Crystal structure of 3,4,7,8-tetraphenyl-2,6-(*N*-ethylimino)-2*H*,6*H*-1,5-dithiocine, C₃₂H₂₇NS₂

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Table 1. Parameters used for the X-ray data collection

Crystal:	colorless platelet, size 0.40 x 0.45 x 0.60 mm
Wavelength:	Mo K α radiation (0.71069 Å)
μ :	2.26 cm ⁻¹
Diffractometer:	Stoe STADI4
Scan mode:	ω/θ
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	50°
$N(hkl)_{\text{unique}}$:	4159
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	425
Programs:	SHELXS-86, SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{iso}
H(1)	2i	0.047(2)	0.360(2)	0.095(1)	0.037(4)
H(4)	2i	0.422(2)	0.188(2)	-0.028(1)	0.031(4)
H(7A)	2i	0.187(2)	0.137(2)	-0.014(2)	0.061(6)
H(7B)	2i	0.052(2)	0.276(2)	-0.038(2)	0.056(6)
H(8A)	2i	0.145(3)	0.210(2)	-0.206(2)	0.077(7)
H(8B)	2i	0.153(3)	0.344(3)	-0.209(2)	0.105(9)
H(8C)	2i	0.291(4)	0.208(3)	-0.183(3)	0.11(1)
H(11)	2i	-0.200(3)	0.440(2)	0.401(2)	0.078(7)
H(10)	2i	-0.091(2)	0.356(2)	0.251(2)	0.065(6)
H(12)	2i	-0.067(3)	0.392(2)	0.568(2)	0.079(7)
H(13)	2i	0.175(3)	0.269(2)	0.576(2)	0.082(8)
H(14)	2i	0.287(2)	0.186(2)	0.423(2)	0.063(6)
H(16)	2i	0.102(2)	0.018(2)	0.346(2)	0.046(5)
H(17)	2i	0.123(3)	-0.148(2)	0.504(2)	0.068(7)
H(18)	2i	0.346(2)	-0.287(2)	0.593(2)	0.073(7)
H(19)	2i	0.548(2)	-0.259(2)	0.513(2)	0.064(6)
H(20)	2i	0.521(2)	-0.090(2)	0.356(2)	0.046(5)
H(22)	2i	0.641(2)	0.235(2)	-0.060(2)	0.058(6)
H(23)	2i	0.892(3)	0.133(2)	-0.028(2)	0.070(7)
H(24)	2i	0.996(3)	0.032(3)	0.149(2)	0.083(8)
H(25)	2i	0.854(3)	0.031(2)	0.309(2)	0.083(8)
H(26)	2i	0.604(2)	0.137(2)	0.283(2)	0.064(6)
H(28)	2i	0.599(2)	0.429(2)	0.079(2)	0.039(5)
H(29)	2i	0.679(2)	0.551(2)	0.147(2)	0.049(5)
H(30)	2i	0.569(2)	0.647(2)	0.295(2)	0.074(7)
H(31)	2i	0.375(3)	0.608(3)	0.374(2)	0.086(8)
H(32)	2i	0.283(2)	0.489(2)	0.306(2)	0.058(6)

Source of material: The compound can be obtained either from the reaction of 3-mercapto-2,3-diphenyl-propenal with 3-ethyl-amino-1,2-diphenyl-prop-2-en-1-thione without any solvents at room temperature, or by heating the educts in acetic acid at 363 K.

The conformations of the rings (C1 N1 C4 C2 C3 S2) and (C1 N1 C4 C6 C5 S1) were found to be twisted. The least-square planes through the atoms (C1 C5 C6 S1 C4) and (C1 C2 C3 C4 S2) form an angle of 73.55°.

C₃₂H₂₇NS₂, triclinic, $P\bar{1}$ (No. 2), $a = 10.419(2)$ Å, $b = 11.700(9)$ Å, $c = 12.234(2)$ Å, $\alpha = 75.083(7)^\circ$, $\beta = 85.391(9)^\circ$, $\gamma = 64.310(7)^\circ$, $V = 1297.8$ Å³, $Z = 2$, $R(F) = 0.030$, $R_w(F^2) = 0.083$.

