



# Redox Control of the Binding Modes of an Organic Receptor

Marco Frasconi,<sup>†,‡</sup> Isurika R. Fernando,<sup>†</sup> Yilei Wu,<sup>†,‡</sup> Zhichang Liu,<sup>†</sup> Wei-Guang Liu,<sup>§</sup>  
Scott M. Dyar,<sup>†,‡</sup> Gokhan Barin,<sup>†,#</sup> Michael R. Wasielewski,<sup>†,‡</sup>  
William A. Goddard III,<sup>§,||</sup> J. Fraser Stoddart<sup>\*,†</sup>

<sup>†</sup>Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, Illinois 60208, USA

<sup>‡</sup>Argonne-Northwestern Solar Energy Research (ANSER) Center, Northwestern University, Evanston, Illinois 60208, USA

<sup>§</sup>Materials and Process Simulation Center, California Institute of Technology, Pasadena, California 91125, USA

<sup>||</sup>NanoCentury KAIST Institute and Graduate School of EEWS (WCU), Korea Advanced Institute of Science and Technology (KAIST), 373-1 Guseong Dong, Yuseong Gu, Daejeon 305-701, Republic of Korea

Present Address:

(M. F.) <sup>‡</sup>Istituto Italiano di Tecnologia (IIT), Via Morego 30, 16163 Genova, Italy

(G. B.) <sup>#</sup>Department of Chemistry, University of California, Berkeley, California 94720-1460, USA

\*e-mail: [stoddart@northwestern.edu](mailto:stoddart@northwestern.edu)

## SUPPORTING INFORMATION

# Table of Contents

**Section A. Materials / General Methods / Instrumentation** **S4**

**Section B. Spectroscopic Characterization** **S5**

**1) *NMR Spectroscopic analysis***

**1.1) *CBPQT•4PF<sub>6</sub>***

**a) *<sup>1</sup>H NMR Spectrum***

**1.2) *Neutral CBPQT***

**a) *<sup>1</sup>H NMR Spectrum***

**b) *<sup>1</sup>H DOSY NMR Spectrum***

**c) *<sup>13</sup>C NMR Spectrum***

**d) *<sup>1</sup>H–<sup>13</sup>C HMBC Spectrum***

**e) *<sup>1</sup>H–<sup>13</sup>C HSQC Spectrum***

**1.3) *Neutral MV***

**a) *<sup>1</sup>H NMR Spectrum***

**b) *<sup>13</sup>C NMR Spectrum***

**1.4) *Inclusion complexes of neutral CBPQT***

**2) *UV–Vis Spectroscopy***

**3) *Electron paramagnetic resonance (EPR) spectroscopy***

**3.1) *Redox titration experiments***

**3.2) *Solid-state EPR spectroscopic analysis***

## Section C. Crystallographic Characterization

S15

### 1) *Neutral CBPQT*

1.1) *Methods*

1.2) *Crystal data*

1.3) *Solid-state structure*

### 2) *Mixed (CBPQT)(CBPQT•2PF<sub>6</sub>)*

2.1) *Methods*

2.2) *Crystal data*

### 3) *Neutral MS*

3.1) *Methods*

3.2) *Crystal data*

### 4) *DCB cCBPQT*

4.1) *Methods*

4.2) *Crystal data*

## Section D. Computational Analysis

S18

### 1) *Methods*

### 2) *Calculated HOMO/LUMO energy levels*

### 3) *Coordinates and energies of each species in different redox states*

## Section E. References

S99

## Section A. Materials / General Methods / Instrumentation

All reagents were purchased from commercial suppliers (Aldrich or VWR) and used without further purification. Cyclobis (paraquat-p-phenylene),<sup>S1</sup> CBPQT·4PF<sub>6</sub>, cyclobis(paraquat-4,4'-biphenylene),<sup>S2</sup> MS·4PF<sub>6</sub>, and dimethyl viologen,<sup>S3</sup> MV·2PF<sub>6</sub>, were prepared according to literature procedures. Bis(cyclopentadienyl)cobalt(II), known as cobaltocene (CoCp<sub>2</sub>), was purchased from Sigma-Aldrich and stored in an Ar glovebox. Under these conditions cobaltocene was found to be stable for several months with purity higher than 99.9%, as assayed in dry solvent by oxidation with a solution of tetrabutylammonium iodide, and by titrating the excess of iodine with aqueous thiosulfate. All experiments were performed in MeCN and DMF solutions, previously degassed, in a glovebox under an Ar atmosphere. In some of the titration experiments, UV–Vis and EPR spectroscopy were measured on the same solutions. UV–Vis Absorbance spectra were recorded using a Varian 100-Bio UV–Vis spectrophotometer in a quartz cell with an optical path-length of 2 or 10 mm containing the solution of interest. Samples were prepared immediately prior to use and the solutions were sealed under Ar with Teflon stoppers. Experimental error: absorption maxima, ±1 nm.

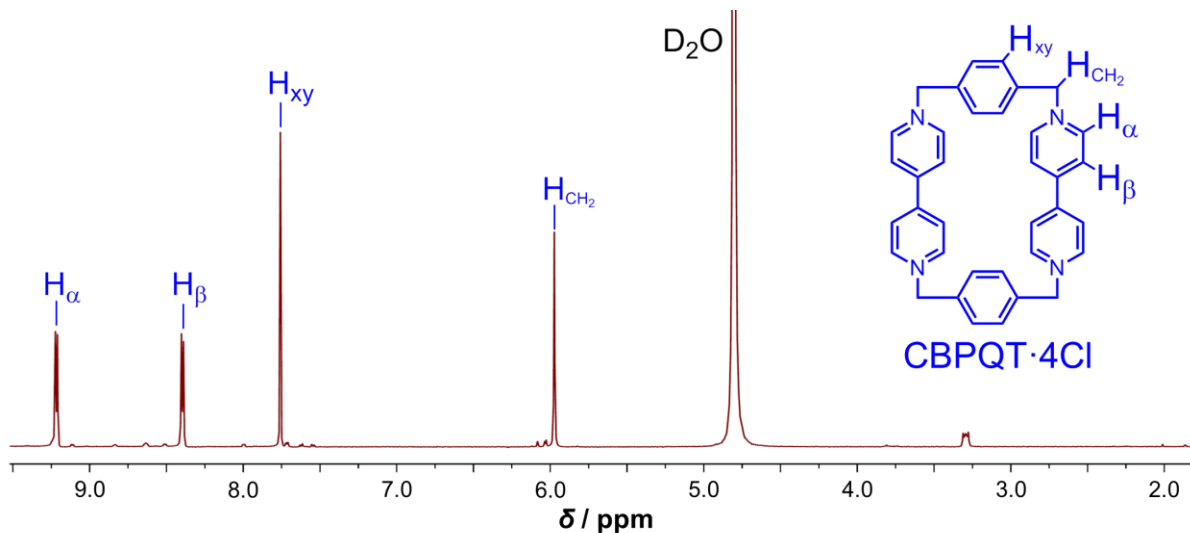
EPR Spectra were recorded using a Bruker Elexsys E580-X EPR spectrometer, equipped with a variable Q dielectric resonator (ER-4118X-MD5-W1). Samples were prepared by titration with cobaltocene and the solution was loaded into quartz 1.4 mm tubes and sealed with a clear ridged UV doming epoxy (IllumaBond 60-7160RCL). The sample was used immediately after preparation. Steady-state solution CW EPR spectra were collected with a 0.25 G modulation amplitude 2.56 ms time constant, and 10.24 ms conversion time, averaging 100 sweeps 50 G wide, centered around 2465 G. Steady-state solid CW EPR spectra were measured with the same parameters with a modulation amplitude of 0.05 G. Nuclear magnetic resonance (NMR) spectra were recorded at 298 K on Bruker Avance 500 and 600 spectrometers, with working frequencies of 500 and 600 MHz for <sup>1</sup>H, and 125 and 150 MHz for <sup>13</sup>C nuclei, respectively. <sup>13</sup>C NMR spectra were recorded with the simultaneous decoupling of proton nuclei. Chemical shifts are reported in ppm relative to the signals corresponding to the residual non-deuterated solvents.<sup>S4</sup> Single crystal X-ray data were measured on a Bruker Kappa APEX CCD diffractometer using Cu-K $\alpha$  radiation. Data collection and structure refinement details can be found in the CIF files. CCDC depositions 985863, 985864, 985865 and 985862 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).

## Section B. Spectroscopic Characterization

### 1) NMR Spectroscopic analysis

#### 1.1) CBPQT•4PF<sub>6</sub>

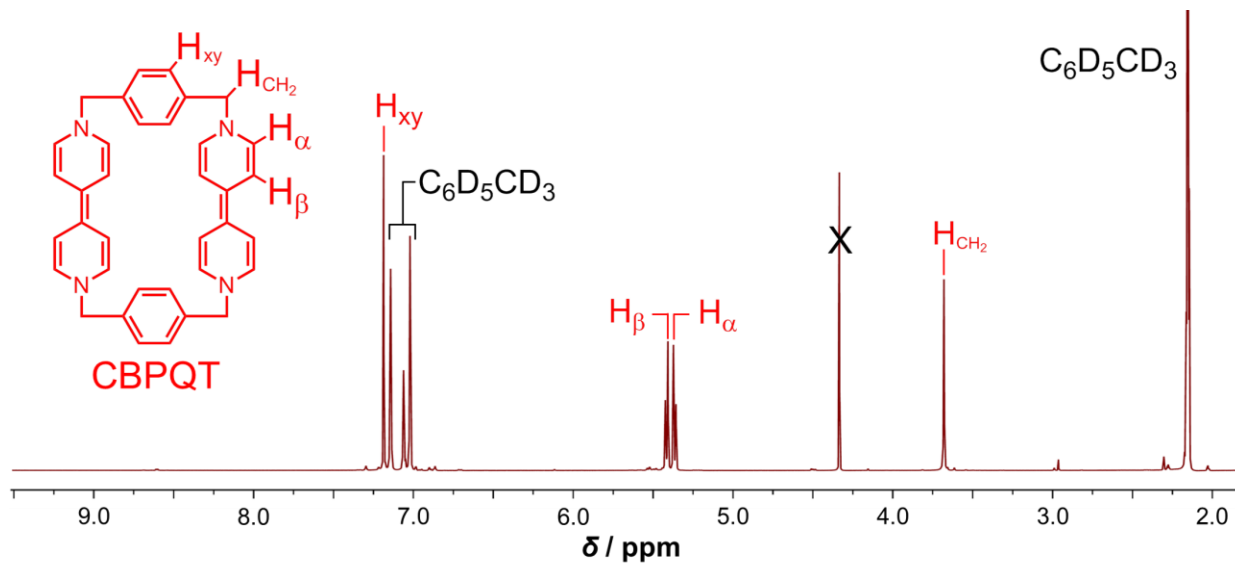
##### a) <sup>1</sup>H NMR Spectrum



**Figure S1.** <sup>1</sup>H NMR spectrum (500 MHz, D<sub>2</sub>O, 298 K) of CBPQT•4Cl recorded in aqueous solution of CO<sub>3</sub><sup>2-</sup>/HCO<sub>3</sub><sup>-</sup> at pH 9.0.

#### 1.2) Neutral CBPQT

##### a) <sup>1</sup>H NMR Spectrum



**Figure S2.** <sup>1</sup>H NMR spectrum (500 MHz, C<sub>6</sub>D<sub>5</sub>CD<sub>3</sub>, 298 K) of neutral CBPQT transferred to C<sub>6</sub>D<sub>5</sub>CD<sub>3</sub> by extraction from the biphasic system.

b)  $^1\text{H}$  DOSY NMR Spectrum

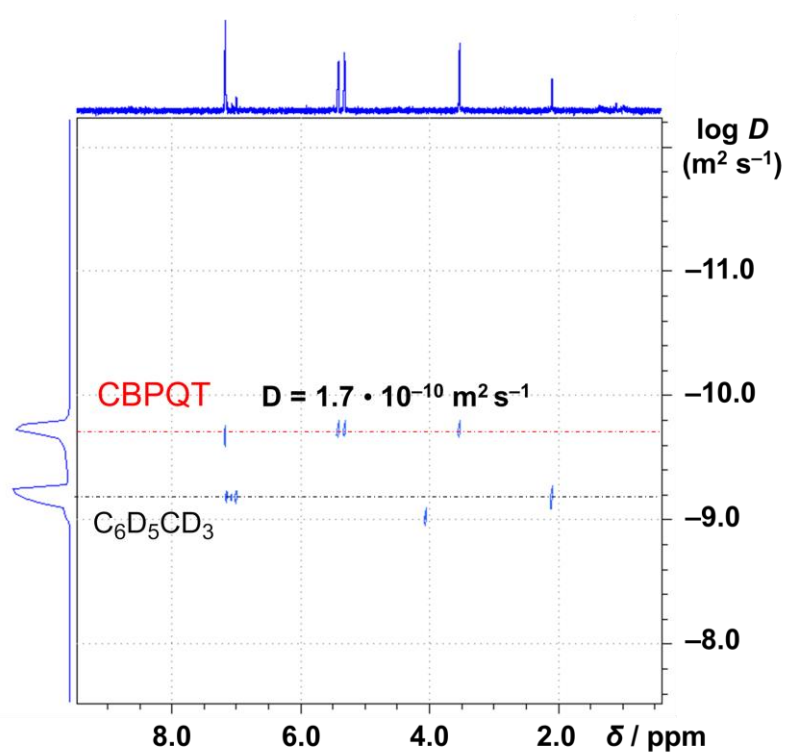


Figure S3.  $^1\text{H}$  DOSY NMR spectrum (600 MHz,  $\text{C}_6\text{D}_5\text{CD}_3$ , 250 K) of neutral CBPQT.

