Supporting Information for

New Insight into the Photo-induced Electron Transfer with a Simple Ubiquinone-based Triphenylamine Model

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General Methods

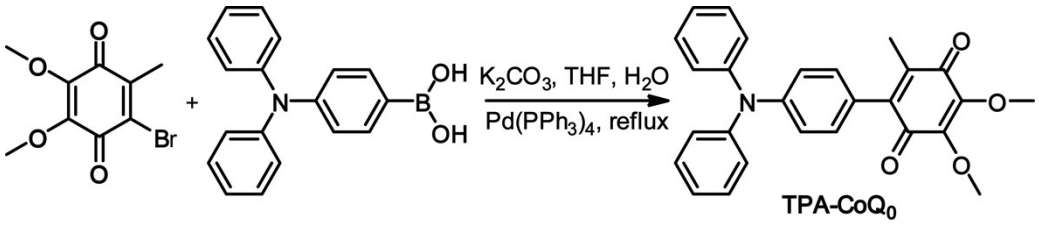
General considerations. HPLC-grade acetonitrile (CH_3CN) and tetrabutylammonium perchlorate (TBAP, 98%) was purchased from Sigma-Aldrich. N_2 (99.998%, prepurified) was gained from Cryogenic Gases. All chemical reagents for synthesis and analysis were analytical grade, obtained from commercial suppliers, and used without further purification unless specified. ^1H NMR and ^{13}C NMR were acquired in $CDCl_3$ on BRUKER AVANCE 500 spectrometer using TMS as an internal standard.

Electrochemical Measurements. PHLC-grade CH_3CN was dried by distillation over CaH_2 before the electrochemical experiments. A three-electrode cell was used for electrochemical measurements. Glassy carbon (GC, 3mm diameter) electrode was used as the work electrode, and platinum wire, Ag/AgCl wire electrode were used as the counter and quasi-reference electrodes, respectively. The measurements were carried out in a test solution containing 1.0 mM TPA-CoQ_0 and 0.1 M tetra-n-butylammonium perchlorate (TBAP). During the measurement, a dry nitrogen purge maintained an oxygen and moisture free environment and the temperature were controlled in 25℃ by using circulating water bath. All the electrochemistry measurements were performed at CHI 660 electrochemical work station (Shanghai Chenhua Co., Ltd., China).

In Situ Spectroelectrochemical and fluorescence spectroelectrochemical Measurements. All the spectroelectrochemical and fluorescence spectroelectrochemical experiments were recorded during redox processes of TPA-CoQ_0 in an optically transparent thin layer electrochemical cell (optical path length is 0.6 mm) via an Ocean Optics DT-minutesi-2 halogen recourse and USB2000+ or USB4000+ spectrometer. Platinum net, a platinum wire and Ag/AgCl wire electrode were used as working electrode, counter electrode and reference electrode, respectively. Electrochemical processes during the spectral measurement were controlled by CHI 660 electrochemical workstation (Shanghai Chenhua Co., Ltd., China).

DFT calculations. Density Functional Theory (DFT) calculations were carried out using the Gaussian 09 software. Geometries of all species in the calculations were optimized at the b3lyp/6-311++g (d, p) lever of theory, and the nature of each stationary point was established by b3lyp/6-311++g (d, p) frequency calculations. Polarizable continuum model (PCM) was used to describe the solvent and the interaction between solvent and solutes.[1]