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
S(1)	2i	0.18135(5)	0.45922(4)	0.12721(4)	0.0395(3)	0.0330(2)	0.0557(3)	-0.0109(2)	0.0058(2)	-0.0109(2)
S(2)	2i	0.41004(5)	0.04077(4)	0.12919(4)	0.0456(3)	0.0350(2)	0.0456(2)	-0.0143(2)	0.0063(2)	-0.0129(2)
N(1)	2i	0.2237(2)	0.2835(1)	0.0124(1)	0.0400(9)	0.0431(8)	0.0385(7)	-0.0180(7)	-0.0002(6)	-0.0093(6)
C(1)	2i	0.1498(2)	0.3223(2)	0.1114(1)	0.034(1)	0.0383(9)	0.0453(9)	-0.0134(8)	0.0003(7)	-0.0079(7)
C(2)	2i	0.1859(2)	0.2168(2)	0.2220(1)	0.0332(9)	0.0391(9)	0.0413(9)	-0.0169(7)	0.0024(7)	-0.0098(7)
C(3)	2i	0.2872(2)	0.0928(2)	0.2331(1)	0.0369(9)	0.0402(9)	0.0392(8)	-0.0191(7)	0.0004(7)	-0.0098(7)
C(4)	2i	0.3735(2)	0.2081(2)	0.0386(1)	0.040(1)	0.0380(9)	0.0354(8)	-0.0164(7)	0.0043(7)	-0.0100(7)
C(5)	2i	0.4420(2)	0.2689(2)	0.0965(1)	0.0360(9)	0.0361(8)	0.0328(8)	-0.0152(7)	0.0036(6)	-0.0093(6)
C(6)	2i	0.3692(2)	0.3778(2)	0.1347(1)	0.040(1)	0.0361(8)	0.0348(8)	-0.0159(7)	0.0049(7)	-0.0075(7)
C(7)	2i	0.1563(2)	0.2278(2)	-0.0473(2)	0.051(1)	0.048(1)	0.051(1)	-0.0240(9)	-0.0095(9)	-0.0078(9)
C(8)	2i	0.1913(3)	0.2434(3)	-0.1701(2)	0.076(2)	0.089(2)	0.055(1)	-0.041(2)	-0.003(1)	-0.029(1)
C(9)	2i	0.1092(2)	0.2631(2)	0.3213(1)	0.042(1)	0.0372(9)	0.0450(9)	-0.0203(8)	0.0054(7)	-0.0096(7)
C(10)	2i	-0.0370(2)	0.3396(2)	0.3183(2)	0.044(1)	0.048(1)	0.059(1)	-0.0200(9)	0.0093(9)	-0.0109(9)
C(11)	2i	-0.1021(3)	0.3884(2)	0.4099(2)	0.053(1)	0.053(1)	0.081(2)	-0.021(1)	0.027(1)	-0.020(1)
C(12)	2i	-0.0242(3)	0.3611(2)	0.5059(2)	0.086(2)	0.071(1)	0.069(2)	-0.040(1)	0.035(1)	-0.037(1)
C(13)	2i	0.1197(3)	0.2845(3)	0.5108(2)	0.085(2)	0.085(2)	0.056(1)	-0.042(2)	0.011(1)	-0.034(1)
C(14)	2i	0.1864(2)	0.2363(2)	0.4198(2)	0.053(1)	0.061(1)	0.054(1)	-0.024(1)	0.0044(9)	-0.0229(9)
C(15)	2i	0.3060(2)	-0.0159(2)	0.3349(1)	0.046(1)	0.0366(8)	0.0409(9)	-0.0193(8)	-0.0010(7)	-0.0104(7)
C(16)	2i	0.1881(2)	-0.0357(2)	0.3798(2)	0.050(1)	0.047(1)	0.049(1)	-0.0242(9)	-0.0018(9)	-0.0080(8)
C(17)	2i	0.2025(3)	-0.1361(2)	0.4743(2)	0.072(2)	0.055(1)	0.055(1)	-0.038(1)	0.010(1)	-0.0095(9)
C(18)	2i	0.3347(3)	-0.2189(2)	0.5248(2)	0.086(2)	0.049(1)	0.043(1)	-0.035(1)	-0.004(1)	-0.0040(9)
C(19)	2i	0.4526(3)	-0.2017(2)	0.4806(2)	0.066(2)	0.048(1)	0.052(1)	-0.021(1)	-0.019(1)	-0.0027(9)
C(20)	2i	0.4390(2)	-0.1010(2)	0.3860(2)	0.048(1)	0.047(1)	0.051(1)	-0.0210(9)	-0.0045(9)	-0.0078(8)
C(21)	2i	0.6002(2)	0.1970(2)	0.1109(1)	0.040(1)	0.0365(8)	0.0453(9)	-0.0167(7)	0.0033(7)	-0.0171(7)
C(22)	2i	0.6867(2)	0.1921(2)	0.0182(2)	0.043(1)	0.055(1)	0.052(1)	-0.0177(9)	0.0088(8)	-0.0234(9)
C(23)	2i	0.8334(2)	0.1328(2)	0.0334(2)	0.047(1)	0.083(2)	0.075(2)	-0.028(1)	0.019(1)	-0.043(1)
C(24)	2i	0.8959(3)	0.0750(3)	0.1403(2)	0.037(1)	0.090(2)	0.093(2)	-0.013(1)	0.000(1)	-0.050(2)
C(25)	2i	0.8114(2)	0.0749(2)	0.2329(2)	0.051(1)	0.077(2)	0.069(1)	-0.013(1)	-0.015(1)	-0.029(1)
C(26)	2i	0.6646(2)	0.1359(2)	0.2186(2)	0.047(1)	0.056(1)	0.048(1)	-0.0183(9)	-0.0013(9)	-0.0185(9)
C(27)	2i	0.4326(2)	0.4468(2)	0.1837(1)	0.047(1)	0.0327(8)	0.0374(8)	-0.0151(7)	0.0010(7)	-0.0077(7)
C(28)	2i	0.5518(2)	0.4651(2)	0.1396(1)	0.048(1)	0.0387(9)	0.0382(9)	-0.0187(8)	-0.0007(8)	-0.0072(7)
C(29)	2i	0.6022(2)	0.5371(2)	0.1820(2)	0.059(1)	0.044(1)	0.054(1)	-0.0255(9)	-0.0085(9)	-0.0042(8)
C(30)	2i	0.5344(3)	0.5926(2)	0.2696(2)	0.081(2)	0.052(1)	0.067(1)	-0.031(1)	-0.012(1)	-0.022(1)
C(31)	2i	0.4180(3)	0.5741(2)	0.3156(2)	0.083(2)	0.066(1)	0.063(1)	-0.028(1)	0.006(1)	-0.037(1)
C(32)	2i	0.3671(2)	0.5022(2)	0.2731(2)	0.060(1)	0.053(1)	0.051(1)	-0.023(1)	0.0098(9)	-0.0229(9)

References

1. Sheldrick, G. M.: Phase Annealing in SHELX-90: Direct Methods for Large Structures. *Acta Crystallogr. A* **46** (1990) 467-473.
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