Supporting Information

Synthesis, Electronic Properties and Electropolymerisation of EDOT-capped σ^3-Phospholes

Vincent Lemau de Talancé, Muriel Hissler,* Ling-Zhi Zhang, Tamás Kárpáti, László Nyulászi,* Dolores Caras-Quintero, Peter Bäuerle* and Régis Réau*

Experimental Section

All experiments were performed under an atmosphere of dry argon using standard Schlenk techniques. Column chromatography was performed in air, unless stated in text. Solvents were freshly distilled under argon from sodium/benzophenone (tetrahydrofurane, diethylether) or from phosphorus pentoxide (pentane, dichloromethane). Triethylamine and diisopropylamine were freshly distilled under argon from potassium hydroxide. Cp_2ZrCl_2, $Pd(PPh_3)_4$ and 1,7-octadiyne were obtained from Alfa Aesar Chem. Co. *n*-BuLi, CuI and I_2 were obtained from Acros Chem. Co. $PdCl_2(PPh_3)_2$ and elemental sulfur were obtained from Aldrich Chem. Co. 3,4-ethylenedioxythiophene (EDOT) was obtained from Bayer Co. All compounds were used as received without further purification. $PPhBr_2$[1] and THTAuCl[2] were prepared as described in the literature. Preparative separations were performed by gravity column chromatography on basic alumina (Aldrich, Type 5016A, 150 mesh, 58 Å) or silica gel (Merck Geduran 60, 0.063-0.200 mm) in 3.5-20 cm columns. ^1H, ^{13}C, and ^{31}P NMR spectra were recorded on Bruker AM300 or DPX200. ^1H and ^{13}C NMR chemical shifts were reported in parts per million (ppm) relative to $Si(CH_3)_4$ as external standard. ^{31}P NMR downfield chemical shifts were expressed with a positive sign, in ppm, relative to external 85 % H_3PO_4. Assignment of proton atoms is based on COSY experiment. Assignment of carbon atoms is based on HMBC, HMQC and DEPT-135 experiments. High-resolution mass spectra were obtained on a Varian MAT 311 or ZabSpec TOF Micromass

---

1. Quin, L. D. ; Gratz, J. P. ; Barket T. P. *J. Org. Chem.* 1968, **33**, 1034.
2 Kaesz H. D. *Inorg. Synth.* 1989, **26**, 86.

instrument at CRMPO, University of Rennes 1. Elemental analyses were performed by the CRMPO, University of Rennes 1.

Synthesis of 2-Iodo-3,4-(ethylenedioxy)thiophene (2). A hexane solution of *n*-BuLi (7.3 mL, 1.6 M 11.6 mmol) was added dropwise to a solution of EDOT (1.5 g, 10.6 mmol) in THF (30 mL) at –78 °C. The mixture was stirred for 1 hour at this temperature. Then iodine (2.7 g, 10.6 mmol) in THF (7 mL) was slowly added while the red color disappeared simultaneously. The mixture was allowed to reach room temperature. After 1 hour of stirring at room temperature, water was added and the mixture was extract with diethyl ether (3 x 30 mL). The combined organic layers were washed with aqueous Na_2SO_3, saturated $NaHCO_3$ solution, water and brine (30 mL each). The organic phase was dried over $MgSO_4$. After filtration and removing the solvent *in vacuo*, the product was purified by recrystallization from ether as white powder (2.5 g, 90%). The solid changes color very rapidly to blue even in the freezer under argon. Purification on the partly decomposed product was achieved by filtration over a short column of silica gel (SiO_2, CH_2Cl_2/diethyl ether, 1/1). δ_H(200 MHz, $CDCl_3$, Me_4Si): 4.21 (2H, m, O$\mathrm{C}H_2$-$\mathrm{C}H_2$O), 4.27 (2H, m, O$\mathrm{C}H_2$-$\mathrm{C}H_2$O), 6.55 (1H, s, $\mathrm{C}H_{\mathrm{edot}}$). δ_C(75 MHz, $CDCl_3$): 49.8 (s, C_{edot}I), 65.1 (s, O$C\mathrm{H}_2$), 65.7 (s, O$C\mathrm{H}_2$), 105.5 (s, $C\mathrm{H}_{\mathrm{edot}}$), 141.5 (s, C_{edot}O), 144.6(s, C_{edot}O). HR-MS (EI): *m/z* : 267.9059 $[M]^{+\cdot}$; calc. for $C_6H_5O_2SI$: 267.90550.