c)  $^{13}\text{C}$  NMR Spectrum

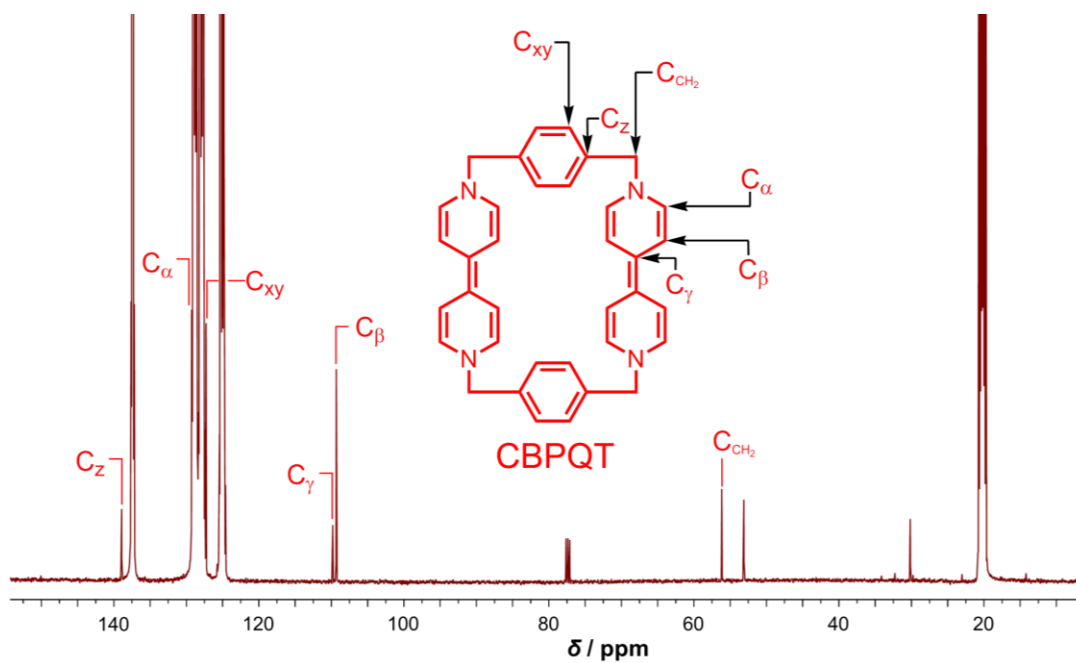
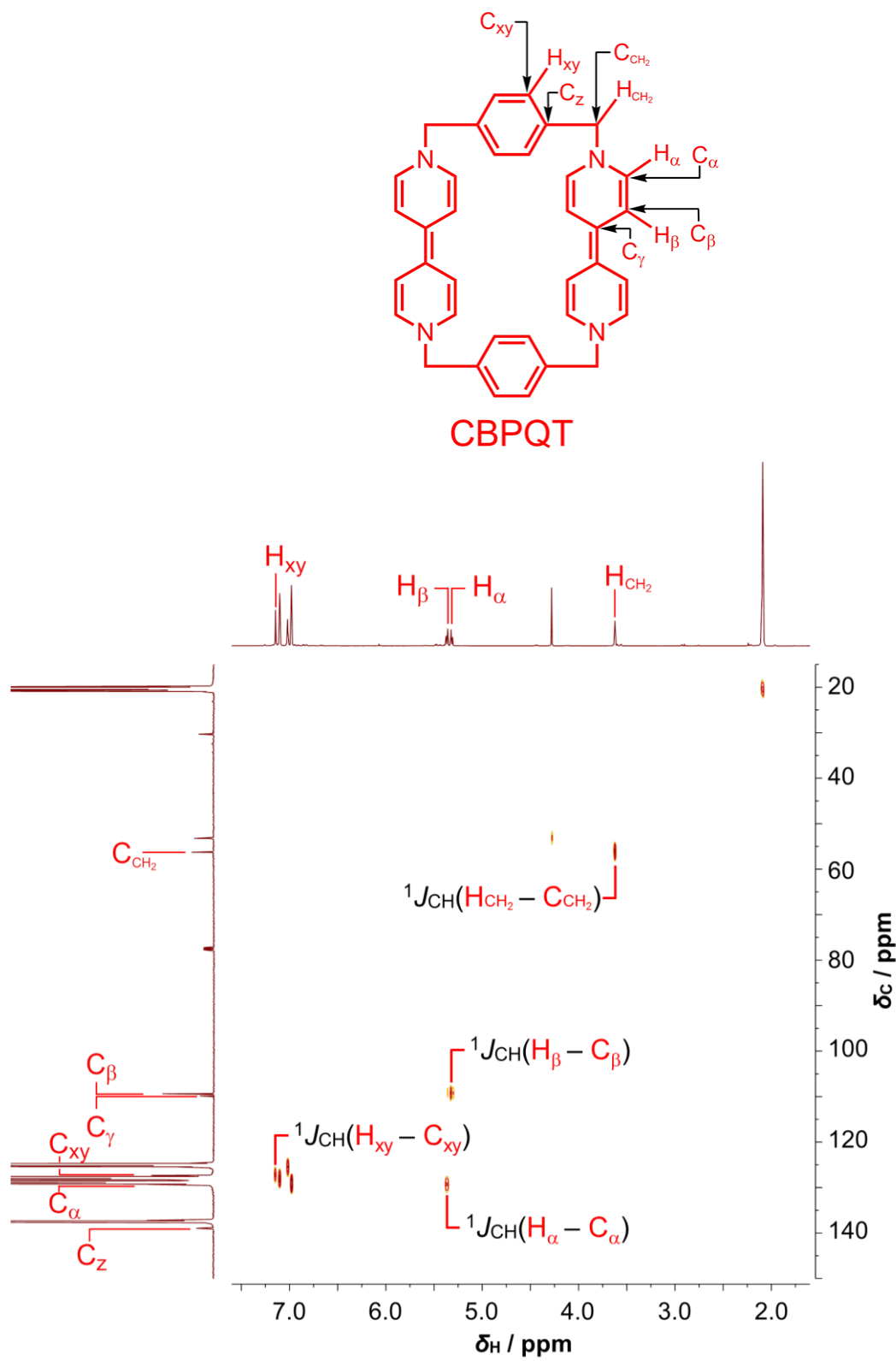


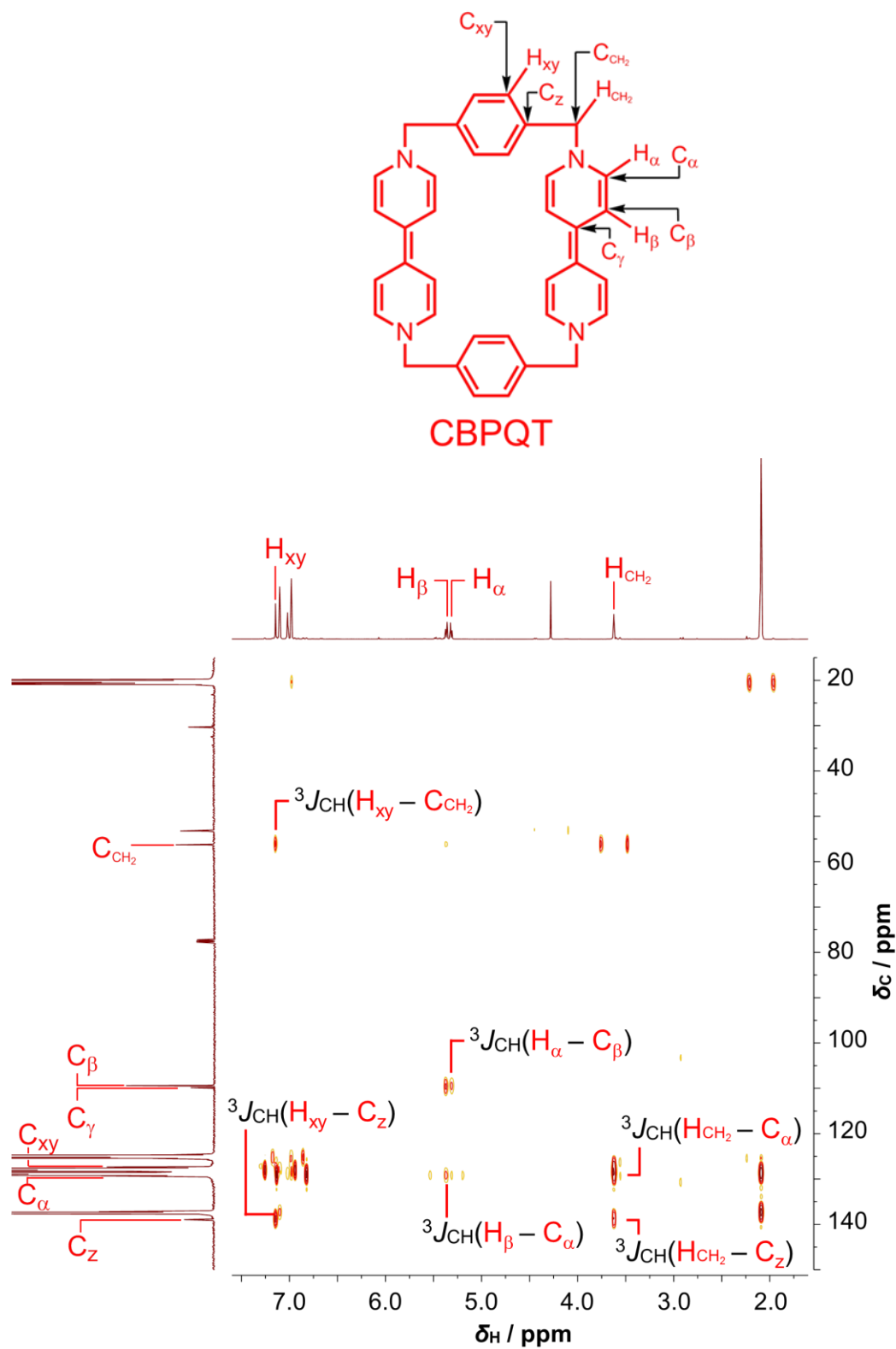
Figure S4.  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{C}_6\text{D}_5\text{CD}_3$ , 298 K) of neutral CBPQT.

d)  $^1\text{H}-^{13}\text{C}$  HSQC Spectrum



**Figure S5.**  $^1\text{H}-^{13}\text{C}$  HSQC spectrum (500 MHz,  $\text{C}_6\text{D}_5\text{CD}_3$ , 298 K) of neutral CBPQT.

e)  $^1\text{H}-^{13}\text{C}$  HMBC Spectrum

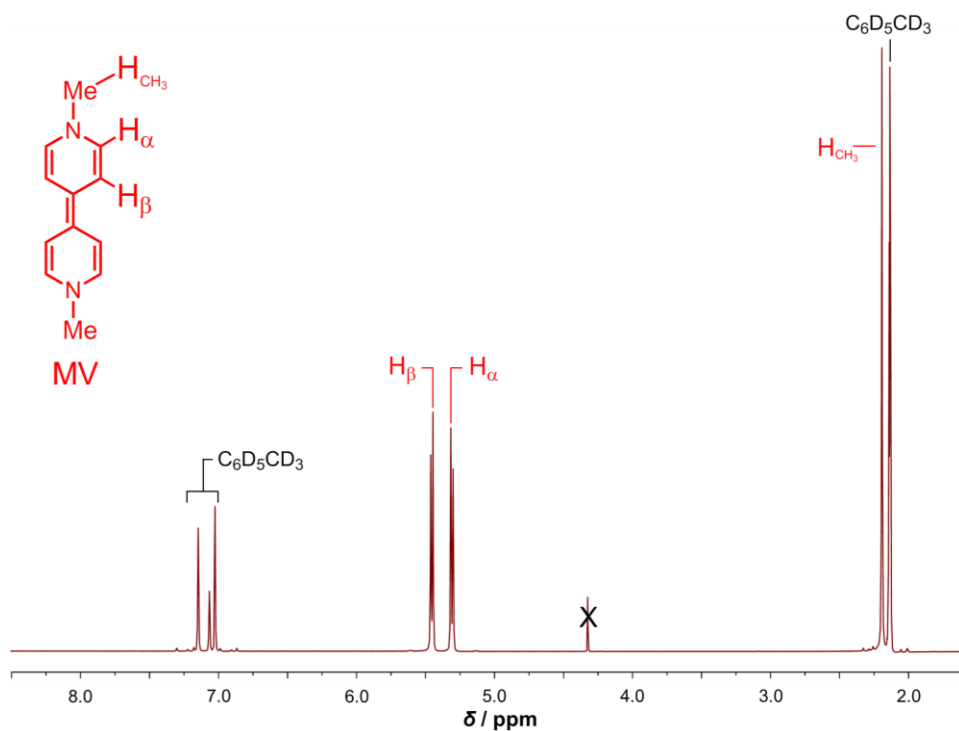


**Figure S6.**  $^1\text{H}-^{13}\text{C}$  HMBC spectrum (500 MHz,  $\text{C}_6\text{D}_5\text{CD}_3$ , 298 K) of neutral CBPQT.



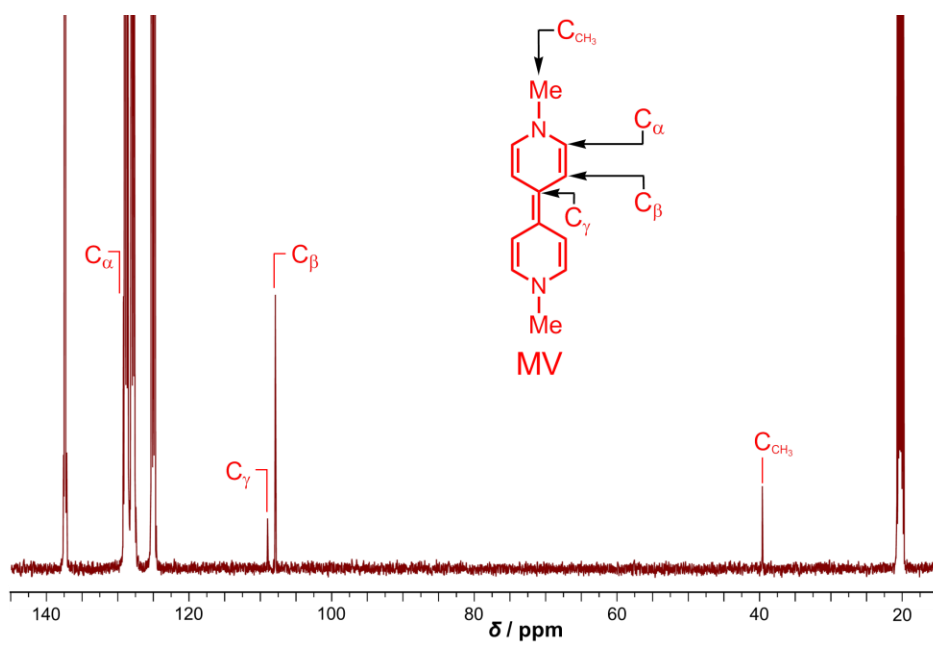
1.3) Neutral MV

a)  $^1\text{H}$  NMR Spectrum



**Figure S7.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{C}_6\text{D}_5\text{CD}_3$ , 298 K) of neutral MV transferred to  $\text{CD}_5\text{CD}_3$  by extraction from the biphasic system.