Synthesis



6-Bormoubiquinone (0.90 g, 3.46 mmol) and K_2CO_3 (0.95 g, 6.92 mmol) were dissolved in a mixture solution of THF (40 mL) and H_2O (10 mL) and the mixture solution was degassed. After 4-(diphenylamino) phenylboronic acid (1.00 g, 3.46 mmol) and $Pd(PPh_3)_4$ (0.04 g, 3.46×10^{-2} mmol) were added, the reaction mixture was stirred and refluxed overnight at 102°C under nitrogen atmosphere. The reaction solution was cooled to room temperature and diluted with water (30 mL), and extracted with CH_2Cl_2 (30 mL ×3). The combined organic phases were washed brine and were dried over anhydrous Na_2SO_4. After evaporation of the solvent, the oily residue was purified by column chromatography to afford TPA-CoQ_0 as a red solid (0.32 g, 24.5%). The structure of TPA-CoQ_0 was confirmed by ^1H and ^{13}C NMR spectroscopy. δ_H (400 MHz, $CDCl_3$) 7.30–7.26 (4 H, m), 7.18–7.12 (4 H, m), 7.06 (4 H, ddd, *J* 5.7, 2.9, 1.1), 7.03–6.99 (2H, m), 4.06 (3 H, s), 4.01 (3 H, s), 2.02 (3 H, s); δ_C (101 MHz, $CDCl_3$) 184.90, 183.92, 148.23, 147.25, 144.97, 143.97, 141.44, 139.18, 130.92, 129.41, 125.27, 123.60, 121.40, 61.37, 61.17, 14.11.