Synthesis of 1-(3,4-(ethylenedioxy)thienyl)]octa-1,7-diyne (3a) and 1,8-di(3,4-(ethylenedioxy)thienyl)]octa-1,7-diyne (3b). A hexane solution of *n*-BuLi (9.7 mL, 1.6 M, 15.5 mmol) was added dropwise to a solution of EDOT (2.0 g, 14.1 mmol) in THF (40 mL) at –78 °C. After 1 hour stirring at –78 °C, iodine (3.6 g, 14.2 mmol) was added. The mixture was allowed to warm to room temperature and stirred for 1 hour. Then the reaction was quenched by water (60 mL). The aqueous phase was extracted with diethyl ether (3×60 mL). Then the combined organic layers were washed with aqueous Na_2SO_3, saturated $NaHCO_3$ solution, water and brine (50 mL each), and dried over $MgSO_4$. After removing part of the solvent *in vacuo*, the residual solution was transferred via cannula to a mixture of $Pd(PPh_3)_4$ (162 mg, 1% mol), CuI (268 mg, 10% mol) and 1,7-octadiyne (0.84 mL, 7.03 mmol) in diisopropylamine (25 ml). The reaction mixture was heated at 40°C for 2 days, protected from light. After evaporating the solvent *in vacuo*, the residue was extracted with diethyl ether. Two products were obtained after purification by column chromatography (silica, ether/heptane, 1/1, **Compound 3a** : R_f = 0.50 , **Compound 3b** : R_f = 0.20) as a yellow oil for **Compound 3a** (0.8 g, 46%) and as a yellow-brown powder for **Compound 3b** (1.01 g, 37%).

1-[2-(3,4-ethylenedioxy)thienyl]octa-1,7-diyne (3a). Found : C, 68.4; H, 5.8; S 13.0. Calc. for $C_{14}H_{14}O_2S$: C, 68.3; H, 5.7; S, 13.0%. δ_H(200 MHz, $CDCl_3$, Me_4Si): 1.62 (4H, m, ≡C-CH_2-C*H*$_2$), 1.89 (1H, t, ^3J(H,H) = 2.6 Hz, ≡C*H*), 2.17 (2H, m, C*H*$_2$-C≡CH), 2.41 (2H, m, C*H*$_2$-C≡), 4.09 (2H, m, OC*H*$_2$), 4.19 (2H, m, OC*H*$_2$), 6.12 (1H, s, C*H*$_{edot}$). δ_C(75 MHz, $CDCl_3$): 16.9 (s, ≡C-*C*H$_2$), 18.4 (s, ≡C-*C*H$_2$), 26.5 (s, ≡C-CH$_2$-*C*H$_2$), 63.3 (s, O*C*H$_2$), 64.0 (s, O*C*H$_2$), 67.5 (s, ≡*C*H), 70.7 (s, *C*≡C), 83.1 (s, *C*≡C), 95.5 (s, *C*≡C), 98.5 (s, *C*$_{edot}$-C≡), 98.6 (s, *C*H$_{edot}$), 139.7 (s, *C*$_{edot}$O), 142.5 (s, *C*$_{edot}$O). HR-MS (EI): *m/z* : 246.0705 $[M]^{+\cdot}$; calc. for $C_{14}H_{14}O_2S$: 246.0715.