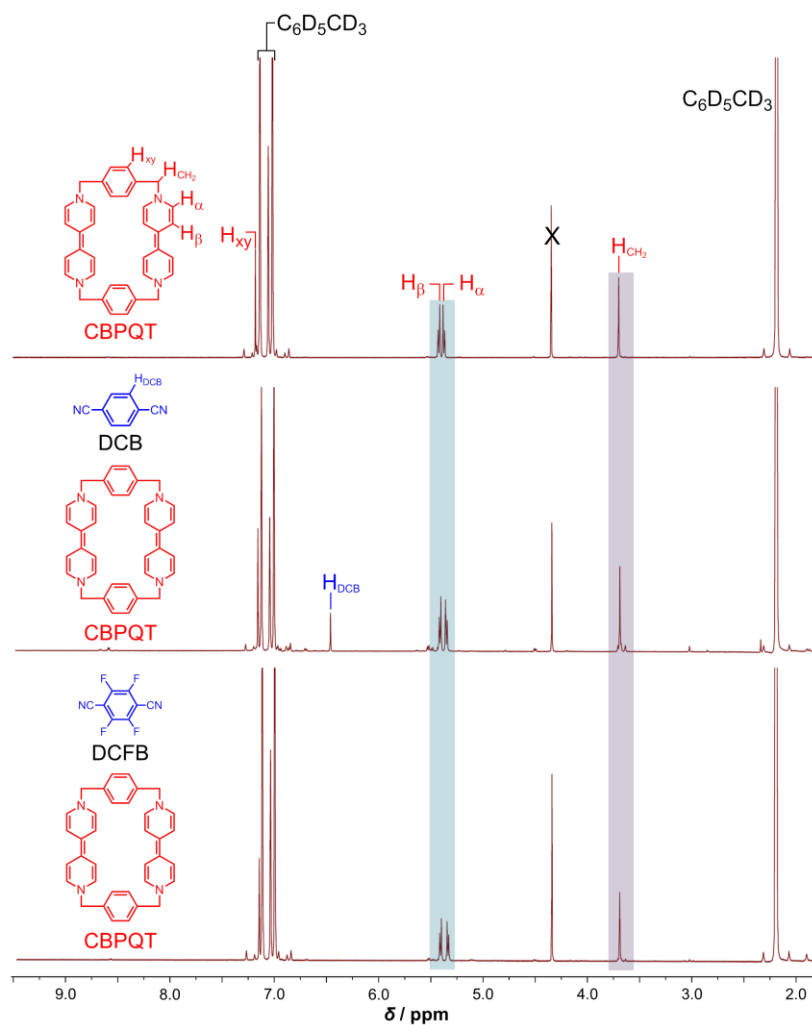
b)  $^{13}\text{C}$  NMR Spectrum



**Figure S8.**  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{C}_6\text{D}_5\text{CD}_3$ , 298 K) of neutral MV.

#### 1.4) Inclusion complexes of neutral CBPQT

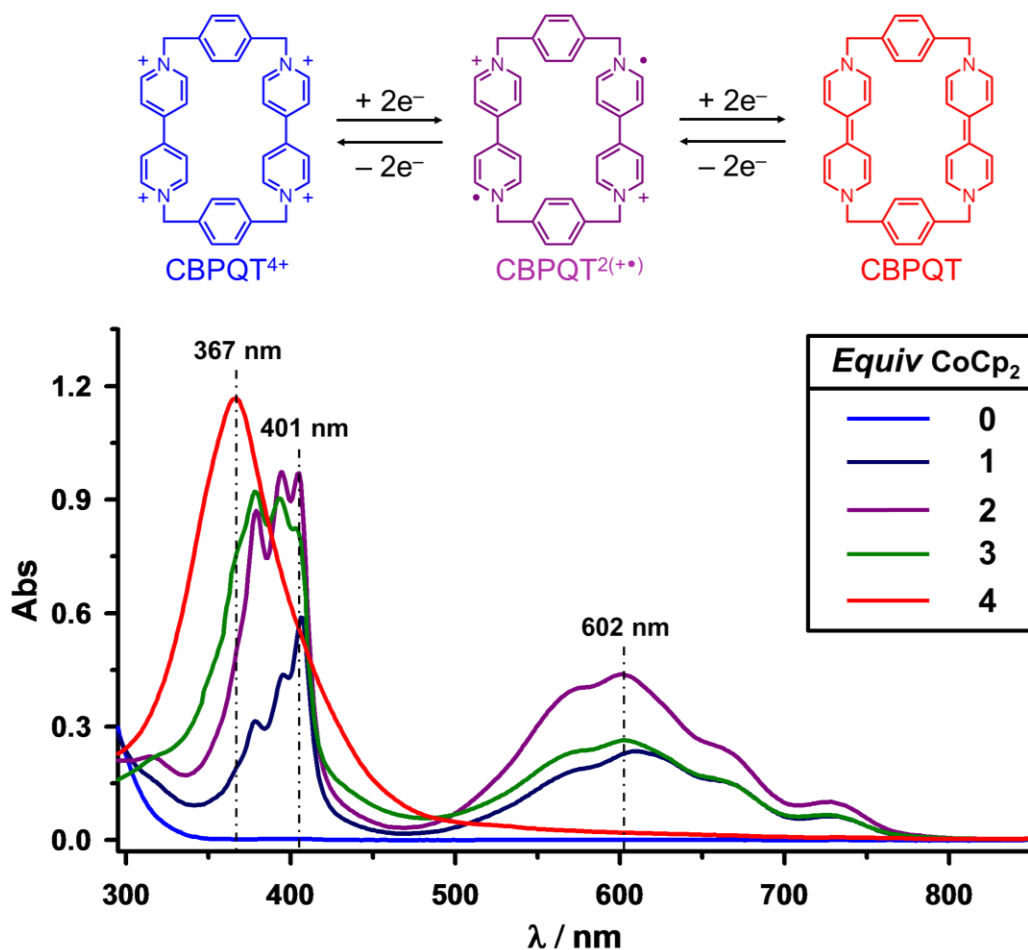
The interaction between the neutral CBPQT and of  $\pi$ -electron poor guests was first investigated in solution by  $^1\text{H}$  NMR spectroscopic analysis. The guest molecule — either 1,4-dicyanobenzene (DCB) or 1,4-dicyanotetrafluorobenzene (DCFB) (100 mM in  $\text{C}_6\text{D}_5\text{CD}_3$ ) — was added to a  $\text{C}_6\text{D}_5\text{CD}_3$  solution of neutral CBPQT (0.7 mM). The solution of neutral CBPQT was transferred to  $\text{C}_6\text{D}_5\text{CD}_3$  by extraction from the biphasic system, followed by dilution to the final concentration. Titrations of the neutral CBPQT with the guests were performed in an Ar glovebox and the solution was loaded in a Wilmad NMR tube and capped. The NMR spectra were measured immediately after mixing the solution. An upfield shift was observed for the resonance associated with the  $\alpha$  proton of the BIPY units of the CBPQT and the signal corresponding to the methylene unit.



**Figure S9.**  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ , 298K) spectra of the neutral CBPQT (top) and a 1:1 mixture of CBPQT and DCB (middle), and DCFB (bottom).

## 2) UV-Vis Spectroscopy

The tetracationic CBPQT<sup>4+</sup> ring undergoes two consecutive reversible two-electron reduction processes to afford firstly the diradical dication CBPQT<sup>2(•+)</sup> and then subsequently the fully reduced CBPQT. The stepwise chemical reduction of a 0.08 mM solution of CBPQT•4PF<sub>6</sub> in MeCN with the one-electron reducing agent CoCp<sub>2</sub> was followed by UV-Vis spectroscopy (Figure S10).

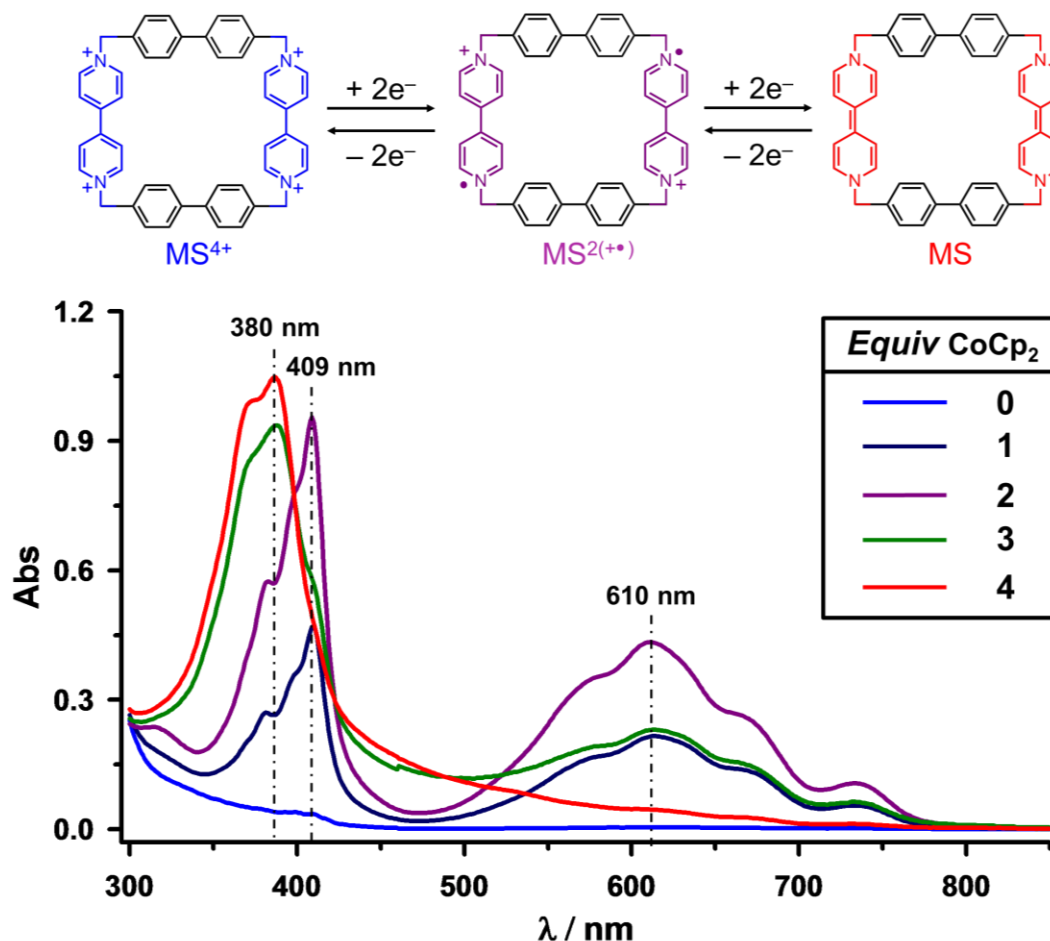


**Figure S10.** UV-Vis Absorption spectra of CBPQT•4PF<sub>6</sub> (0.08 mM in MeCN, 0.2 cm path-length) and the reduced states arising from the stepwise addition of 1.0-4.0 equiv of CoCp<sub>2</sub> in a MeCN solution. All spectra were recorded in Ar-purged MeCN solutions at 298 K.

Addition of 1 equiv of CoCp<sub>2</sub> to a solution of CBPQT•4PF<sub>6</sub> leads to the emergence of the characteristic absorbances of the radical-cation BIPY<sup>•+</sup> species at 401 and 602 nm. The intensity of these peaks increases with the addition of 2 equiv of CoCp<sub>2</sub>, resulting in the quantitative conversion of CBPQT<sup>4+</sup> to its diradical dication form. As more than 2 equiv of reductant is added, the bands centered at 401 and 602 nm start to decrease, while a new adsorption band appears at 367 nm in the spectrum. This band can be attributed to the formation of the fully

reduced BIPY unit in the cyclophane. The generation of the neutral CBPQT in quantitative yield was achieved by addition of 4 equiv of  $\text{CoCp}_2$  as evidenced by the presence of the strong absorption band at 367 nm and the concomitant disappearance of the absorption bands associated with the radical cation species.

The reduced states of the cyclophane  $\text{MS}^{4+}$  were also characterized (Figure S11) by UV–Vis spectroscopy. The chemical reduction of  $\text{MS}^{4+}$  was performed in DMF on account of the low solubility of its reduced forms in MeCN.