NMR spectra

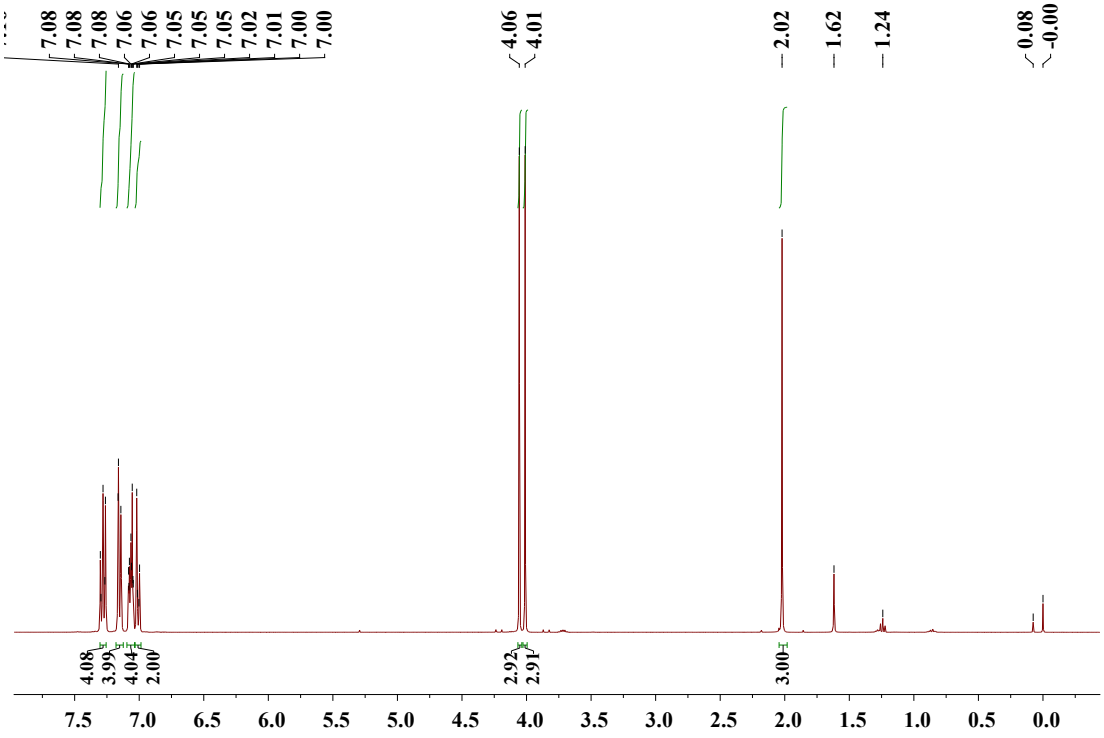


Figure S1. ^{1}H NMR spectrum of TPA-CoQ_0 in $CDCl_3$

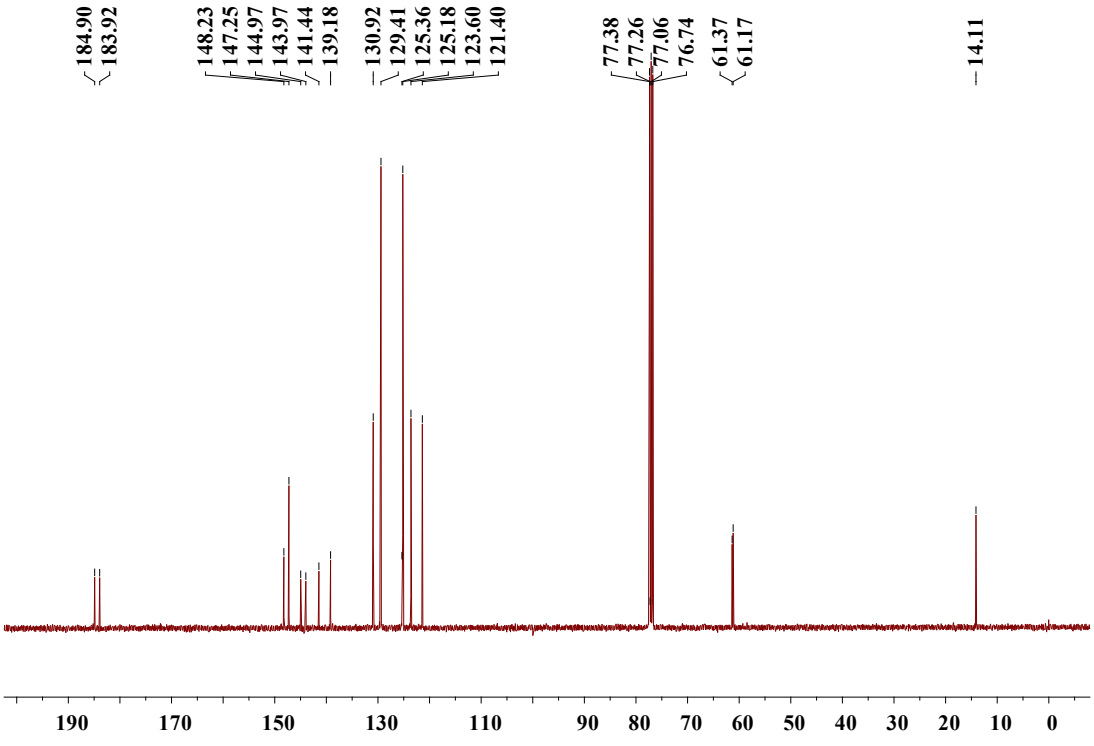


Figure S2. ^{13}C NMR spectrum of TPA-CoQ_0 in $CDCl_3$

References

1. Namazian, M. & Coote, M.L. Accurate Calculation of Absolute One-Electron Redox Potentials of Some para-Quinone Derivatives in Acetonitrile. J. Phys. Chem. A **111**, 7227-7232 (2007).

Single Crystal Data

Table 1. Crystal data and structure refinement for TPA-CoQ_0.