1,8-di[2-(3,4-ethylenedioxy)thienyl]octa-1,7-diyne (3b). Found : C, 62.2; H, 4.9; S 16.2. Calc. for $C_{20}H_{18}O_4S_2$: C, 62.15; H, 4.7; S, 16.5%. δ_H(200 MHz, $CDCl_3$, Me_4Si): 1.77 (4H, m**,** ≡C-CH$_2$-C*H*$_2$), 2.52 (4H, m, ≡C-C*H*$_2$), 4.21 (4H, m, OC*H*$_2$), 4.27 (4H, m, OC*H*$_2$), 6.21 (2H, s, C*H*$_{edot}$). δ_C(75 MHz, $CDCl_3$): 19.3 (s, ≡C-*C*H$_2$), 27.9 (s, ≡C-CH$_2$-*C*H$_2$), 64.5 (s, O*C*H$_2$), 65.1 (s, O*C*H$_2$), 71.3 (s, *C*≡C), 96.4 (s, *C*≡C), 99.0 (s, *C*$_{edot}$-C≡), 99.4 (s, *C*H$_{edot}$), 141.0 (s, *C*$_{edot}$O), 143.7 (s, *C*$_{edot}$O). HR-MS (EI): *m/z* : 386.0617 $[M]^{+\cdot}$; calc. for $C_{20}H_{18}O_4S_2$: 386.0647.

Synthesis of 1-phenyl-2,5-bis(2-(3,4-ethylenedioxy)thienyl)-phosphole (4) . To a THF solution (5 mL) of Cp_2ZrCl_2 (0.12 g, 0.39 mmol) was added dropwise, at -78°C, a hexane solution of 1.6 M *n*-BuLi (0.52 mL, 0.82 mmol). After one hour stirring, 1,8-di[2-(3,4-ethylenedioxy)thienyl]octa-1,7-diyne (0.15 mg, 0.39 mmol) was added to the reaction mixture. The solution was warmed to room temperature, and stirred for 12h. To this solution was added, at -78°C, freshly distilled $PhPBr_2$ (0.09 mL, 0.43 mmol). The reaction mixture was allowed to warm to room temperature and stirred for 7h. After filtration on basic alumina (THF) and evaporation of the volatile materials under vacuo, the

1-phenyl-2,5-bis(2-(3,4-ethylenedioxy)thienyl)-phosphole (4) was obtained as a yellow solid (0.064 g, 33%). Found : C, 63.2; H, 4.8; S 13.2. Calc. for $C_{26}H_{23}O_4S_2P$: C, 63.1; H, 4.7; S, 13.0%. δ_H(200 MHz, $CDCl_3$, Me_4Si): 1.73 (4H, m, =C-CH_2-CH_2), 2.66 (4H, m, =C-CH_2), 4.27 (8H, m, OCH_2), 6.31 (2H, s, CH_{edot}), 7.20 (3H, m, C$H_{\text{Ph-meta and para}}$), 7.28 (2H, m, C$H_{\text{Ph-ortho}}$). ^{31}P NMR (81 MHz, CD_2Cl_2): δ 16.4 (s). HR-MS (EI): *m/z* : 494.0753 $[M]^{+\cdot}$; calc. for $C_{26}H_{23}O_4S_2P$: 494.07754.