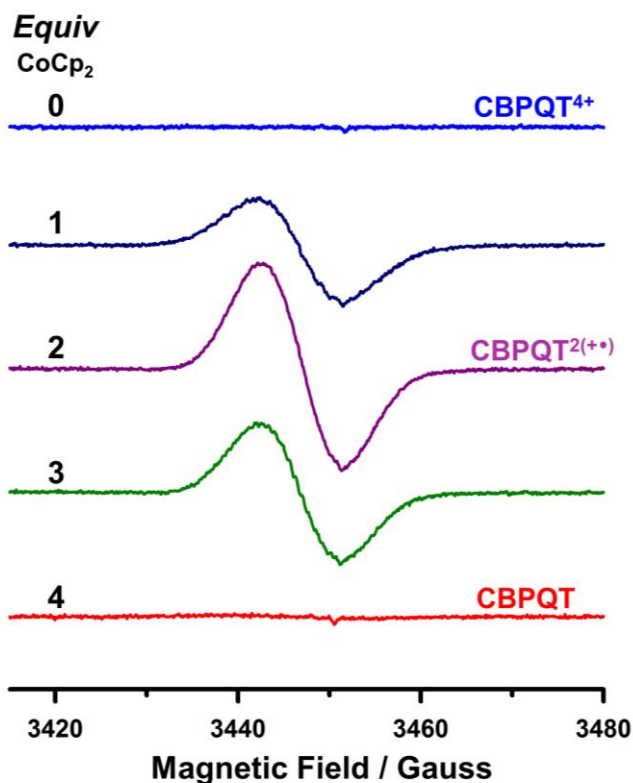
**Figure S11.** UV–Vis Absorption spectra of  $\text{MS}\cdot 4\text{PF}_6$  (0.08 mM in DMF, 0.2 cm path-length) recorded upon the addition of up to 4.0 equiv  $\text{CoCp}_2$  (in DMF solution). All spectra were recorded in Ar-purged DMF solutions at 298 K.

Upon stepwise addition of the reductant, the DMF solution of  $\text{MS}\cdot 4\text{PF}_6$  becomes blue and two sets of finely structured absorptions at 409 and 610 nm appear on account of the generation of the diradical-dication  $\text{MS}^{2(\bullet\bullet)}$ . As more than 2 equiv of  $\text{CoCp}_2$  is added, these absorption features are followed by the emergence of an intense band at 380 nm. Titration with up to 4 equiv of  $\text{CoCp}_2$  yielded to an intense red solution of the fully reduced  $\text{MS}$  cyclophane.

### 3) Electron paramagnetic resonance (EPR) spectroscopy

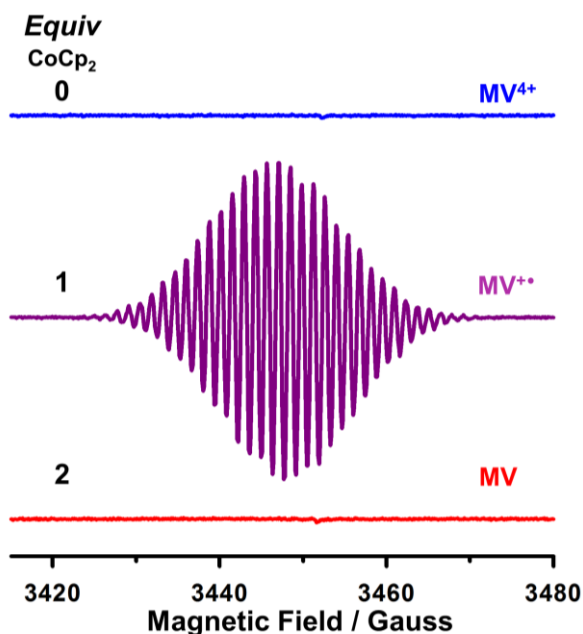
#### 3.1) Redox titration experiments

Further spectroscopic evidence for the occurrence of the reduction of the tetracationic CBPQT<sup>4+</sup> to the neutral CBPQT by CoCp<sub>2</sub> was provided by EPR spectroscopy. A gradual increase in the radical signal intensity was observed (Figure S12) upon addition of CoCp<sub>2</sub> to a MeCN solution of the cyclophane.



**Figure S12.** Continuous-wave EPR spectra of CBPQT<sup>4+</sup> (0.20 mM in MeCN, 298 K) recorded during a stepwise titration with CoCp<sub>2</sub> from 1 to 4 equiv.

Titration up to 2 equiv yielded a symmetric derivative EPR signal. The absence of the hyperfine structure is consistent with EPR spectra previously measured<sup>S5</sup> on a solution of CBPQT<sup>2(++)</sup>, generated by electrochemical reduction. During the titration with cobaltocene we found that, by measuring the UV–Vis spectra from the same solution used for the EPR spectroscopy, the increase in the intensity of the EPR signal is proportional to the height of the visible band associated with the radical cationic species in the UV–Vis spectra. Addition of up to 4 equiv of CoCp<sub>2</sub> results in the formation of neutral CBPQT, comprising dihydrobipyridyl units, which have no radical character and are EPR silent. A stepwise titration with CoCp<sub>2</sub> of a MeCN solution of MV<sup>2+</sup> was also performed and the resulting EPR spectra are reported in Figure S13.

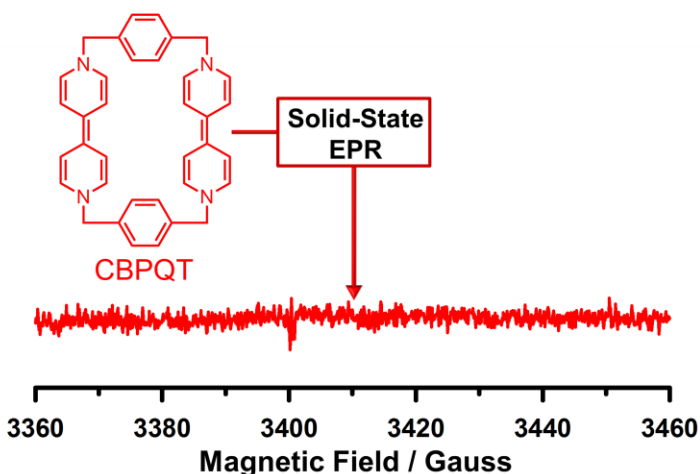


**Figure S13.** Continuous-wave EPR spectra of  $MV^{2+}$  (0.20 mM in MeCN, 298 K) recorded upon the addition of 1 and 2 equiv of  $CoCp_2$ .

Reduction to the radical cation  $MV^{\bullet+}$  results in an EPR spectrum with a strong hyperfine splitting pattern, as observed previously with other viologen radicals.<sup>S6,S7</sup> Titration with up to 2 equiv yielded to the fully neutral  $MV$  and the disappearance of the EPR signal.

### 3.2) Solid-state EPR spectroscopic analysis

Solid-state EPR spectroscopic analysis was performed on single crystals of neutral CBPQT (Figure S14).



**Figure S14.** Solid-state CW EPR spectrum of single crystals of neutral CBPQT.

The absence of an EPR signal provides further evidence for the complete reduction of the CBPQT to the neutral state and the lack of free radicals in the crystals. This result supports the data obtained by X-ray diffraction analysis of single CBPQT crystals.

## C. Crystallographic Characterization

All crystallographic data has been deposited with the Cambridge Crystallographic Data Centre (CCDC) as supplementary publications, and are available free of charge via [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).

### 1) Neutral CBPQT

#### 1.1) Methods

Single crystals of CBPQT were grown at 4 °C by slow vapor diffusion of *n*-hexane into a MeCN solution under inert (Ar) atmosphere. The single crystals were mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa APEX CCD area detector, equipped with a CuK $\alpha$  microsource with MX optics.

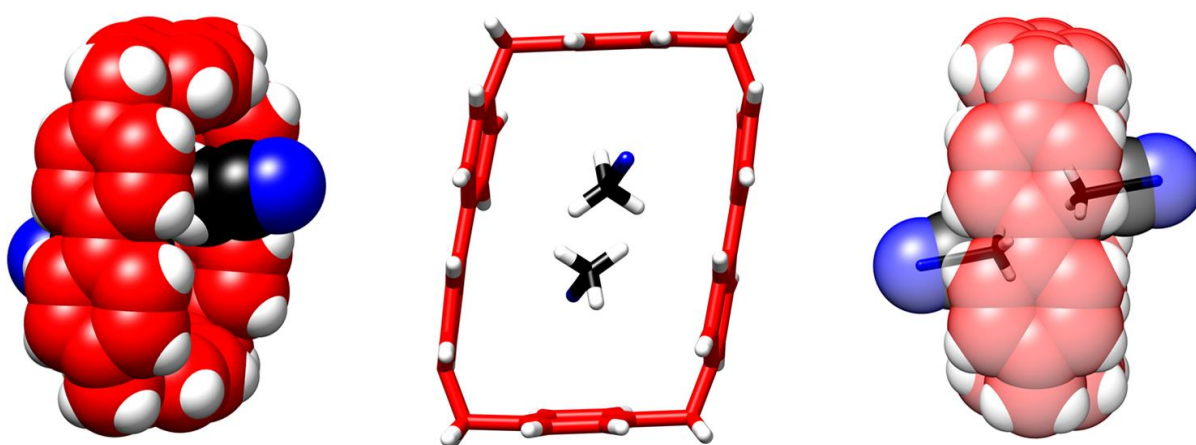
#### 1.2) Crystal data

3(C<sub>36</sub>H<sub>32</sub>N<sub>4</sub>) • 7(CH<sub>3</sub>CN),  $M = 1849.34$ , trigonal, space group  $R\bar{3}$  (no. 148),  $a = 22.3679(12)$ ,  $c = 17.9046(10)$  Å,  $V = 7757.9(9)$  Å<sup>3</sup>,  $T = 99.99$  K,  $Z = 3$ ,  $\mu(\text{CuK}\alpha) = 0.554$ . A total of 40341 reflections were collected, of which 3124 were unique ( $R_{\text{int}} = 0.0236$ ). Final  $wR(F_2) = 0.0946$ . CCDC number: 985863.

No special restraints or constraints were used in the refinement. Hydrogen atoms were located from the residual electron density and freely refined, except for those on solvent molecules.

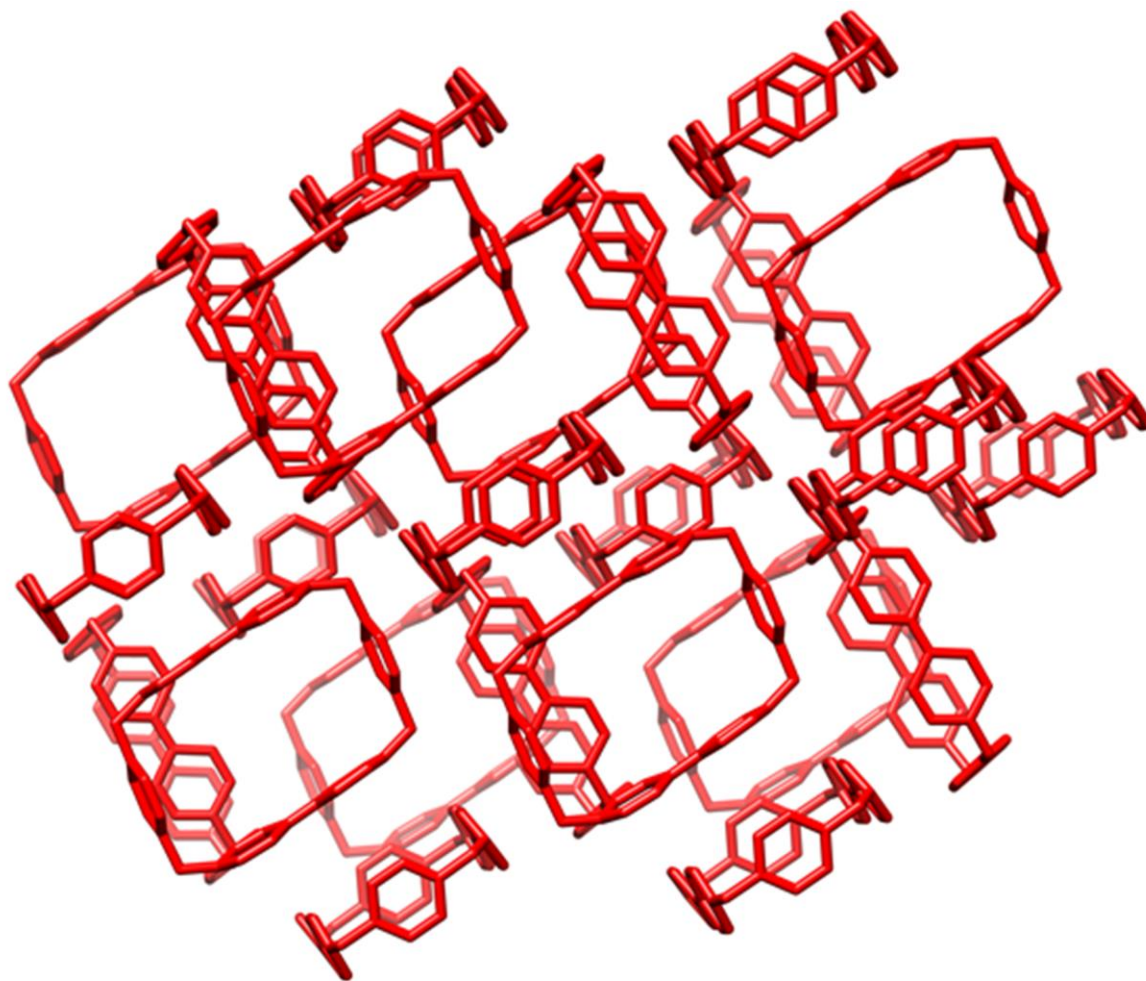
#### 1.3) Solid-state superstructure

The solid-state superstructure of fully reduce CBPQT reveals (Figure S15) the presence of two MeCN molecules in proximity of the cavity of the macrocycle.



**Figure S15.** Perspective (left), plan (center) and lateral (right) views of the solid-state structure of the neutral CBPQT showing the presence of two MeCN molecules in the cell unit.

The extended supramolecular solid-state structure of the neutral CBPQT is shown in Figure S16.



**Figure S16.** Plan view along the  $a$ -axis of the long range packing of neutral CBPQT, revealing the absence of interaction between the CBPQT rings.

The separation between the CBPQT units indicates that the molecules are not interacting in the long-range packing order, precluding any possibility of conformational distortion arising from lattice effects.

## 2) *Mixed (CBPQT)(CBPQT•2PF<sub>6</sub>)*

### 2.1) *Methods*

Single crystals of  $(\text{CBPQT})(\text{CBPQT}\cdot 2\text{PF}_6)$  were grown under inert (Ar) atmosphere at 4 °C by slow vapor diffusion of  $i\text{Pr}_2\text{O}$  into a DMF solution containing CBPQT and  $\text{CBPQT}\cdot 2\text{PF}_6$  in equimolar mixture. The single crystals were mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa APEX CCD area detector, equipped with a  $\text{CuK}\alpha$  microsource with MX optics. TWINABS-2008/4 (Bruker 2010) was used for absorption correction.



