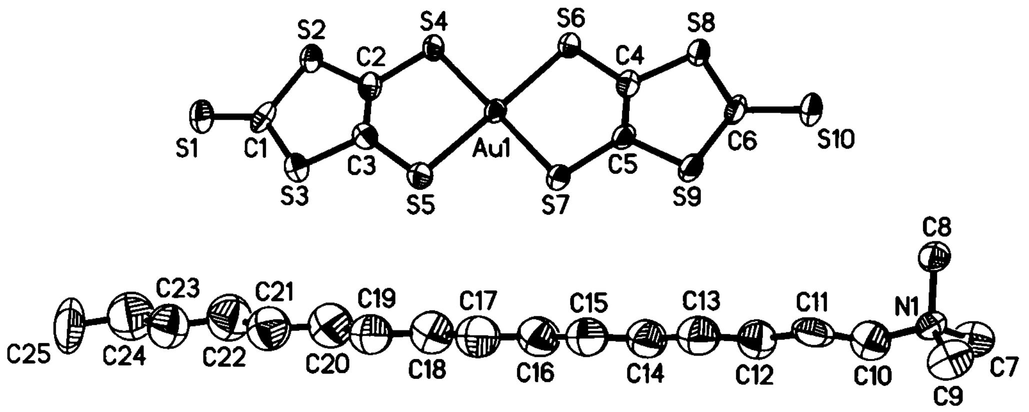

Abstract

$C_{25}H_{42}AuNS_{10}$, triclinic, $P\bar{1}$ (no. 2), a = 9.806(5) Å, b = 10.298(5) Å, c = 18.660(5) Å, α = 85.925(5)°, β = 79.413(5)°, γ = 73.551(5)°, V = 1776.1 Å^3, Z = 2, $R_{gt}(F)$ = 0.061, $wR_{ref}(F^2)$ = 0.164, T = 293 K.

Source of material

The synthesis route was the same as reported in [1-3]. A crystal suitable for X-ray structure analysis was obtained by slow evaporation from acetonitrile.

Discussion

Many of 4,5-dimercapto-1,3-dithiole-2-thione (dmit) derivatives have been paid much attention and have been extensively studied as heterocyclic compounds, coordination compounds, precursors of tetrathiafulvalene derivatives and organic conductors [1-6]. For exploring the nonlinear optical property of this kind of material we synthesized $[C_{19}H_{42}N][Au(dmit)_2]$ compound and report here the structure. Bond lengths and angles within the two independent $Au(dmit)_2$ complexes are similar to each other and to those observed for the related gold(III)$[dmit]_2$ structures of [5-7].

Table 1. Data collection and handling.

Crystal:	red platelet, size 0.04 × 0.13 × 0.36 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	47.47 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{max}$:	50.02°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	7497, 6169
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 4361
$N(param)_{refined}$:	334
Program:	SHELXTL [8]

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Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(7A)	2i	1.1963	−0.2055	0.9089	0.167
H(7B)	2i	1.3297	−0.2816	0.8526	0.167
H(7C)	2i	1.2631	−0.3621	0.9177	0.167
H(8A)	2i	0.9620	−0.2957	0.9146	0.123
H(8B)	2i	1.0803	−0.4325	0.9222	0.123
H(8C)	2i	0.9870	−0.4132	0.8605	0.123
H(9A)	2i	1.2577	−0.4934	0.8047	0.191
H(9B)	2i	1.3019	−0.3755	0.7570	0.191
H(9C)	2i	1.1606	−0.4121	0.7494	0.191
H(10A)	2i	1.0280	−0.1137	0.8620	0.164
H(10B)	2i	1.1478	−0.1230	0.7929	0.164
H(11A)	2i	0.8919	−0.1917	0.7910	0.160
H(11B)	2i	1.0079	−0.1821	0.7225	0.160
H(12A)	2i	0.8295	0.0407	0.8044	0.164
H(12B)	2i	0.9509	0.0533	0.7394	0.164
H(13A)	2i	0.7087	−0.0231	0.7232	0.179
H(13B)	2i	0.8275	0.0003	0.6592	0.179
H(14A)	2i	0.6361	0.2065	0.7483	0.166
H(14B)	2i	0.7576	0.2313	0.6863	0.166
H(15A)	2i	0.5250	0.1460	0.6608	0.179
H(15B)	2i	0.6437	0.1792	0.5998	0.179
H(16A)	2i	0.5617	0.4068	0.6332	0.189
H(16B)	2i	0.4407	0.3725	0.6924	0.189
H(17A)	2i	0.4579	0.3547	0.5413	0.207
H(17B)	2i	0.3411	0.3103	0.5988	0.207
H(18A)	2i	0.2416	0.5302	0.6355	0.206
H(18B)	2i	0.3602	0.5759	0.5804	0.206
H(19A)	2i	0.2627	0.5400	0.4850	0.191
H(19B)	2i	0.1495	0.4819	0.5375	0.191
H(20A)	2i	0.1573	0.7485	0.5366	0.225
H(20B)	2i	0.0421	0.6894	0.5866	0.225
H(21A)	2i	−0.0442	0.6559	0.4846	0.210
H(21B)	2i	0.0672	0.7217	0.4366	0.210
H(22A)	2i	−0.1699	0.8549	0.5344	0.245
H(22B)	2i	−0.0531	0.9238	0.4958	0.245
H(23A)	2i	−0.1227	0.9136	0.3880	0.211
H(23B)	2i	−0.2398	0.8455	0.4268	0.211
H(24A)	2i	−0.2491	1.1107	0.4414	0.270