Synthesis of 1-Phenyl-2,5-bis[2-ethylenedioxylthiophene]-thiooxophosphole (5) . To a THF solution (5 mL) of Cp_2ZrCl_2 (0.12, 0.39 mmol) was added dropwise, at -78°C, a hexane solution of 1.6 M *n*-BuLi (0.52 mL, 0.82 mmol). After one hour stirring, 1,8-di[2-(3,4-ethylenedioxy)thienyl]octa-1,7-diyne (0.15 mg, 0.39 mmol) was added to the reaction mixture. The solution was warmed to room temperature, and stirred for 12h. To this solution was added, at -78°C, freshly distilled $PhPBr_2$ (0.09 mL, 0.43 mmol). The reaction mixture was allowed to warm to room temperature and stirred for 7h. After filtration on basic alumina (THF) and evaporation of the volatile materials under *vacuo*, the 1-phenyl-2,5-bis(2-(3,4-ethylenedioxy)thienyl)-phosphole was dissolved in dichloromethane (10 mL) and a large excess of S_8 was added. The mixture was stirred at room temperature for 3 days. After evaporation of the solvent *in vacuo*, the product was purified by column chromatography (alumina, ether/heptane, 1/1, R_f = 0.10) to give orange powder (0.155 g, 76%). Found : C, 59.5; H, 4.6; S 18.5. Calc. for $C_{26}H_{23}O_4PS_3$: C, 59.3; H, 4.4; S, 18.3%. δ_H(500 MHz, $CDCl_3$, Me_4Si): 1.70 (4H, m, =C-CH_2-CH_2), 2.61 (2H, m, =C-CH_2), 2.72 (2H, m, =C-CH_2), 3.96 (4H, m, OCH_2), 4.05 (4H, m, OCH_2), 6.23 (2H, s, CH_{edot}), 7.29 (2H, td, ^4J(H,H) = 3.0 Hz, ^3J(H,H) = 7.2 Hz ^3J(H,H) = 7.5 Hz, C$H_{\text{Ph- meta}}$), 7.36 (1H, dd, ^4J(H,H) = 5.5 Hz, ^3J(H,H) = 7.5 Hz, C$H_{\text{Ph- para}}$), 7.77 (2H, dd, ^3J(H,H) = 7.2 Hz, ^3J(P,H) = 14.0 Hz, C$H_{\text{Ph-ortho}}$). δ_C(125 MHz, $CDCl_3$): 21.5 (s, =C-CH_2-CH_2), 27.3 (s, =C-CH_2), 63.3 (s, OCH_2), 100.3 (s, CH$_{\text{edot}}$), 108.3 (d, *J*(P,C) = 13.8 Hz, C_{edot}-C=), 125.8 (d, *J*(P,C) = 84.3 Hz, P*C*=C),127.1 (d, *J*(P,C) = 12.6 Hz, CH$_{\text{Ph-meta}}$), 129.9 (d, *J*(P,C) = 45 Hz, $C_{\text{Ph-ipso}}$), 129.9 (d, *J*(P,C) = 11.6 Hz, CH$_{\text{Ph-ortho}}$), 130.4 (s, CH$_{\text{Ph-para}}$), 138.5 (s, C_{edot}O), 140.1 (s, C_{edot}O), 147.5 (d, *J*(P,C) = 22.8 Hz, PC=*C*). δ_P(81 MHz, $CDCl_3$, H_3PO_4 85%): 55.2. HR-MS (EI): *m/z* : 526.0479 $[M]^{+\cdot}$; calc. for $C_{26}H_{23}O_4S_3P$: 526.04961.

Synthesis of [1-phenyl-2,5-bis[2-ethylenedioxylthiophene]-phosphole]gold chloride complex (6). To a THF solution (5 mL) of Cp_2ZrCl_2 (0.12 g, 0.39 mmol) was added dropwise, at -78°C, a hexane solution of 1.6 M *n*-BuLi (0.52 mL, 0.82 mmol). After one hour stirring, 1,8-di[2-(3,4-ethylenedioxy)thienyl]octa-1,7-diyne (0.15 mg, 0.39 mmol) was added to the reaction mixture. The solution was warmed to room temperature, and stirred for 12h. To this solution was added, at -78°C, freshly distilled $PhPBr_2$ (0.09 mL, 0.43 mmol). The reaction mixture was allowed to warm to room temperature and stirred for 7h. After filtration on basic alumina (THF) and evaporation of the volatile materials under *vacuo*, the 1-phenyl-2,5-bis(2-(3,4-ethylenedioxy)thienyl)-phosphole was dissolved in dichloromethane (10 mL) and THTAuCl complex (132 mg, 0.41 mmol) was added. The mixture was stirred at room temperature for 1 hour. After evaporation of the solvent *in vacuo*, the product was purified by column chromatography (alumina, ether/heptane, 1/1, R_f = 0.15) to give a yellow powder (0.263 g, 93%). Found : C, 43.1; H, 3.0; S 9.0. Calc. for $C_{26}H_{23}O_4S_2AuClP$: C, 43.0; H, 3.2; S, 8.8%. δ_H(200 MHz, $CDCl_3$, Me_4Si): 1.86 (4H, m, =C-CH$_2$-C*H*$_2$), 2.68-3.08 (4H, m, =C-C*H*$_2$), 4.15 (8H, m, OC*H*$_2$), 6.43 (2H, s, C*H*$_{edot}$), 7.41 (3H, m, C*H*$_{Ph\text{-}meta\ and\ para}$), 7.55 (2H, m, C*H*$_{Ph\text{-}ortho}$). δ_C(125 MHz, $CDCl_3$): 21.7 (s, =C-CH$_2$-C*H*$_2$), 28.3 (s, =C-C*H*$_2$), 28.4 (s, =C-C*H*$_2$), 64.4 (s, O*C*H$_2$), 64.8 (s, O*C*H$_2$), 100.4 (s, *C*H$_{edot}$), 110.1 (d, ^2J(P,C) = 16.8 Hz, *C*$_{edot}$-C=), 124.2 (d, *J*(P,C) = 59.1 Hz, P*C*=C), 126.0 (d, *J*(P,C) = 52.5 Hz, *C*$_{Ph\text{-}ipso}$), 127.8 (d, *J*(P,C) = 12.5 Hz, *C*H$_{Ph\text{-}meta}$), 130.9 (d, *J*(P,C) = 2.4 Hz, *C*H$_{Ph\text{-}para}$), 132.8 (d, *J*(P,C) = 13.9 Hz, *C*H$_{Ph\text{-}ortho}$), 138.5 (d, *J*(P,C) = 3.9 Hz, *C*$_{edot}$O), 140.9 (s, *C*$_{edot}$O), 147.8 (d, *J*(P,C) = 15.3 Hz, PC=*C*). δ_P(81 MHz, CD_2Cl_2, H_3PO_4 85%): 43.7 (s). HR-MS (FAB, *m*NBA): *m/z* : 726.0128 $[M]^{+\cdot}$; calc. for $C_{26}H_{23}O_4S_2P$ AuCl: 726.0130.