Identification code	TPA-CoQ_0	
Empirical formula	C27 H23 N O4	
Formula weight	425.46	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 9.7269(19) Å	α= 90°.
	b = 7.7811(15) Å	β= 95.907(4)°.
	c = 28.607(5) Å	γ = 90°.
Volume	2153.6(7) $Å^3$	
Z	4	
Density (calculated)	1.312 Mg/m^3	
Absorption coefficient	0.088 mm^{-1}	
F(000)	896	
Crystal size	0.211 x 0.165 x 0.112 mm^3	
Theta range for data collection	2.105 to 25.497°.	
Index ranges	-7<=h<=11, -8<=k<=9, -34<=l<=34	
Reflections collected	11839	
Independent reflections	4008 [R(int) = 0.0522]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6285	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4008 / 38 / 312	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2sigma(I)]	R1 = 0.0497, wR2 = 0.1198	
R indices (all data)	R1 = 0.0653, wR2 = 0.1291	
Extinction coefficient	0.0015(10)	
Largest diff. peak and hole	0.223 and -0.219 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for TPA-CoQ_0. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	5584(2)	8249(2)	3670(1)	41(1)
O(1)	264(1)	9254(2)	2329(1)	50(1)
O(2)	-1722(1)	8462(2)	1604(1)	65(1)
O(4)	1966(2)	8786(2)	682(1)	68(1)
C(1)	654(2)	8750(2)	1963(1)	38(1)
C(2)	-355(2)	8488(3)	1546(1)	45(1)
C(3)	76(2)	8491(3)	1119(1)	47(1)
C(4)	1573(2)	8592(3)	1067(1)	44(1)
C(5)	2592(2)	8417(2)	1490(1)	38(1)
C(6)	2161(2)	8474(2)	1922(1)	35(1)
C(7)	3062(2)	8404(2)	2371(1)	33(1)
C(8)	4265(2)	9376(2)	2444(1)	36(1)
C(9)	5094(2)	9341(2)	2865(1)	36(1)
C(10)	4755(2)	8310(2)	3233(1)	34(1)
C(11)	3554(2)	7324(2)	3164(1)	36(1)
C(12)	2725(2)	7382(2)	2744(1)	34(1)
C(13)	7047(2)	8412(2)	3702(1)	37(1)
C(14)	7783(2)	7874(3)	3341(1)	42(1)
C(15)	9201(2)	8053(3)	3373(1)	52(1)
C(16)	9909(2)	8728(3)	3771(1)	64(1)
C(17)	9193(2)	9240(3)	4131(1)	67(1)
C(18)	7771(2)	9097(3)	4099(1)	54(1)
C(19)	4898(2)	8292(2)	4087(1)	39(1)
C(20)	5248(2)	7151(3)	4450(1)	54(1)
C(21)	4550(3)	7214(3)	4844(1)	70(1)
C(22)	3504(3)	8374(3)	4879(1)	66(1)
C(23)	3169(2)	9525(3)	4523(1)	57(1)
C(24)	3869(2)	9493(3)	4130(1)	46(1)
C(25)	4055(2)	8208(3)	1384(1)	50(1)
C(26)	-2148(2)	7360(4)	1961(1)	68(1)
O(3)	-848(10)	8243(14)	726(6)	66(2)
C(27)	-1116(8)	9686(11)	432(3)	101(2)
O(3')	-640(20)	8480(30)	703(11)	71(2)
C(27')	-1801(7)	9564(10)	602(2)	81(2)

Table 3. Bond lengths [Å] and angles [°] for TPA-CoQ_0.

N(1)-C(10)	1.415(2)
N(1)-C(13)	1.422(2)
N(1)-C(19)	1.428(2)
O(1)-C(1)	1.214(2)
O(2)-C(2)	1.357(2)
O(2)-C(26)	1.426(3)
O(4)-C(4)	1.212(2)
C(1)-C(2)	1.479(3)
C(1)-C(6)	1.498(2)
C(2)-C(3)	1.332(3)
C(3)-O(3')	1.31(3)
C(3)-O(3)	1.378(14)
C(3)-C(4)	1.481(3)
C(4)-C(5)	1.490(3)
C(5)-C(6)	1.345(2)
C(5)-C(25)	1.494(3)
C(6)-C(7)	1.481(2)
C(7)-C(8)	1.391(2)
C(7)-C(12)	1.396(2)
C(8)-C(9)	1.378(2)
C(8)-H(8)	0.9300
C(9)-C(10)	1.391(2)
C(9)-H(9)	0.9300
C(10)-C(11)	1.395(2)
C(11)-C(12)	1.377(2)
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(13)-C(14)	1.379(3)
C(13)-C(18)	1.381(3)
C(14)-C(15)	1.380(3)
C(14)-H(14)	0.9300
C(15)-C(16)	1.372(3)
C(15)-H(15)	0.9300
C(16)-C(17)	1.361(3)
C(16)-H(16)	0.9300
C(17)-C(18)	1.382(3)