Table 2. Continued.

Atom	Site	*x*	*y*	*z*	U_{iso}
H(24B)	2*i*	–0.3662	1.0426	0.4813	0.270
H(25A)	2*i*	–0.4522	1.1708	0.3903	0.351
H(25B)	2*i*	–0.4258	1.0196	0.3698	0.351
H(25C)	2*i*	–0.3164	1.1004	0.3338	0.351

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	2*i*	–0.264(1)	0.547(1)	0.7529(7)	0.041(6)	0.062(8)	0.11(1)	–0.009(5)	–0.026(6)	–0.021(7)
C(2)	2*i*	–0.122(1)	0.362(1)	0.8411(6)	0.058(7)	0.047(7)	0.063(8)	–0.005(5)	–0.018(6)	–0.007(5)
C(3)	2*i*	–0.031(1)	0.358(1)	0.7808(6)	0.070(7)	0.055(7)	0.055(7)	–0.024(6)	–0.018(6)	0.001(5)
C(4)	2*i*	0.346(1)	–0.067(1)	0.9713(6)	0.052(6)	0.037(6)	0.076(8)	–0.013(5)	–0.024(6)	–0.002(5)
C(5)	2*i*	0.436(1)	–0.069(1)	0.9080(6)	0.037(6)	0.045(6)	0.074(8)	–0.005(5)	–0.008(5)	0.000(5)
C(6)	2*i*	0.582(1)	–0.248(1)	0.9887(7)	0.039(6)	0.050(7)	0.11(1)	–0.008(5)	–0.030(6)	0.008(6)
C(7)	2*i*	1.242(2)	–0.289(2)	0.8832(9)	0.13(1)	0.13(1)	0.11(1)	–0.08(1)	–0.02(1)	–0.02(1)
C(8)	2*i*	1.033(1)	–0.369(1)	0.8883(8)	0.069(8)	0.069(9)	0.12(1)	–0.034(7)	–0.017(8)	0.011(8)
C(9)	2*i*	1.222(2)	–0.406(2)	0.7828(9)	0.118(9)	0.14(1)	0.13(1)	–0.049(8)	–0.007(8)	–0.037(8)
C(10)	2*i*	1.072(2)	–0.163(2)	0.817(1)	0.14(1)	0.13(1)	0.14(1)	–0.042(8)	–0.021(8)	0.004(8)
C(11)	2*i*	0.961(2)	–0.143(2)	0.7695(9)	0.13(2)	0.17(2)	0.11(1)	–0.08(2)	–0.00(1)	0.04(1)
C(12)	2*i*	0.880(2)	0.004(2)	0.758(1)	0.13(1)	0.14(1)	0.15(1)	–0.046(8)	–0.031(8)	0.013(8)
C(13)	2*i*	0.776(2)	0.031(2)	0.707(1)	0.14(1)	0.15(1)	0.16(1)	–0.048(8)	–0.014(8)	0.009(8)
C(14)	2*i*	0.690(2)	0.177(2)	0.701(1)	0.14(1)	0.14(1)	0.14(1)	–0.046(8)	–0.018(8)	0.006(8)
C(15)	2*i*	0.589(2)	0.204(2)	0.648(1)	0.14(1)	0.15(1)	0.15(1)	–0.042(8)	–0.010(8)	0.008(8)
C(16)	2*i*	0.498(2)	0.348(2)	0.645(1)	0.16(1)	0.15(1)	0.17(1)	–0.054(9)	–0.021(9)	0.017(8)
C(17)	2*i*	0.399(2)	0.374(2)	0.589(1)	0.17(1)	0.18(1)	0.17(1)	–0.047(9)	–0.016(9)	0.006(9)
C(18)	2*i*	0.301(2)	0.513(2)	0.588(1)	0.17(1)	0.17(1)	0.17(1)	–0.049(9)	–0.028(9)	0.004(9)