X-ray Crystallographic Study of compound 4 :

Single crystals suitable for X-Ray crystal analysis were obtained by slow evaporation of a CH_2Cl_2 solution of **4** at room temperature. Single crystal data collection were performed at room temperature with a Nonius KappaCCD diffractometer (Center de Diffractométrie, Université de Rennes 1, France), with Mo-$K\alpha$ radiation (λ = 0.71073 Å). Reflections were indexed, Lorentz-polarization corrected and integrated by the *DENZO* program of the KappaCCD software package. The data merging process was performed using the SCALEPACK program.[3] Structure determinations were performed by direct methods with the solving program SIR97,[4] that revealed all the non hydrogen atoms. SHELXL program[5] was used to refine the structures by full-matrix least-squares based on F^2. All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were included in idealised positions and refined with isotropic displacement parameters. Atomic scattering factors for all atoms were taken from International Tables for X-ray Crystallography.[2 6 2] CCDC reference number "CCDC 671173" contain the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retreving.html or from the Cambridge Crystallographic Data Center, 12 union Road, Cambridge CB2 1EZ, UK; Fax: (internat.) + 44-1223-336-033; E-mail: deposit@ccdc.cam.ac.uk].

Crystallographic data :

Crystal data **4** : $C_{26}H_{23}O_4PS_2$, M_r = 494.53, 0.30 x 0.25 x 0.20 mm^3, monoclinic, *P21/c*, *a* = 11.081(2), *b* = 14.186(3), *c* = 15.345(3) Å, β = 104.749(7)°, *V* = 2332.7(1)Å^3, *T* = 120(2) K, *Z* = 4, ρ_{calcd} = 1.408 g cm^{-3}, μ = 0.329 mm^{-1}, *F*(000) = 1032, 10378 reflections were collected in the range 2.91≤ θ ≤ 27.46° of which 5329 were unique, $\lambda(Mo_{K\alpha})$ = 0.71069 Å, R_{int} = 0.0200, 299 parameters, $R1(F_0)$ = 0.0507, $\omega R2(F_0^2)$ = 0.1416

---

3. Otwinowski, Z.; Minor, W. In Methods in Enzymology, (Ed.: C.W. Carter, Jr. & R.M. Sweet), New York:Academic Press, 1997, 276, 307.