C(17)-H(17)	0.9300
C(18)-H(18)	0.9300
C(19)-C(20)	1.382(3)
C(19)-C(24)	1.383(3)
C(20)-C(21)	1.375(3)
C(20)-H(20)	0.9300
C(21)-C(22)	1.372(4)
C(21)-H(21)	0.9300
C(22)-C(23)	1.369(3)
C(22)-H(22)	0.9300
C(23)-C(24)	1.376(3)
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
O(3)-C(27)	1.410(12)
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
O(3')-C(27')	1.418(17)
C(27')-H(27D)	0.9600
C(27')-H(27E)	0.9600
C(27')-H(27F)	0.9600

C(10)-N(1)-C(13)	121.95(14)
C(10)-N(1)-C(19)	117.63(14)
C(13)-N(1)-C(19)	119.70(14)
C(2)-O(2)-C(26)	117.19(16)
O(1)-C(1)-C(2)	119.96(16)
O(1)-C(1)-C(6)	120.69(17)
C(2)-C(1)-C(6)	119.28(15)
C(3)-C(2)-O(2)	121.12(17)
C(3)-C(2)-C(1)	119.69(17)
O(2)-C(2)-C(1)	118.68(16)

O(3')-C(3)-C(2)	130.2(11)
C(2)-C(3)-O(3)	120.5(6)
O(3')-C(3)-C(4)	110.0(11)
C(2)-C(3)-C(4)	119.82(17)
O(3)-C(3)-C(4)	119.4(6)
O(4)-C(4)-C(3)	120.24(18)
O(4)-C(4)-C(5)	120.28(18)
C(3)-C(4)-C(5)	119.46(15)
C(6)-C(5)-C(4)	119.95(16)
C(6)-C(5)-C(25)	125.66(17)
C(4)-C(5)-C(25)	114.39(15)
C(5)-C(6)-C(7)	125.71(16)
C(5)-C(6)-C(1)	118.53(16)
C(7)-C(6)-C(1)	115.63(14)
C(8)-C(7)-C(12)	117.08(15)
C(8)-C(7)-C(6)	121.60(15)
C(12)-C(7)-C(6)	121.31(15)
C(9)-C(8)-C(7)	121.83(16)
C(9)-C(8)-H(8)	119.1
C(7)-C(8)-H(8)	119.1
C(8)-C(9)-C(10)	120.71(16)
C(8)-C(9)-H(9)	119.6
C(10)-C(9)-H(9)	119.6
C(9)-C(10)-C(11)	118.01(15)
C(9)-C(10)-N(1)	121.99(16)
C(11)-C(10)-N(1)	120.01(15)
C(12)-C(11)-C(10)	120.84(15)
C(12)-C(11)-H(11)	119.6
C(10)-C(11)-H(11)	119.6
C(11)-C(12)-C(7)	121.53(16)
C(11)-C(12)-H(12)	119.2
C(7)-C(12)-H(12)	119.2
C(14)-C(13)-C(18)	118.21(17)
C(14)-C(13)-N(1)	121.18(16)
C(18)-C(13)-N(1)	120.60(16)
C(13)-C(14)-C(15)	120.79(19)
C(13)-C(14)-H(14)	119.6
C(15)-C(14)-H(14)	119.6