## 2.2) Crystal data

(C<sub>36</sub>H<sub>32</sub>N<sub>4</sub>) • 2(PF<sub>6</sub>),  $M = 665.62$ , monoclinic, space group  $P2_1/m$  (no. 11),  $a = 9.9084(4)$ ,  $b = 26.6982(9)$  Å,  $\beta = 99.632(2)^\circ$ ,  $V = 4129.1(3)$  Å<sup>3</sup>,  $T = 99.99$  K,  $Z = 4$ ,  $\mu(\text{CuK}\alpha) = 1.048$  mm<sup>-1</sup>. A total of 6777 reflections were collected, of which 6766 were unique. Final  $wR(F_2) = 0.2768$ . CCDC no.: 985865.

Chemically equivalent N-C and C-C distances in the disordered pyridine ring were refined with similarity restraints (SADI). All disordered C and N atoms were refined with the enhanced rigid-bond restraint (SHELX keyword RIGU).<sup>S8</sup> This crystal was found to be non-merohedrally twinned. The orientation matrices for the two components were identified using the program Cell\_Now (Sheldrick, 2005), and the data were processed using both orientation matrices with SAINT. The exact twin matrix identified by the integration program was found to be  $-0.25993$ ,  $0.00122$ ,  $-0.63215$ ,  $-0.01145$ ,  $-0.99999$ ,  $-0.00507$ ,  $-1.47499$ ,  $0.00170$ ,  $0.25994$ . The second domain is rotated from first domain by 180 % about the reciprocal lattice [101] axis. The absorption correction was carried out using TWINABS V2008/4 (Sheldrick, 2008) to create a "detwinned" HKLF4 format file which was used in all refinements. The solvent masking procedure as implemented in Olex2 was used to remove the electronic contribution of solvent molecules from the refinement.

## 3) Neutral MS

### 3.1) Methods

Single crystals of **MS** were grown at 4 °C by slow vapor diffusion of *t*Pr<sub>2</sub>O into a DMF solution under inert (Ar) atmosphere. The single crystals were mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa APEX CCD area detector, equipped with a CuK $\alpha$  microsource with MX optics. SADABS-2008/1 (Bruker 2008) was used for absorption correction.

### 3.2) Crystal data

C<sub>48</sub>H<sub>40</sub>N<sub>4</sub>,  $M = 672.84$ , monoclinic, space group  $P2_1/n$  (no. 14),  $a = 5.7756(3)$ ,  $b = 23.3531(17)$  Å,  $V = 1956.4(2)$  Å<sup>3</sup>,  $T = 100.01$  K,  $Z = 2$ ,  $\mu(\text{CuK}\alpha) = 0.515$ . A total of 10353 reflections were collected, of which 2041 were unique ( $R_{\text{int}} = 0.0539$ ). Final  $wR(F_2) = 0.2101$ . CCDC number: 985864.

The enhanced rigid-bond restraint (SHELX keyword RIGU) was used in the refinement.<sup>S8</sup>

The solvent masking procedure as implemented in Olex2 was used to remove the electronic contribution of solvent molecules from the refinement.

#### 4) DCB ⊂ CBPQT

##### 4.1) Methods

Single crystals of (DCB ⊂ CBPQT) were grown under inert (Ar) atmosphere at 4 °C by slow vapor diffusion of *n*-hexane into a MeCN solution containing CBPQT and DCB in equimolar mixture. The single crystals were mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa APEX CCD area detector, equipped with a CuK $\alpha$  microsource with MX optics.

##### 4.2) Crystal data

(C<sub>36</sub>H<sub>32</sub>N<sub>4</sub> • C<sub>8</sub>H<sub>4</sub>N<sub>2</sub>), *M* = 662.47, trigonal, space group *R*-3 (no. 148), *a* = 22.2705(9), *c* = 17.9544(7) Å, *V* = 7711.9(7) Å<sup>3</sup>, *T* = 99.99 K, *Z* = 9,  $\mu$ (CuK $\alpha$ ) = 0.599 mm<sup>-1</sup>. A total of 16258 reflections were collected, (6.726 ≤ 2 $\theta$  ≤ 130.08), 2933 unique (*R*<sub>int</sub> = 0.0197, *R*<sub>sigma</sub> = 0.0133) which were used in all calculations. Final *wR*(*F*<sub>2</sub>) = 0.0803. CCDC no.: 985862.

No special restraints or constraints were used in the refinement of this structure.

## D. Computational Analysis

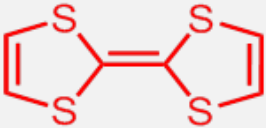
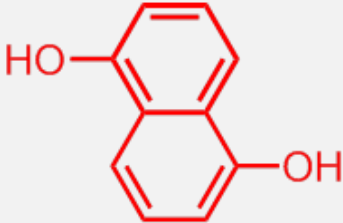


### 1) Methods

DFT Calculations were performed with the M06 functional at M06<sup>1</sup>/6-311++G\*\*//M06/6-31G\* level as implemented in with Jaguar 7.7.<sup>S9</sup> The geometries were optimized at 6-31G\* level in the presence of the Poisson-Boltzmann solvation model for acetonitrile ( $\epsilon$ =37.5 and *R*<sub>0</sub>= 2.18 Å). Single point energies were refined at 6-311++G\*\* level.<sup>S10</sup> For S atom, the basis of 6-311++G(2d) was used. For inclusion complexes with the cyclophane in 4+ and 0 charge, the ground state is close shell. For inclusion complexes in 2+ charge, the ground state is open-shell singlet with one BIPY<sup>++</sup> spin up and the other BIPY<sup>++</sup> spin down. However, the energy of the triplet and the open-shell singlet states are almost degenerate.

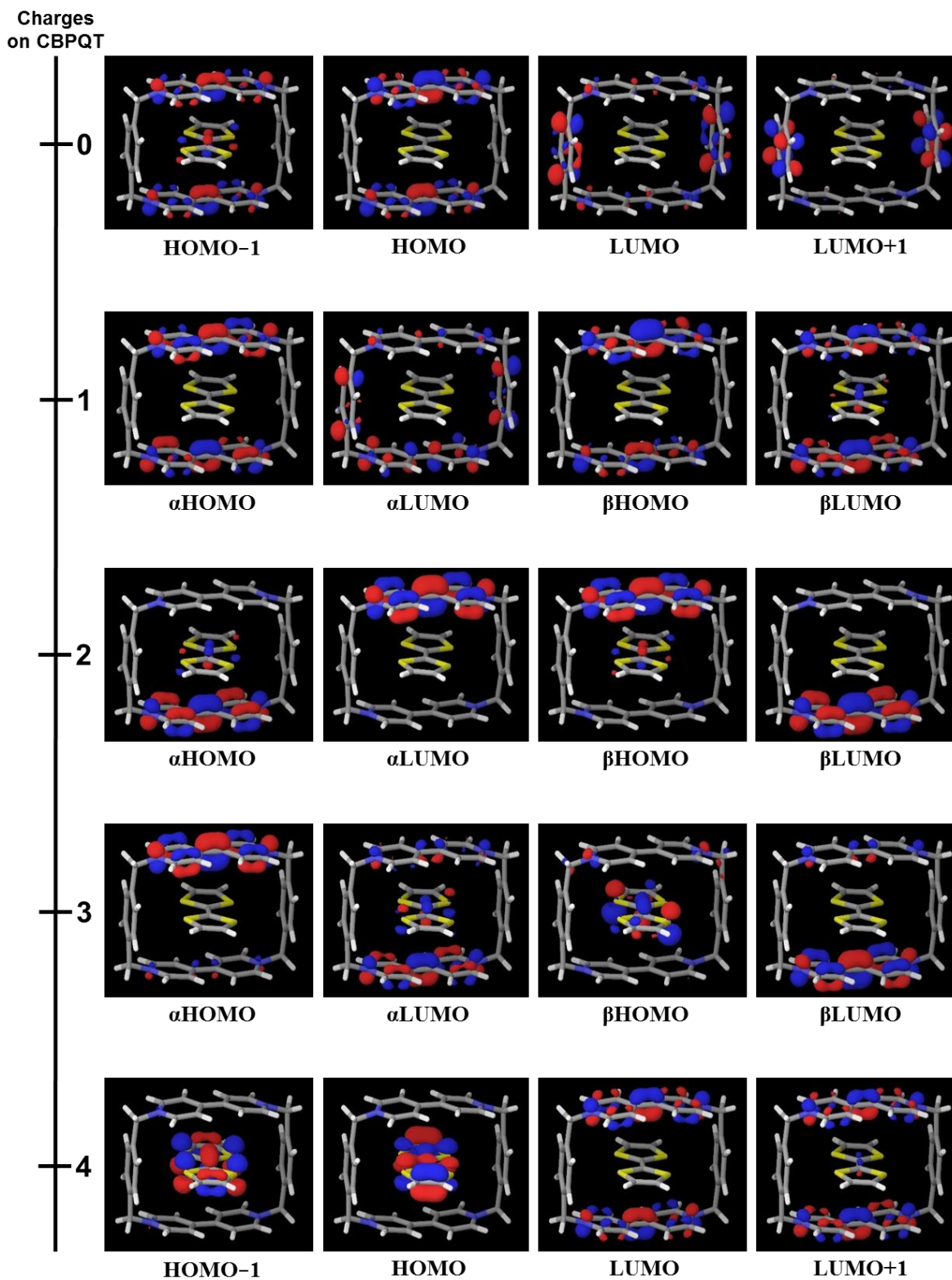
### 2) Calculated HOMO/LUMO energy levels

In order to understand the relative energetics which govern the binding mode of the CBPQT host in different oxidation states we have calculated the complexation energies (Table S1) for the formation of 1:1 inclusion complexes of several electron rich and electron poor guests. The guest molecules investigated comprise tetrathiafulvalene (TTF), 1,5-dihydroxynaphthalene (DNP), 1,2,4,5-tetrafluorobenzene (TFB) and 1,4-dicyanobenzene (DCB). The complexation enthalpy increases in the tetracationic state with the electron donating properties of the guest, while, for the electron poor guests, the energies calculated for the complexation increase by reducing the charges on the cyclophane.

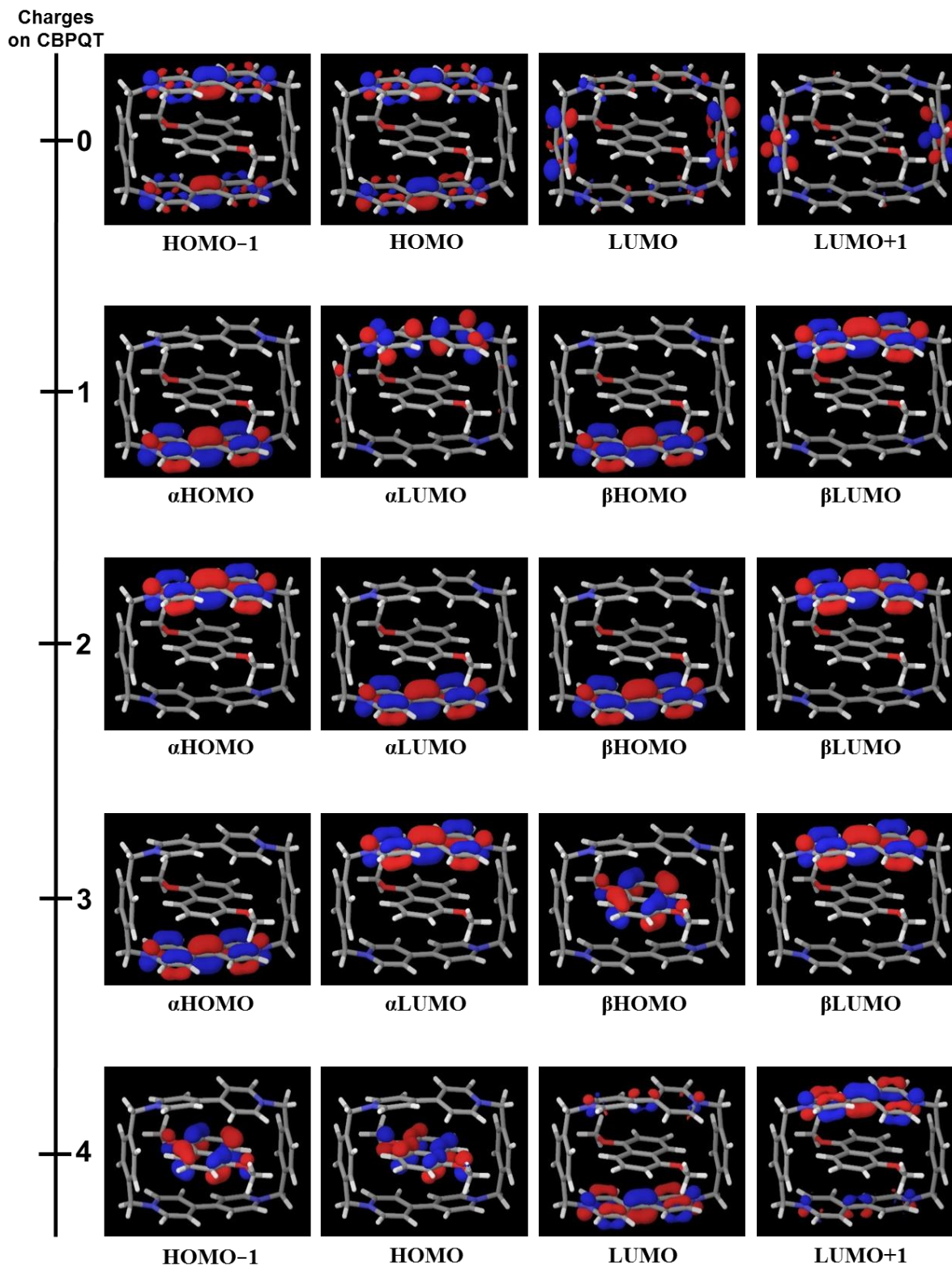
**Table S1. Complexation Enthalpies Between the Cyclophane in Different Oxidation States and Guests Comprising Electron Rich as well as Electron Poor Molecules.**