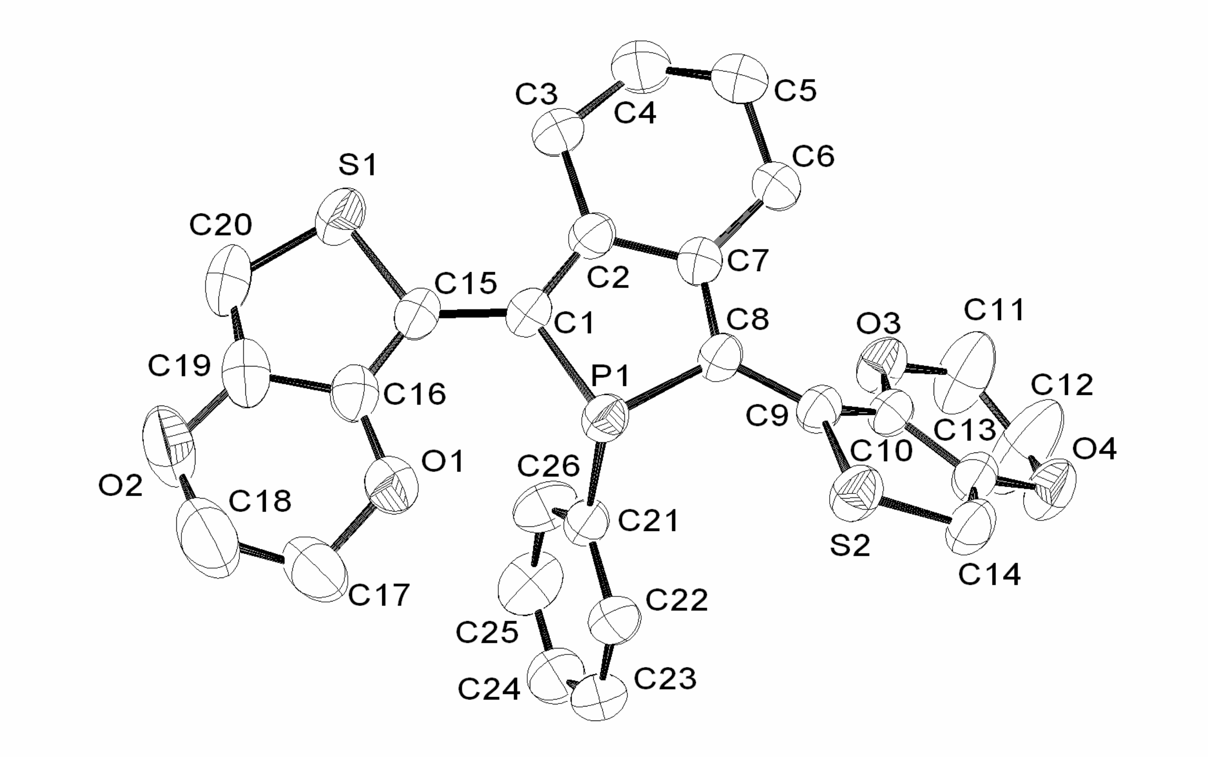
4. Altomare, A.; Burla, M.C.; Camalli, M.; Cascarano, G.; Giacovazzo, C.; Guagliardi, A.; Moliterni, A.G.G., Polidori, G.; Spagna, R. J. of Applied Cryst. **1999**, 32, 115.

5. Sheldrick G.M., SHELX97, Program for the Refinement of Crystal Structures, University of Göttingen, Germany, 1997.

6. International Tables for X-ray Crystallography, vol C, Ed. Kluwer, Dordrech, 1992.

and GOF = 1.059 for 4042 reflections with $I \geq 2\sigma(I)$ ($R1(F_0) = 0.0680$, $\omega R2(F_0^2) = 0.1570$ for all data), max/min residual density 0.503/-0.431 e.Å^{-3}.

Figure S1. Molecular structure of the derivative **4** (thermal ellipsoids 50% probability). Hydrogen atoms have been omitted for clarity.



B3LYP/6-31G* optimized data for the phosphole derivatives A1' and 4.

1-phenyl-2,5-bis(2-thienyl)-phosphole (A1')

Total energy:

E_tot (B3LYP/6-31G*) = -1831.431115 a.u.

