New synthetic routes to highly-extended tetrathiafulvalenes

Piétrick Hudhomme,* Marc Sallé,* Nicolas Gautier, Ahmed Belyasmine, and Alain Gorgues

Laboratoire de Chimie et Ingénierie Moléculaire des Matériaux d'Angers (CIMMA), Groupe Synthèse Organique et Matériaux Fonctionnels, UMR CNRS 6200, Université d'Angers, 2 Bd Lavoisier, F-49045 Angers, France
E-mail: pietrick.hudhomme@univ-angers.fr, marc.salle@univ-angers.fr

Dedicated to Prof. Armand LATTES on the occasion of his 50th anniversary of teaching and research activities and for his involvement as a President of the "Société Française de Chimie"

Supplementary Information

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CIF file of compound **26**

Table 1. Crystal data and structure refinement for **26**.

Identification code	**26**
Empirical formula	C28 N2 S6
Formula weight	556.70
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 1 21/m 1
Unit cell dimensions	a = 5.754(2) A alpha = 90 deg. b = 25.392(9) A beta = 90.90(5) deg. c = 9.862(5) A gamma = 90 deg.
Volume	1441(1) A^3
Z, Calculated density	2, 1.28 Mg/m^3
Absorption coefficient	0.493 mm^-1
F(000)	556
Crystal size	0.60 x 0.23 x 0.20 mm
Theta range for data collection	2.5 to 29.98 deg.
Limiting indices	0<=h<=7, 0<=k<=34, -13<=l<=13
Absorption correction	DIFABS
Max. and min. transmission	0.4854 and 1.0000
Refinement method	Full-matrix least-squares on F
Data / restraints / parameters	4606 / 52 / 166
Number of data with I > 3 s(I)	1687
Goodness-of-fit on F^2	1.042
Final R indices [I>3sigma(I)]	R1 = 0.055, wR2 = 0.063
R indices (all data)	R1 = 0.119, wR2 = 0.101
Largest diff. peak and hole	0.229 and -0.177 e.A^-3

Table 2. Atomic coordinates and equivalent isotropic displacement parameters for **26**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S1	0.3603(3)	0.31528(7)	0.5312(1)	0.115(2)
S2	0.6172(2)	0.30767(6)	0.2725(1)	0.069(2)
S3	0.0384(2)	0.30793(5)	0.0560(1)	0.054(2)
N	0.1042(8)	0.5075(2)	0.7076(5)	0.101(4)
C1	0.1043(9)	0.2775(2)	0.5624(7)	0.090(5)
C2	0.4953(7)	0.2763(2)	0.4097(4)	0.050(3)
C3	0.7536(7)	0.2500	0.2124(5)	0.033(3)
C4	0.9219(9)	0.2500	0.1235(5)	0.045(2)
C5	0.2713(7)	0.2776(2)	0.9772(4)	0.039(2)
C6	0.4511(7)	0.3097(2)	0.9152(3)	0.055(2)
C7	0.4487(7)	0.3634(2)	0.9282(4)	0.053(2)
C8	0.6210(7)	0.3974(2)	0.8663(4)	0.050(2)
C9	0.6246(9)	0.4504(2)	0.9017(6)	0.172(7)
C10	0.7867(8)	0.3825(2)	0.7754(4)	0.065(3)
C11	0.7796(9)	0.4863(2)	0.8486(6)	0.182(7)
C12	0.9447(8)	0.4170(2)	0.7235(4)	0.074(4)
C13	0.9395(8)	0.4718(2)	0.7613(5)	0.078(4)
C14	0.0775(9)	0.5649(2)	0.7398(7)	0.23(1)
C15	0.2764(9)	0.4910(2)	0.6071(6)	0.094(5)

Table 3. Bond lengths [A] for **26**.