C(16)-C(15)-C(14)	120.41(19)
C(16)-C(15)-H(15)	119.8
C(14)-C(15)-H(15)	119.8
C(17)-C(16)-C(15)	119.2(2)
C(17)-C(16)-H(16)	120.4
C(15)-C(16)-H(16)	120.4
C(16)-C(17)-C(18)	120.8(2)
C(16)-C(17)-H(17)	119.6
C(18)-C(17)-H(17)	119.6
C(17)-C(18)-C(13)	120.5(2)
C(17)-C(18)-H(18)	119.7
C(13)-C(18)-H(18)	119.7
C(20)-C(19)-C(24)	119.55(17)
C(20)-C(19)-N(1)	120.88(18)
C(24)-C(19)-N(1)	119.57(17)
C(21)-C(20)-C(19)	119.3(2)
C(21)-C(20)-H(20)	120.4
C(19)-C(20)-H(20)	120.4
C(22)-C(21)-C(20)	121.0(2)
C(22)-C(21)-H(21)	119.5
C(20)-C(21)-H(21)	119.5
C(23)-C(22)-C(21)	119.9(2)
C(23)-C(22)-H(22)	120.0
C(21)-C(22)-H(22)	120.0
C(22)-C(23)-C(24)	119.8(2)
C(22)-C(23)-H(23)	120.1
C(24)-C(23)-H(23)	120.1
C(23)-C(24)-C(19)	120.5(2)
C(23)-C(24)-H(24)	119.8
C(19)-C(24)-H(24)	119.8
C(5)-C(25)-H(25A)	109.5
C(5)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(5)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
O(2)-C(26)-H(26A)	109.5
O(2)-C(26)-H(26B)	109.5

H(26A)-C(26)-H(26B)	109.5
O(2)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(3)-O(3)-C(27)	116.0(9)
O(3)-C(27)-H(27A)	109.5
O(3)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
O(3)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(3)-O(3')-C(27')	121(2)
O(3')-C(27')-H(27D)	109.5
O(3')-C(27')-H(27E)	109.5
H(27D)-C(27')-H(27E)	109.5
O(3')-C(27')-H(27F)	109.5
H(27D)-C(27')-H(27F)	109.5
H(27E)-C(27')-H(27F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for cd214669. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	30(1)	64(1)	30(1)	-1(1)	3(1)	-1(1)
O(1)	39(1)	70(1)	43(1)	-7(1)	8(1)	5(1)
O(2)	33(1)	100(1)	59(1)	15(1)	-3(1)	7(1)
O(4)	72(1)	98(1)	33(1)	4(1)	9(1)	13(1)
C(1)	35(1)	43(1)	37(1)	3(1)	5(1)	3(1)
C(2)	33(1)	53(1)	45(1)	4(1)	-3(1)	7(1)
C(3)	48(1)	53(1)	37(1)	1(1)	-8(1)	9(1)
C(4)	54(1)	47(1)	32(1)	1(1)	4(1)	8(1)
C(5)	40(1)	39(1)	37(1)	3(1)	6(1)	4(1)
C(6)	33(1)	38(1)	34(1)	2(1)	2(1)	1(1)
C(7)	29(1)	37(1)	32(1)	0(1)	5(1)	3(1)
C(8)	36(1)	39(1)	35(1)	7(1)	7(1)	0(1)