Structural data in cartesian coordinates:

P	0.000670	-0.132082	-0.983517
C	-0.003217	1.504204	-0.122571
C	-0.001234	1.626253	1.275733
C	-0.004383	2.885292	1.871983
C	-0.009597	4.037979	1.080107
C	-0.011648	3.926993	-0.309506
C	-0.008430	2.664253	-0.908339
H	-0.009940	2.579966	-1.992264
H	-0.015692	4.819531	-0.929578
H	-0.012036	5.018823	1.548228
H	-0.002794	2.969561	2.955594
H	0.002775	0.732503	1.893045
C	-1.304099	-1.099316	-0.119400
C	1.309071	-1.093605	-0.118610
C	-0.715885	-2.115851	0.585454
C	0.724856	-2.112713	0.585876
C	-2.715787	-0.843805	-0.285399
C	2.719744	-0.831943	-0.283712
S	-3.917645	-1.586026	0.767703
S	3.924311	-1.570181	0.769109
C	-5.218499	-0.792767	-0.063133
C	5.222124	-0.770440	-0.060271

C	-4.759698	-0.001081	-1.080259
C	4.760384	0.020440	-1.076691
C	-3.342884	-0.027330	-1.206185
C	3.343753	-0.011743	-1.203284
H	-2.796568	0.522178	-1.965155
H	2.795429	0.536366	-1.961820
H	-5.410734	0.581071	-1.723552
H	5.409199	0.606132	-1.719012
H	-6.240123	-0.956133	0.252740
H	6.244300	-0.929810	0.255856
H	-1.281129	-2.897067	1.089092
H	1.293182	-2.891481	1.089836

1-phenyl-2,5-bis(2-(3,4-ethylenedioxy)thienyl)-phosphole (4)

Total energy:

E_tot (B3LYP/6-31G*) = -2443.156195 a.u.

Structural data in cartesian coordinates:

C	-0.782612	-3.018084	0.013674
C	-0.398158	-1.734108	0.421369
C	-0.073085	-1.517359	1.769470
C	-0.134093	-2.563890	2.687742
C	-0.519335	-3.841784	2.271370
C	-0.842470	-4.067890	0.933756
P	-0.332310	-0.390540	-0.847827
C	1.254884	0.458928	-0.533128
C	2.538298	-0.153361	-0.820773

S	2.759867	-1.218594	-2.208914
C	4.407940	-1.566578	-1.783407
C	4.767272	-0.903900	-0.645384
C	3.711382	-0.103876	-0.098113
O	3.856533	0.583435	1.081607
C	5.228270	0.753969	1.451990
C	5.997810	-0.550238	1.298991
O	6.008478	-0.974582	-0.067843
C	1.012363	1.745726	-0.131120
C	-0.391290	2.053231	0.125151
C	-0.689319	3.470917	0.545937
C	0.015979	4.505604	-0.369207
C	1.467646	4.118254	-0.765660
C	1.999427	2.875735	-0.018239
C	-1.259090	1.005329	-0.085061
C	-2.686053	0.931907	0.154165
C	-3.600588	0.045566	-0.385039
C	-4.933415	0.187160	0.116887
C	-5.052531	1.170340	1.055769
S	-3.524545	1.943729	1.338628
O	-3.279565	-0.908646	-1.314365
C	-4.425743	-1.420753	-2.003190
C	-5.532713	-1.760052	-1.016324
O	-5.973444	-0.584532	-0.327759
H	-1.762196	3.675718	0.555572
H	2.971777	2.580914	-0.421162
H	-0.339416	3.612927	1.579907
H	2.164174	3.119899	1.041778
H	-0.585709	4.629246	-1.276625

H	1.506344	3.903375	-1.839881
H	0.003355	5.476089	0.140603
H	2.147875	4.961181	-0.595741
H	-5.943630	1.476481	1.583985
H	5.018781	-2.224789	-2.383794
H	0.230240	-0.526163	2.094709
H	-1.035223	-3.194378	-1.028270
H	-1.139479	-5.060299	0.604019
H	-0.565207	-4.657186	2.988792
H	7.044574	-0.422153	1.586937
H	5.544264	-1.329095	1.927834
H	5.222698	1.085512	2.493698
H	5.688841	1.533704	0.828989
H	-4.085853	-2.311599	-2.536946
H	-4.782738	-0.678520	-2.730180
H	-6.410544	-2.156900	-1.532868
H	-5.173512	-2.503870	-0.291825
H	0.119414	-2.384313	3.729556

Full reference 5 entry:

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. G. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, *GAUSSIAN 03*, Gaussian, Inc., Wallingford, CT, 2004