Guests	Complexation Enthalpy / kcal mol <sup>-1</sup>				
	Charge on CBPQT				
	4	3	2	1	0
 <b>TTF</b>	-23.3	-19.5	-15.7	-9.9	-5.8
 <b>DNP</b>	-19.6	-15.5	-13.6	-7.3	-3.5
 <b>DCB</b>	-6.2	-8.6	-11.5	-10.7	-12.0
 <b>DCFB</b>	5.7	1.0	-6.6	-11.5	-14.8

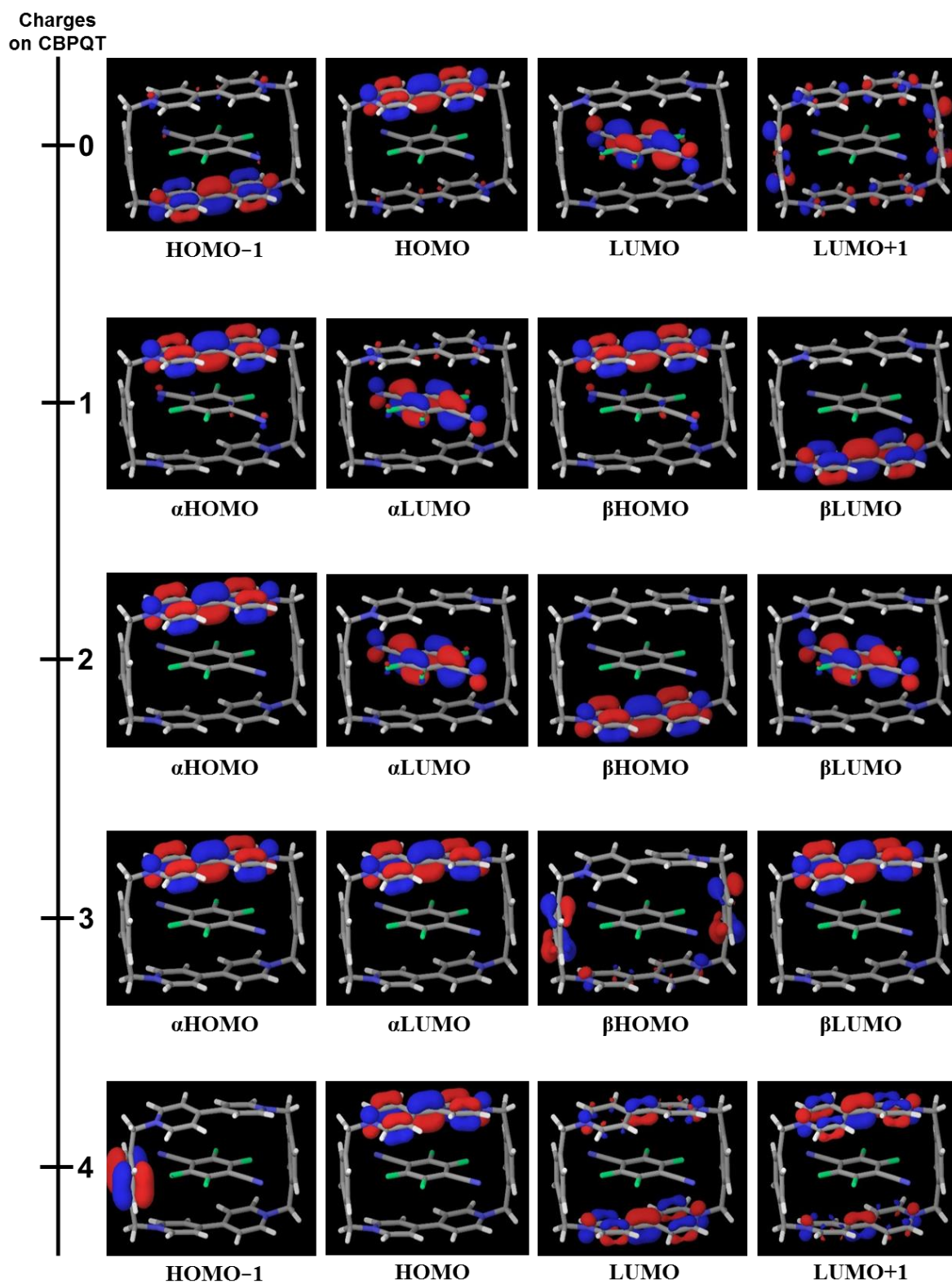
The HOMO/LUMO electron density distributions for the different complexes were also calculated and the frontiers molecular orbitals are represented in Figure S17–S20.



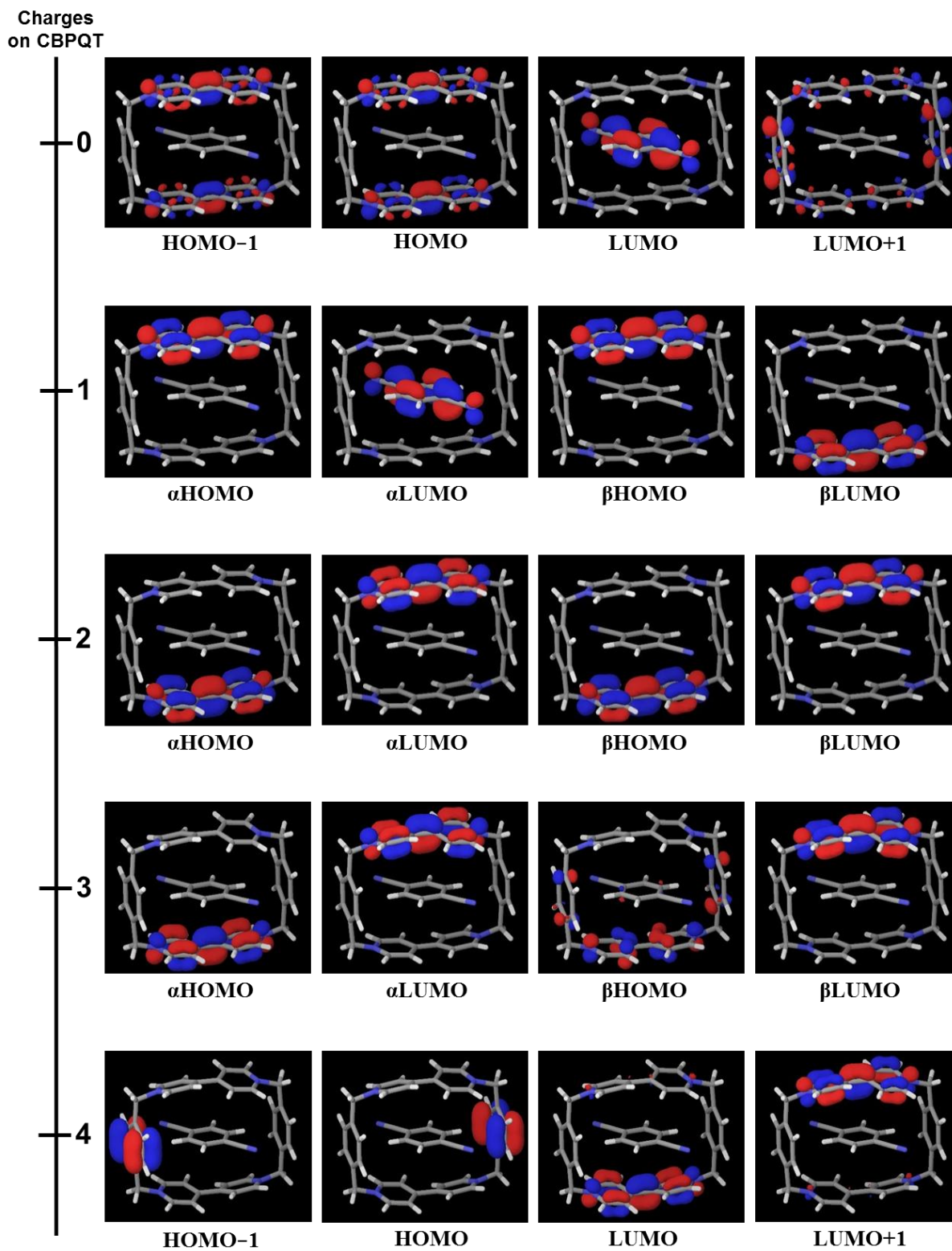
**Figure S17.** Frontier molecular orbitals and energies for the HOMO and LUMO levels of the 1:1 inclusion complexes between the CBPQT ring in different oxidation states and TTF.



**Figure S18.** Frontier molecular orbitals and energies for the HOMO and LUMO levels of the 1:1 inclusion complexes between the CBPQT ring in different oxidation states and DNP.



**Figure S19.** Frontier molecular orbitals and energies for the HOMO and LUMO levels of the 1:1 inclusion complexes between the CBPQT ring in different oxidation states and DCFB.



**Figure S20.** Frontier molecular orbitals and energies for the HOMO and LUMO levels of the 1:1 inclusion complexes between the CBPQT ring in different oxidation states and DCB.

### 3) Coordinates and energies of each species in different redox states

The coordinates of optimized complexes were reported in XYZ format. The energies were reported in the following format: (1) M06/6-31G\* (in CH<sub>3</sub>CN), (2) M06/6-31G\* (in gas phase), (3) M06/6-311++G\*\* (in gas phase), and (4) the total energy, which is (1)-(2)+(3).

#### 1. (CBPQT-2CH<sub>3</sub>CN)<sup>0</sup>

	-1874.191835	-1874.156434	-1874.601735	-1874.637136
H1	-4.9283983278	-1.6245438811	-2.8670089126	
H2	5.6023414456	1.7168085372	-3.0013721348	
H3	2.2450335948	-1.4490486085	-2.9903392588	
H4	-1.5648108973	1.5130008642	-3.1970331616	
H5	-4.1360391822	-3.1990771249	-2.6839664736	
H6	4.8100667253	3.2968334825	-3.1463811497	
H7	4.3603734203	-0.2648463450	-3.0100000956	
H8	-3.6843920266	0.3492784838	-3.0171094286	
C9	2.2234068192	-0.3606761534	-3.0054536812	
C10	-1.5462708751	0.4372148530	-3.0348483088	
C11	-2.7396814376	-0.1894388181	-2.9450634560	
C12	3.4136822037	0.2755111894	-3.0229508103	
C13	-0.2778684110	-0.2728892373	-2.9494479592	
C14	0.9526823214	0.3491317719	-3.0259210593	
H15	0.4103456972	-2.3688476436	-2.7310843185	
H16	0.2584221015	2.4436453816	-3.2230480846	
C17	-0.4550144910	-1.7097947445	-2.7922021155	
C18	1.1251802537	1.7892989220	-3.1434555571	
N19	-2.8548276498	-1.5618088324	-2.7943073891	
N20	3.5284652182	1.6575163259	-3.1134936432	
C21	-1.6730974051	-2.2851928938	-2.7036297932	
C22	2.3386992576	2.3779055543	-3.1567828948	
H23	-1.7994079987	-3.3591972015	-2.5683312076	
H24	2.4595701881	3.4584995619	-3.2348502687	
C25	-4.1142515443	-2.1519572158	-2.3478143701	



C26	4.7490824863	2.3165049639	-2.6507717759
C27	-4.2974441132	-2.0679033929	-0.8520631421
C28	4.7844995331	2.4742123459	-1.1511928285
H29	-5.0364093306	-0.0408845874	-0.8948867770
H30	5.6182164661	0.5176221640	-0.7963700609
H31	-3.6323184275	-4.0810724008	-0.4701257355
H32	3.9958540740	4.4791294709	-1.1645208851
C33	-4.7422187616	-0.8809399814	-0.2621994039
C34	5.2153248167	1.4232233065	-0.3373334084
C35	-3.9632447543	-3.1398388594	-0.0248185722
C36	4.3118629589	3.6379881606	-0.5433329654
C37	-4.8247037729	-0.7620618752	1.1195991331
C38	5.1443406799	1.5222799276	1.0480126682
C39	-4.0457082460	-3.0203082158	1.3604936593
C40	4.2390837319	3.7367720882	0.8437356173
H41	-5.1842874989	0.1689743046	1.5628456618
H42	5.4936939538	0.6939498711	1.6682372816
H43	-3.7798238271	-3.8689584351	1.9947750152
H44	3.8628113352	4.6542149934	1.3026656245
C45	-4.4648708827	-1.8268957706	1.9494769888
C46	4.6368513763	2.6743667081	1.6562166605
C47	-4.4515096896	-1.6531566716	3.4470534377
C48	4.4524735749	2.7380273793	3.1520393829
H49	-2.1746853727	-2.8111614517	4.0339518056
H50	2.1457599866	3.9607716266	3.3441065168
N51	-3.2302773250	-1.0007787061	3.9227115918
N52	3.1840306916	2.1560270184	3.5901835899
C53	-2.0458432211	-1.7332412813	3.9404895687
C54	2.0097257851	2.8856689615	3.4600380408
H55	3.9903130217	0.2243043557	3.7334166353
H56	-4.0426663922	0.9288157330	3.7880876117
H57	-5.3043626124	-1.0446483450	3.7808231525
H58	5.2598838512	2.2006753122	3.6705154024