C(9)	30(1)	40(1)	40(1)	0(1)	5(1)	-5(1)
C(10)	30(1)	42(1)	30(1)	-2(1)	4(1)	2(1)
C(11)	34(1)	43(1)	32(1)	6(1)	9(1)	0(1)
C(12)	27(1)	40(1)	37(1)	-2(1)	6(1)	-4(1)
C(13)	31(1)	40(1)	39(1)	0(1)	0(1)	0(1)
C(14)	34(1)	48(1)	43(1)	-3(1)	3(1)	-2(1)
C(15)	37(1)	59(1)	62(1)	1(1)	12(1)	1(1)
C(16)	33(1)	78(2)	79(2)	-3(1)	-1(1)	-7(1)
C(17)	45(1)	82(2)	69(2)	-17(1)	-12(1)	-12(1)
C(18)	44(1)	68(1)	48(1)	-15(1)	-1(1)	-2(1)
C(19)	37(1)	49(1)	32(1)	-4(1)	4(1)	-7(1)
C(20)	75(2)	49(1)	38(1)	0(1)	8(1)	4(1)
C(21)	118(2)	54(1)	38(1)	2(1)	18(1)	-9(2)
C(22)	88(2)	68(2)	48(1)	-17(1)	33(1)	-26(1)
C(23)	46(1)	71(2)	56(1)	-18(1)	16(1)	-8(1)
C(24)	38(1)	58(1)	40(1)	-1(1)	2(1)	-3(1)
C(25)	46(1)	64(1)	42(1)	4(1)	14(1)	4(1)
C(26)	44(1)	91(2)	69(2)	5(1)	5(1)	-15(1)
O(3)	62(3)	84(3)	47(2)	0(2)	-20(2)	5(2)
C(27)	99(5)	110(4)	86(4)	27(4)	-36(4)	9(4)
O(3')	66(4)	93(4)	50(3)	1(4)	-21(4)	17(4)
C(27')	76(4)	94(4)	65(3)	5(3)	-23(3)	27(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for TPA-CoQ_0.

	x	y	z	U(eq)
H(8)	4518	10068	2202	44
H(9)	5887	10015	2903	44
H(11)	3309	6619	3405	43
H(12)	1923	6724	2708	41
H(14)	7318	7384	3073	50
H(15)	9680	7715	3124	63
H(16)	10866	8835	3794	76
H(17)	9668	9692	4402	80
H(18)	7297	9465	4347	65

H(20)	5948	6350	4428	65
H(21)	4791	6458	5091	83
H(22)	3022	8379	5143	80
H(23)	2470	10326	4548	68
H(24)	3650	10284	3890	55
H(25A)	4429	9311	1315	75
H(25B)	4085	7464	1118	75
H(25C)	4592	7717	1651	75
H(26A)	-1494	6441	2017	102
H(26B)	-3043	6894	1860	102
H(26C)	-2193	8005	2245	102
H(27A)	-1520	10581	604	152
H(27B)	-1743	9369	165	152
H(27C)	-266	10089	328	152
H(27D)	-2555	9142	761	121
H(27E)	-2064	9574	269	121
H(27F)	-1571	10709	707	121

Table 6. Torsion angles [°] for TPA-CoQ_0.

C(26)-O(2)-C(2)-C(3)	137.7(2)
C(26)-O(2)-C(2)-C(1)	-50.5(3)
O(1)-C(1)-C(2)-C(3)	158.1(2)
C(6)-C(1)-C(2)-C(3)	-18.8(3)
O(1)-C(1)-C(2)-O(2)	-13.8(3)
C(6)-C(1)-C(2)-O(2)	169.27(18)
O(2)-C(2)-C(3)-O(3')	0.3(13)
C(1)-C(2)-C(3)-O(3')	-171.4(13)
O(2)-C(2)-C(3)-O(3)	-8.6(6)
C(1)-C(2)-C(3)-O(3)	179.8(5)
O(2)-C(2)-C(3)-C(4)	177.46(18)
C(1)-C(2)-C(3)-C(4)	5.8(3)
O(3')-C(3)-C(4)-O(4)	5.8(11)
C(2)-C(3)-C(4)-O(4)	-171.9(2)
O(3)-C(3)-C(4)-O(4)	14.0(6)
O(3')-C(3)-C(4)-C(5)	-172.9(10)
C(2)-C(3)-C(4)-C(5)	9.4(3)
O(3)-C(3)-C(4)-C(5)	-164.7(5)