C(19)	2*i*	0.204(2)	0.548(2)	0.533(1)	0.15(1)	0.17(1)	0.16(1)	–0.047(9)	–0.016(9)	0.006(9)
C(20)	2*i*	0.102(3)	0.683(2)	0.539(1)	0.19(1)	0.19(1)	0.19(1)	–0.051(9)	–0.033(9)	0.001(9)
C(21)	2*i*	0.006(3)	0.724(2)	0.484(1)	0.18(1)	0.18(1)	0.17(1)	–0.054(9)	–0.032(9)	–0.011(9)
C(22)	2*i*	–0.103(3)	0.857(3)	0.489(1)	0.20(1)	0.21(1)	0.21(1)	–0.059(9)	–0.042(9)	0.000(9)
C(23)	2*i*	–0.190(3)	0.912(2)	0.433(1)	0.17(1)	0.18(1)	0.18(1)	–0.050(9)	–0.041(9)	–0.007(9)
C(24)	2*i*	–0.298(3)	1.043(3)	0.437(1)	0.23(2)	0.23(2)	0.22(2)	–0.06(1)	–0.04(1)	–0.00(1)
C(25)	2*i*	–0.380(3)	1.087(3)	0.378(1)	0.22(3)	0.25(3)	0.28(4)	–0.07(3)	–0.17(3)	0.08(3)
N(1)	2*i*	1.143(1)	–0.314(1)	0.8376(6)	0.059(6)	0.052(6)	0.095(8)	–0.016(5)	–0.001(5)	–0.008(5)
S(1)	2*i*	–0.3879(4)	0.6637(4)	0.7238(2)	0.078(2)	0.096(3)	0.123(3)	–0.006(2)	–0.042(2)	0.038(2)
S(2)	2*i*	–0.2930(3)	0.4752(3)	0.8453(2)	0.052(2)	0.061(2)	0.085(2)	0.001(1)	–0.019(2)	0.012(2)
S(3)	2*i*	–0.0965(4)	0.4675(3)	0.7099(2)	0.072(2)	0.074(2)	0.073(2)	–0.016(2)	–0.023(2)	0.019(2)
S(4)	2*i*	–0.0802(3)	0.2645(3)	0.9194(2)	0.046(2)	0.065(2)	0.069(2)	0.004(1)	–0.009(1)	0.016(2)
S(5)	2*i*	0.1467(3)	0.2555(3)	0.7634(2)	0.056(2)	0.070(2)	0.067(2)	–0.006(2)	–0.006(1)	0.012(2)
S(6)	2*i*	0.1678(3)	0.0322(3)	0.9871(2)	0.044(1)	0.052(2)	0.065(2)	–0.002(1)	–0.009(1)	0.006(1)
S(7)	2*i*	0.3950(3)	0.0328(3)	0.8314(2)	0.043(2)	0.062(2)	0.078(2)	–0.004(1)	–0.008(1)	0.014(2)
S(8)	2*i*	0.4133(3)	–0.1816(3)	1.0387(2)	0.048(2)	0.057(2)	0.079(2)	–0.011(1)	–0.019(1)	0.012(2)
S(9)	2*i*	0.6069(3)	–0.1823(3)	0.9028(2)	0.039(2)	0.061(2)	0.091(2)	–0.003(1)	–0.011(1)	0.006(2)
S(10)	2*i*	0.7096(4)	–0.3698(4)	1.0211(2)	0.056(2)	0.079(2)	0.118(3)	0.001(2)	–0.030(2)	0.028(2)
Au(1)	2*i*	0.15819(4)	0.14829(4)	0.87646(2)	0.0395(2)	0.0388(3)	0.0653(3)	–0.0076(2)	–0.0117(2)	0.0041(2)

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