C59	-3.1020201901	0.3778034900	3.7909743456
C60	3.0521949817	0.7758353848	3.6727096946
H61	-4.5258207251	-2.6278768061	3.9513228978
H62	4.4753838078	3.7804647128	3.5018845177
C63	-0.8286884520	-1.1594509555	3.8880360859
C64	0.7857343507	2.3190562133	3.5056662360
H65	0.0324104698	-1.8223768505	3.9481366421
H66	-0.0719499750	2.9854799775	3.4231553578
C67	1.8529177190	0.1578078569	3.7195384953
C68	-1.9070285522	1.0021511964	3.7331446431
C69	-0.6439763989	0.2771640711	3.7489987206
C70	0.5928955352	0.8837680947	3.6560542059
H71	1.8609232105	-0.9260951424	3.8187216354
H72	-1.9189827922	2.0900228850	3.6925146104
C73	1.9392256235	0.3796606838	0.2955038681
N74	1.6263406381	1.4947072402	0.2243285094
C75	2.3054002471	-1.0201210657	0.3919874571
H76	2.8818447785	-1.1934463865	1.3105754590
H77	1.3883918463	-1.6206251804	0.4195249847
H78	2.9088794944	-1.3105056097	-0.4765216419
N79	-1.1080232632	-1.1846365197	0.4766843188
C80	-1.3333933382	-0.0465390096	0.4665095885
C81	-1.5964367418	1.3788231727	0.4524851034
H82	-0.8177749671	1.8823243824	1.0402500024
H83	-1.5657358890	1.7510410813	-0.5802616296
H84	-2.5809494809	1.5903415342	0.8876300653

## 2. (CBPQT-2CH<sub>3</sub>CN)<sup>+1</sup>

-1874.078946	-1873.998344	-1874.43287	-1874.513472
H1	-5.0252636796	-1.6061637218	-2.9154537719
H2	5.4731393658	1.5941360945	-2.9334242161
H3	2.1028115754	-1.5238165984	-2.9874007743
H4	-1.6444108860	1.4528330565	-3.3967784900
H5	-4.2513176523	-3.1961195766	-2.7739951287

H6	4.6938394879	3.1786232666	-3.1000236988
H7	4.2326682302	-0.3459701602	-2.8266305329
H8	-3.7831071629	0.3110768457	-3.1406354587
C9	2.0894068957	-0.4373131709	-2.9829566647
C10	-1.6350523473	0.3867810327	-3.1841675091
C11	-2.8427641668	-0.2289166301	-3.0528386299
C12	3.2926105497	0.1977805491	-2.8986873588
C13	-0.4123421984	-0.3378396010	-3.0532110966
C14	0.8658079140	0.2952682910	-3.0706635146
H15	0.2919081563	-2.4020624586	-2.7816402194
H16	0.1639520800	2.3729677933	-3.2444494172
C17	-0.5673087344	-1.7423980227	-2.8650624850
C18	1.0209888257	1.7119751733	-3.1426641829
N19	-2.9427139441	-1.5702230466	-2.8194538707
N20	3.3894035252	1.5612138214	-2.9151016005
C21	-1.7973814779	-2.3096652711	-2.7384319379
C22	2.2459078270	2.2981180541	-3.0467434701
H23	-1.9295018555	-3.3748715338	-2.5599857756
H24	2.3752878496	3.3785947533	-3.0652913150
C25	-4.2296216388	-2.1630062416	-2.4050182462
C26	4.6582627317	2.2255581923	-2.5571668652
C27	-4.3694042590	-2.1023240173	-0.9078426869
C28	4.7487049768	2.4302269072	-1.0684281521
H29	-5.1531395305	-0.0922798717	-0.9003062250
H30	5.5312196048	0.4568803491	-0.6807445838
H31	-3.6461759530	-4.1054887578	-0.5827284948
H32	4.0169388747	4.4570830083	-1.1226631356
C33	-4.8112980419	-0.9309419849	-0.2905567516
C34	5.1736093465	1.3895393293	-0.2395714723
C35	-3.9722709651	-3.1756262679	-0.1132214782
C36	4.3304318703	3.6264173629	-0.4870372318
C37	-4.8243620720	-0.8270456753	1.0934914534
C38	5.1475730380	1.5322168622	1.1418678291

C39	-3.9817508946	-3.0679734100	1.2735190418
C40	4.3041547546	3.7670816356	0.8976731816
H41	-5.1825147522	0.0906814153	1.5635660197
H42	5.4879630749	0.7116835284	1.7761333279
H43	-3.6631598415	-3.9145981030	1.8848646411
H44	3.9715943346	4.7088075099	1.3396369013
C45	-4.3907352667	-1.8881286471	1.8911680516
C46	4.6943425804	2.7167862732	1.7278469349
C47	-4.2879095856	-1.7237952354	3.3856714433
C48	4.5520704700	2.8203902251	3.2247902543
H49	-1.9709685546	-2.8584166079	3.8318019524
H50	2.2288102145	4.0133332938	3.4423330265
N51	-3.0482941635	-1.0592943893	3.7852645507
N52	3.3032409996	2.2314711820	3.7050936070
C53	-1.8571341137	-1.7756771343	3.7870610597
C54	2.1144509266	2.9346431085	3.5478356528
H55	4.1435892014	0.3255957976	3.9523826198
H56	-3.8930163210	0.8559853045	3.6626785916
H57	-5.1258102927	-1.1275198163	3.7747877187
H58	5.3791300312	2.3054133240	3.7341995014
C59	-2.9440807995	0.3203518240	3.6767883722
C60	3.1970625882	0.8504289143	3.8245679528
H61	-4.3196483126	-2.7016612900	3.8870181531
H62	4.5724704708	3.8722452161	3.5448609254
C63	-0.6468803583	-1.1816501249	3.7729107246
C64	0.9048892077	2.3402646939	3.5666034461
H65	0.2240068009	-1.8347293818	3.8093899358
H66	0.0349968649	2.9900627898	3.4838032950
C67	2.0113560741	0.2061973571	3.8424237568
C68	-1.7585297340	0.9631793973	3.6479715388
C69	-0.4843995545	0.2623248977	3.6978695677
C70	0.7406263231	0.8996092528	3.6949273071
H71	2.0367705579	-0.8699716883	4.0035109185

H72	-1.7903723355	2.0510322020	3.6208268512
C73	1.8332434383	0.4060918097	0.4095274918
N74	1.5906798793	1.5157385271	0.1758477688
C75	2.1118852500	-0.9877873976	0.6869801681
H76	2.7559340729	-1.0749938435	1.5704758215
H77	1.1607069588	-1.5007403024	0.8801581271
H78	2.6099905844	-1.4591689701	-0.1693949471
N79	-1.1886983275	-0.8859605160	0.2965214257
C80	-1.4334367949	0.2486443612	0.3232268308
C81	-1.7336001372	1.6668920337	0.3370425289
H82	-1.0740444939	2.1752443495	1.0582178269
H83	-1.5560076380	2.0975598406	-0.6593691836
H84	-2.7823000095	1.8370602823	0.6243676570

### 3. (CBPQT-2CH<sub>3</sub>CN)<sup>+2</sup>

-1873.962456	-1873.758777	-1874.181018	-1874.384697
H1	-4.9032916581	-1.7214006690	-2.9362802920
H2	5.5296503545	1.6872313972	-3.0187506465
H3	2.2033038933	-1.4667700229	-3.1438756229
H4	-1.5977676390	1.4271904517	-3.3807852449
H5	-4.0850783417	-3.2831377828	-2.7442584545
H6	4.7369409715	3.2703718756	-3.1400010219
H7	4.3230359231	-0.2588139603	-3.0410053544
H8	-3.7130280555	0.2369542656	-3.1130782303
C9	2.1758122063	-0.3821546318	-3.0760998471
C10	-1.5654272881	0.3671792620	-3.1398846172
C11	-2.7599867836	-0.2773329788	-3.0030767377
C12	3.3720841233	0.2698191254	-3.0287892547
C13	-0.3252694334	-0.3277415189	-3.0028131938
C14	0.9388070359	0.3306094703	-3.0637545204
H15	0.4288513386	-2.3655827931	-2.6683576182
H16	0.1929602885	2.3973943675	-3.1034151767
C17	-0.4469930231	-1.7300677358	-2.7731278469
C18	1.0657432773	1.7502080847	-3.0832311130

N19	-2.8295303856	-1.6172413678	-2.7454933092
N20	3.4457752173	1.6332811726	-2.9839583856
C21	-1.6648875423	-2.3249144782	-2.6341241657
C22	2.2843975155	2.3546972330	-3.0198891377
H23	-1.7702799813	-3.3885296451	-2.4291419348
H24	2.3947718467	3.4367532515	-2.9875434218
C25	-4.1147578077	-2.2470951359	-2.3836399749
C26	4.7110896656	2.3024173278	-2.6237257760
C27	-4.3277997103	-2.1832443658	-0.8946305837
C28	4.7971981630	2.4696717285	-1.1281712001
H29	-5.2213098176	-0.2179603326	-0.9383942006
H30	5.4123734390	0.4268022721	-0.7801138152
H31	-3.5184359825	-4.1477698919	-0.5217529347
H32	4.2320958249	4.5506012791	-1.1432009454
C33	-4.8560056228	-1.0311131550	-0.3076501711
C34	5.1218871020	1.3753114771	-0.3216598455
C35	-3.9050422009	-3.2298542310	-0.0748535382
C36	4.4676027341	3.6821278598	-0.5243864843
C37	-4.9070032395	-0.9069732920	1.0756573984
C38	5.0815290947	1.4851701510	1.0607039851
C39	-3.9568848446	-3.1059754648	1.3100095254
C40	4.4261314410	3.7919883202	0.8633637376
H41	-5.3111001028	0.0036676877	1.5231030244
H42	5.3410036746	0.6226075360	1.6782847400
H43	-3.6097334720	-3.9270595803	1.9405803226
H44	4.1575418410	4.7458288595	1.3236125868
C45	-4.4307947485	-1.9327660101	1.8964818209
C46	4.7156145806	2.6910901660	1.6664879716
C47	-4.3154178756	-1.7228683820	3.3825076296
C48	4.5508760297	2.7620932695	3.1621507300
H49	-1.9997331967	-2.8552186445	3.7904156087
H50	2.2289180751	3.9431936844	3.2256180016
N51	-3.0414172148	-1.0475656979	3.6988166686

N52	3.2628669608	2.1605625079	3.5615529031
C53	-1.8849503745	-1.7735667970	3.7831210566
C54	2.1086699890	2.8820029720	3.4365848695
H55	4.1225664373	0.3018055366	3.9577977798
H56	-3.9068382878	0.8513184621	3.6509503369
H57	-5.1242666168	-1.0936985000	3.7746291248
H58	5.3425353168	2.2141817963	3.6887092377
C59	-2.9597139346	0.3163536650	3.6903615316
C60	3.1763414242	0.8233090550	3.8293596580
H61	-4.3302228424	-2.6722514422	3.9319406084
H62	4.5632627615	3.7988637850	3.5217014186
C63	-0.6633457564	-1.1732578148	3.8543456662
C64	0.8832539874	2.2997174301	3.5613894901
H65	0.2050425944	-1.8235756441	3.9183823656
H66	0.0164101019	2.9460183019	3.4491419968
C67	1.9745890187	0.1895561651	3.9463661744
C68	-1.7608411668	0.9640807256	3.7492628490
C69	-0.5276034185	0.2470225740	3.8046856226
C70	0.7442715505	0.8961865787	3.7824814390
H71	1.9935060534	-0.8693698024	4.1892328687
H72	-1.7852532162	2.0507965881	3.7688374490
C73	1.6397822876	0.3484750812	0.3951113149
N74	1.4987539711	1.4983305402	0.2971157682
C75	1.8088334162	-1.0842757952	0.5209120925
H76	2.3658869833	-1.3262498738	1.4321352635
H77	0.8165814448	-1.5506214581	0.5702250268
H78	2.3569855170	-1.4837041662	-0.3400867918
N79	-1.4257194434	-0.6902914243	0.4497410965
C80	-1.5892114948	0.4567441232	0.3631828405
C81	-1.8022206619	1.8876368119	0.2623108279
H82	-0.9846194994	2.4169083319	0.7712864708
H83	-1.8146142198	2.2005599585	-0.7893323909
H84	-2.7581923494	2.1681835978	0.7206541330

#### 4. (CBPQT-2CH<sub>3</sub>CN)<sup>+3</sup>

	-1873.813423	-1873.382349	-1873.798255	-1874.229328
H1	-4.8364224271	-1.8627672605	-2.9686456317	
H2	5.4035042570	1.8222621075	-3.0715659594	
H3	2.1689826317	-1.3410247682	-3.5791359608	
H4	-1.6149921830	1.2493845413	-3.8114466751	
H5	-3.9826668145	-3.3980039466	-2.7202603782	
H6	4.5754594006	3.3912156508	-3.1244415797	
H7	4.2826943752	-0.0633307345	-3.3654132148	
H8	-3.7249081379	0.0001007066	-3.4608412965	
C9	2.1285980633	-0.2856840618	-3.3185505514	
C10	-1.5750953020	0.2465826028	-3.3927190759	
C11	-2.7595761835	-0.4368029276	-3.2158652656	
C12	3.3152134885	0.4096040313	-3.2145350377	
C13	-0.3634833323	-0.3629470397	-3.0517027551	
C14	0.9148695021	0.3749272172	-3.1002224431	
H15	0.5034215880	-2.2194892882	-2.3131895651	
H16	0.0469914804	2.3264324125	-2.6670225301	
C17	-0.3999423278	-1.6808208195	-2.5879487879	
C18	0.9511953390	1.7486890249	-2.8425186435	
N19	-2.7648231554	-1.6908584469	-2.7254069967	
N20	3.3189259198	1.7229483765	-2.9111025478	
C21	-1.6105108211	-2.3165864196	-2.4249086922	
C22	2.1634247558	2.3943897940	-2.7414075839	
H23	-1.6871460438	-3.3303566904	-2.0413473081	
H24	2.2420880136	3.4516280460	-2.4998079972	
C25	-4.0606704874	-2.3606714086	-2.3781411828	
C26	4.6106984003	2.4230594114	-2.6132234969	
C27	-4.2899131969	-2.2526232619	-0.8972344985	
C28	4.7617167356	2.5567388995	-1.1236557839	
H29	-5.1203804367	-0.2645853969	-1.0167357720	
H30	5.3749580029	0.5037061932	-0.8565968387	
H31	-3.5565685780	-4.2339339687	-0.4572750442	