O(4)-C(4)-C(5)-C(6)	169.57(19)
C(3)-C(4)-C(5)-C(6)	-11.7(3)
O(4)-C(4)-C(5)-C(25)	-9.7(3)
C(3)-C(4)-C(5)-C(25)	169.04(18)
C(4)-C(5)-C(6)-C(7)	-176.78(17)
C(25)-C(5)-C(6)-C(7)	2.4(3)
C(4)-C(5)-C(6)-C(1)	-1.2(3)
C(25)-C(5)-C(6)-C(1)	177.94(18)
O(1)-C(1)-C(6)-C(5)	-160.59(18)
C(2)-C(1)-C(6)-C(5)	16.3(3)
O(1)-C(1)-C(6)-C(7)	15.4(3)
C(2)-C(1)-C(6)-C(7)	-167.68(16)
C(5)-C(6)-C(7)-C(8)	45.2(3)
C(1)-C(6)-C(7)-C(8)	-130.47(17)
C(5)-C(6)-C(7)-C(12)	-135.98(19)
C(1)-C(6)-C(7)-C(12)	48.3(2)
C(12)-C(7)-C(8)-C(9)	-0.1(3)
C(6)-C(7)-C(8)-C(9)	178.72(16)
C(7)-C(8)-C(9)-C(10)	0.6(3)
C(8)-C(9)-C(10)-C(11)	-0.3(3)
C(8)-C(9)-C(10)-N(1)	-179.92(16)
C(13)-N(1)-C(10)-C(9)	-34.0(3)
C(19)-N(1)-C(10)-C(9)	136.21(18)
C(13)-N(1)-C(10)-C(11)	146.36(17)
C(19)-N(1)-C(10)-C(11)	-43.4(2)
C(9)-C(10)-C(11)-C(12)	-0.4(3)
N(1)-C(10)-C(11)-C(12)	179.23(16)
C(10)-C(11)-C(12)-C(7)	0.9(3)
C(8)-C(7)-C(12)-C(11)	-0.6(3)
C(6)-C(7)-C(12)-C(11)	-179.44(16)
C(10)-N(1)-C(13)-C(14)	-29.7(3)
C(19)-N(1)-C(13)-C(14)	160.22(18)
C(10)-N(1)-C(13)-C(18)	151.13(19)
C(19)-N(1)-C(13)-C(18)	-18.9(3)
C(18)-C(13)-C(14)-C(15)	-1.5(3)
N(1)-C(13)-C(14)-C(15)	179.34(18)
C(13)-C(14)-C(15)-C(16)	1.9(3)
C(14)-C(15)-C(16)-C(17)	-0.9(4)

C(15)-C(16)-C(17)-C(18)	-0.4(4)
C(16)-C(17)-C(18)-C(13)	0.7(4)
C(14)-C(13)-C(18)-C(17)	0.3(3)
N(1)-C(13)-C(18)-C(17)	179.4(2)
C(10)-N(1)-C(19)-C(20)	133.2(2)
C(13)-N(1)-C(19)-C(20)	-56.4(3)
C(10)-N(1)-C(19)-C(24)	-46.9(2)
C(13)-N(1)-C(19)-C(24)	123.5(2)
C(24)-C(19)-C(20)-C(21)	1.1(3)
N(1)-C(19)-C(20)-C(21)	-179.0(2)
C(19)-C(20)-C(21)-C(22)	0.8(4)
C(20)-C(21)-C(22)-C(23)	-1.9(4)
C(21)-C(22)-C(23)-C(24)	1.1(3)
C(22)-C(23)-C(24)-C(19)	0.8(3)
C(20)-C(19)-C(24)-C(23)	-1.9(3)
N(1)-C(19)-C(24)-C(23)	178.21(18)
O(3')-C(3)-O(3)-C(27)	-35(7)
C(2)-C(3)-O(3)-C(27)	110.3(9)
C(4)-C(3)-O(3)-C(27)	-75.7(11)
C(2)-C(3)-O(3')-C(27')	45(2)
O(3)-C(3)-O(3')-C(27')	84(7)
C(4)-C(3)-O(3')-C(27')	-132.6(16)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for TPA-CoQ_0 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)