S1	C1	1.789(5)
S1	C2	1.746(4)
S2	C2	1.728(4)
S2	C3	1.768(3)
S3	C4	1.752(3)
S3	C5	1.739(4)
N	C13	1.420(7)
N	C14	1.500(8)
N	C15	1.473(7)
C3	C4	1.32(1)
C5	C6	1.459(8)
C6	C7	1.370(8)
C7	C8	1.456(8)
C8	C9	1.390(8)
C8	C10	1.372(7)
C9	C11	1.38(1)
C10	C11	1.368(8)
C11	C13	1.33(1)
C12	C13	1.441(8)

Table 4. Bond angles [deg] for **26**.

C1	S1	C2	100.9(2)
C2	S2	C3	93.9(2)
C4	S3	C5	95.7(2)
C13	N	C14	118.0(4)
C13	N	C15	121.9(4)
C14	N	C15	119.4(4)
S1	C2	S2	117.8(2)
S2	C3	S2	111.8(3)
S2	C3	C4	123.9(2)
S3	C4	S3	114.1(3)
S3	C4	C3	122.8(2)
S3	C5	C6	119.7(2)
C5	C6	C7	120.5(3)
C6	C7	C8	122.9(4)
C7	C8	C9	118.4(4)
C7	C8	C10	126.5(3)
C9	C8	C10	115.0(4)
C8	C9	C11	123.3(5)
C8	C10	C12	122.7(4)
C9	C11	C13	121.4(4)
C10	C12	C13	120.3(4)
N	C13	C11	122.7(4)
N	C13	C12	120.2(4)
C11	C13	C12	117.0(4)

Table 5. Anisotropic displacement parameters for **26**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12	
S1	0.115(1)	0.126()	0.079(1)	-0.009(1)	0.017(1)	-0.040(1)	O
S2	0.069(1)	0.061(1)	0.064(1)	0.002(1)	-0.001(1)	-0.005(1)	O
S3	0.054(1)	0.057(1)	0.079(1)	0.005(1)	0.005(1)	0.004(1)	O
N	0.101(3)	0.103(3)	0.114(3)	-0.036(3)	0.002(3)	0.013(3)	N
C1	0.090(4)	0.146(5)	0.210(5)	0.001(4)	0.041(4)	-0.029(4)	C
C2	0.051(6)	0.089(3)	0.034(2)	0.005(2)	-0.019(2)	-0.004(2)	C
C3	0.034(4)	0.051(3)	0.051(2)	0.001(2)	-0.018(2)	0.000(2)	C
C4	0.045(4)	0.047(3)	0.046(2)	0.001(2)	-0.007(2)	0.000(2)	C
C5	0.039(2)	0.058(2)	0.035(2)	-0.008(2)	-0.018(2)	-0.001(2)	C
C6	0.055(2)	0.059(2)	0.036(2)	-0.018(3)	-0.020(2)	0.012(2)	C
C7	0.053(3)	0.056(2)	0.069(3)	-0.008(2)	-0.006(2)	0.009(2)	C
C8	0.050(3)	0.049(3)	0.050(2)	-0.002(2)	-0.010(2)	-0.003(2)	C
C9	0.172(5)	0.061(3)	0.196(5)	-0.036(3)	0.115(3)	-0.035(3)	C
C10	0.065(3)	0.063(2)	0.075(3)	0.004(3)	0.024(2)	0.015(2)	C
C11	0.182(4)	0.077(3)	0.162(4)	-0.051(3)	0.111(3)	-0.052(3)	C
C12	0.074(3)	0.064(3)	0.087(3)	0.010(3)	0.009(3)	0.011(5)	C
C13	0.078(3)	0.083(3)	0.060(3)	-0.025(3)	-0.009(3)	0.009(2)	C
C14	0.237(5)	0.056(3)	0.199(5)	-0.069(4)	0.069(5)	-0.027(3)	C
C15	0.094(4)	0.126(5)	0.156(5)	-0.003(4)	0.046(4)	0.044(4)	C