H32	4.2180461141	4.6426016347	-1.0686302405
C33	-4.7924416492	-1.0684219364	-0.3557646144
C34	5.1099607191	1.4397092969	-0.3614322062
C35	-3.9140272481	-3.2891220217	-0.0444590367
C36	4.4618288646	3.7557511047	-0.4816033552
C37	-4.8645358134	-0.9036687803	1.0203857553
C38	5.1057407255	1.5092673936	1.0233018215
C39	-3.9842098525	-3.1211155724	1.3342669117
C40	4.4580957445	3.8236505907	0.9086770555
H41	-5.2518546985	0.0287159665	1.4341541224
H42	5.3686099937	0.6271544879	1.6095740088
H43	-3.6778813325	-3.9344865887	1.9939004224
H44	4.2107572243	4.7640306358	1.4034109016
C45	-4.4307266201	-1.9177958634	1.8766129041
C46	4.7511387292	2.6953010747	1.6706176702
C47	-4.3370759476	-1.6676878940	3.3597056862
C48	4.5828461422	2.7114543475	3.1682367689
H49	-2.0390627589	-2.8168462644	3.7845040115
H50	2.2754183346	3.9105364473	3.1576368256
N51	-3.0592407411	-0.9993515364	3.6775272681
N52	3.2809074639	2.1211596012	3.5370415529
C53	-1.9123440728	-1.7364630502	3.7708071571
C54	2.1380512010	2.8555146673	3.3843007325
H55	4.1112995538	0.2658084381	4.0093650849
H56	-3.9068987090	0.9075066469	3.6303424648
H57	-5.1449331104	-1.0203877843	3.7207094677
H58	5.3612352934	2.1305478282	3.6773806154
C59	-2.9653767419	0.3635735601	3.6698621159
C60	3.1745360240	0.7960657427	3.8499966745
H61	-4.3726520540	-2.6020040420	3.9329740608
H62	4.6112254619	3.7326709900	3.5675023459
C63	-0.6860845450	-1.1500008104	3.8477239601
C64	0.9040160410	2.2960395350	3.5138897479

H65	0.1732056684	-1.8108602357	3.9288983024
H66	0.0475993710	2.9544523916	3.3916934449
C67	1.9615150229	0.1868846618	3.9791454004
C68	-1.7605893378	0.9975048344	3.7334238739
C69	-0.5352721794	0.2673790057	3.7926363091
C70	0.7427288956	0.9017592933	3.7709803742
H71	1.9611061484	-0.8597304873	4.2737710149
H72	-1.7737334552	2.0837297676	3.7634166624
C73	1.7340015194	-0.0116034580	0.4677038832
N74	1.7311306541	1.1157651962	0.1859690564
C75	1.7234396679	-1.4186165321	0.8177925915
H76	2.2907842555	-1.5881115819	1.7413566047
H77	0.6851037185	-1.7526105892	0.9626373108
H78	2.1846686201	-2.0230543147	0.0257211775
N79	-1.4959117909	-0.4199695333	0.2807518791
C80	-1.5716373354	0.7383680416	0.3525883694
C81	-1.6680236267	2.1825539921	0.4370633358
H82	-0.7382136269	2.5946601521	0.8522619367
H83	-1.8240852469	2.6178155457	-0.5563869987
H84	-2.5137335690	2.4748437167	1.0728161563

### 5. (CBPQT-2CH<sub>3</sub>CN)<sup>+4</sup>

-1873.656765	-1872.920998	-1873.330031	-1874.065798
H1	-4.7900396968	-2.0145869573	-2.9529879567
H2	5.3584788250	1.9096150164	-3.0725569998
H3	2.1931402330	-1.3072502616	-3.6964071395
H4	-1.6301430257	1.1205153421	-3.9640466433
H5	-3.8949555446	-3.5164934907	-2.6083803822
H6	4.4867463051	3.4657572246	-3.0377123581
H7	4.2785436317	0.0153266519	-3.4441653384
H8	-3.7140121509	-0.1696458609	-3.5711753578
C9	2.1313912961	-0.2639749777	-3.3913811841
C10	-1.5715032420	0.1470169071	-3.4846533044
C11	-2.7397805153	-0.5597894106	-3.2860521391

C12	3.3004593822	0.4574359919	-3.2673905085
C13	-0.3525667547	-0.4116221744	-3.0917684665
C14	0.9069400877	0.3569387598	-3.1299787450
H15	0.5579272480	-2.2022962428	-2.2655937159
H16	-0.0117048619	2.2635841268	-2.6205151232
C17	-0.3573954775	-1.7046772681	-2.5734331233
C18	0.9077046951	1.7184558837	-2.8226101878
N19	-2.7192732058	-1.7808322558	-2.7221572823
N20	3.2735803317	1.7552886779	-2.9050718334
C21	-1.5527559699	-2.3629635522	-2.3898044001
C22	2.1038583854	2.3927250924	-2.7112645679
H23	-1.6064090909	-3.3580692675	-1.9609456203
H24	2.1568973775	3.4457832789	-2.4456970073
C25	-3.9991841588	-2.4592623250	-2.3394759187
C26	4.5516042677	2.4692782017	-2.5851946673
C27	-4.2366073578	-2.2588268858	-0.8680500415
C28	4.7137804234	2.5214468504	-1.0912381890
H29	-5.2570455167	-0.3755826058	-1.1290772777
H30	5.6074038173	0.5588883796	-0.9659837212
H31	-3.3324472241	-4.1310589086	-0.2848155883
H32	3.9179500168	4.5175412560	-0.8939713001
C33	-4.8560858390	-1.0954154300	-0.4126581614
C34	5.2300349074	1.4190510482	-0.4091653264
C35	-3.7745321802	-3.1939812853	0.0572529920
C36	4.2860654166	3.6338230746	-0.3707200930
C37	-4.9654667813	-0.8456952193	0.9502416135
C38	5.2716425276	1.4114854155	0.9794606643
C39	-3.8701435299	-2.9372656046	1.4188711726
C40	4.3144823231	3.6208663614	1.0181669880
H41	-5.4713401977	0.0574248541	1.2964360020
H42	5.6957486082	0.5526489178	1.5022987781
H43	-3.4939293310	-3.6709049537	2.1337147973
H44	3.9617615886	4.4917309156	1.5726013913

C45	-4.4404323267	-1.7495655883	1.8740003355
C46	4.7823435601	2.5009883515	1.7022845805
C47	-4.4090171114	-1.4199760703	3.3405648463
C48	4.6854796785	2.4448250742	3.1998139044
H49	-2.3011400824	-2.5844410583	4.3528447762
H50	2.5459972007	3.7900060010	3.8415263864
N51	-3.0893204411	-0.7890318573	3.6679190953
N52	3.3459887736	1.8928816481	3.5781112365
C53	-2.0754066721	-1.5460243186	4.1202085469
C54	2.3199338202	2.7264701490	3.8126531640
H55	4.0388164676	-0.0622894191	3.4186140424
H56	-3.7789701815	1.0747084840	3.0714063708
H57	-5.1879741476	-0.7060125728	3.6326618044
H58	5.4397411497	1.7885621364	3.6488569842
C59	-2.9003415258	0.5181195058	3.3931773932
C60	3.1578944807	0.5581253761	3.5718173505
H61	-4.4968577197	-2.3080476403	3.9749400685
H62	4.7647740853	3.4331173225	3.6655766267
C63	-0.8105845571	-1.0171345440	4.2639635547
C64	1.0421472678	2.2407330479	3.9955748896
H65	-0.0278769165	-1.6667497023	4.6457163354
H66	0.2503022394	2.9538673473	4.2018450269
C67	1.9013087419	0.0246588653	3.7333432591
C68	-1.6549381428	1.0918500268	3.5122923099
C69	-0.5666508331	0.3148283022	3.9193482043
C70	0.8011456466	0.8687286168	3.9096812264
H71	1.7947454922	-1.0551603751	3.6799551898
H72	-1.5453167896	2.1433418239	3.2566946373
C73	2.0679482275	0.1438656567	0.3925688664
N74	1.6321100774	1.2172069506	0.3745875540
C75	2.5886516561	-1.2058197997	0.4570405761
H76	3.3952015515	-1.2569674690	1.1942126975
H77	1.7986262944	-1.9122782499	0.7433566375

H78	2.9849979736	-1.5128452530	-0.5113594045
N79	-1.4662697770	-0.2251518337	0.1173956026
C80	-1.9918511688	0.8060213489	0.0973374889
C81	-2.6435662371	2.1042617939	0.0994924097
H82	-1.9672584391	2.8684698916	0.5077119351
H83	-2.9185807798	2.4040358401	-0.9184774282
H84	-3.5522667362	2.0724086248	0.7151037508

**6. (TTF  $\subset$  CBPQT)<sup>0</sup>**

-3432.305387	-3432.275903	-3432.822596	-3432.852079
H2	-5.2698098221	1.6740294061	3.3441339452
H3	-5.5350365173	-0.0771721194	3.3397171497
H4	-3.7184689479	-1.5685366600	3.3581675656
C5	-2.9933614831	-0.7549376686	3.3862907667
H6	1.3401230516	2.0152610695	3.4715748794
H7	3.7184689479	1.5685366600	3.3581675656
H8	-1.3401230516	-2.0152610695	3.4715748794
N9	-3.5447183390	0.5206509422	3.3701925773
H10	5.5350365173	0.0771721194	3.3397171497
C11	-1.6645759164	-0.9767972344	3.4476320811
C12	1.6645759164	0.9767972344	3.4476320811
C13	2.9933614831	0.7549376686	3.3862907667
H14	5.2698098221	-1.6740294061	3.3441339452
C15	-2.6474896444	1.5826597679	3.3651682181
C16	-0.6840234590	0.0990955457	3.4472831500
C17	-1.3109372643	1.4114137521	3.4230137471
C18	0.6840234590	-0.0990955457	3.4472831500
H19	-3.1049225634	2.5712171706	3.3421027311
H20	-0.6996438418	2.3117428270	3.4385598326
N21	3.5447183390	-0.5206509422	3.3701925773
C22	1.3109372643	-1.4114137521	3.4230137471
H23	0.6996438418	-2.3117428270	3.4385598326
C24	2.6474896444	-1.5826597679	3.3651682181
C25	-4.9170879968	0.7257373566	2.9117064176

H26	3.1049225634	-2.5712171706	3.3421027311
C27	4.9170879968	-0.7257373566	2.9117064176
C28	-5.0486638592	0.7491428788	1.4077072967
H29	-4.5284678022	2.8329489024	1.2274278923
C30	5.0486638592	-0.7491428788	1.4077072967
H31	-5.6363179034	-1.3172473056	1.2421743692
H33	5.6363179034	1.3172473056	1.2421743692
H34	4.5284678022	-2.8329489024	1.2274278923
C36	-4.7615512006	1.9117280179	0.6900782836
C37	-5.3829651558	-0.4045448985	0.6971970034
C38	5.3829651558	0.4045448985	0.6971970034
C39	4.7615512006	-1.9117280179	0.6900782836
H42	3.3029407458	2.6977012221	0.0625853626
S42	-2.1376336804	-0.5513684440	-0.0047519190
C44	2.2931610266	2.2921726770	0.0388714513
S44	2.1376336804	0.5513684440	-0.0047519190
C46	0.3666950145	0.5648511550	-0.0061955751
C48	-0.3666950145	-0.5648511550	-0.0061955751
H50	-3.3029407458	-2.6977012221	0.0625853626
H51	1.1527196206	4.1187875492	0.0609890527
C52	1.1793936640	3.0315375013	0.0375046559
C53	-2.2931610266	-2.2921726770	0.0388714513
S53	-0.3626925763	2.1897309776	-0.0083871536
S57	0.3626925763	-2.1897309776	-0.0083871536
C59	-1.1793936640	-3.0315375013	0.0375046559
H61	-1.1527196206	-4.1187875492	0.0609890527
C66	-4.7623375106	1.9086922307	-0.6994965415
C67	-5.3835546710	-0.4077835826	-0.6960480556
C68	5.3835546710	0.4077835826	-0.6960480556
C69	4.7623375106	-1.9086922307	-0.6994965415
H70	-4.5302828712	2.8277074804	-1.2411332791
H71	-5.6365893979	-1.3230567530	-1.2368973434
H72	5.6365893979	1.3230567530	-1.2368973434

C73	-5.0505177206	0.7429068757	-1.4118707646
H74	4.5302828712	-2.8277074804	-1.2411332791
C75	5.0505177206	-0.7429068757	-1.4118707646
C76	-4.9193595048	0.7125841257	-2.9158055401
H77	-3.1123151362	2.5614230029	-3.3436791543
C78	4.9193595048	-0.7125841257	-2.9158055401
C79	-2.6522071938	1.5741680935	-3.3683656992
N80	-3.5463255672	0.5096969736	-3.3730684643
H81	-5.2743110316	1.6582050609	-3.3522645149
H82	3.7137334322	1.5804935175	-3.3636955564
C83	-1.3152256649	1.4069322632	-3.4267341145
H84	-5.5353551917	-0.0936925505	-3.3403020964
C85	-2.9915589688	-0.7643209201	-3.3915507374
H86	-0.7066039801	2.3091010275	-3.4405194655
C87	2.9915589688	0.7643209201	-3.3915507374
N88	3.5463255672	-0.5096969736	-3.3730684643
H89	-3.7137334322	-1.5804935175	-3.3636955564
C90	-0.6843129614	0.0966890632	-3.4520308868
C91	1.6619476569	0.9823651354	-3.4534791940
C92	-1.6619476569	-0.9823651354	-3.4534791940
C93	0.6843129614	-0.0966890632	-3.4520308868
H94	1.3345398058	2.0199518961	-3.4797958698
C95	2.6522071938	-1.5741680935	-3.3683656992
H96	-1.3345398058	-2.0199518961	-3.4797958698
H97	3.1123151362	-2.5614230029	-3.3436791543
H98	5.5353551917	0.0936925505	-3.3403020964
C99	1.3152256649	-1.4069322632	-3.4267341145
H100	5.2743110316	-1.6582050609	-3.3522645149
H101	0.7066039801	-2.3091010275	-3.4405194655

**7. (TTF  $\subset$  CBPQT)<sup>+1</sup>**

	-3432.202502	-3432.133188	-3432.665655	-3432.734969
H2	-5.2728138041	1.6284959886	3.3768554039	
H3	-5.5243852305	-0.1258801660	3.3467360863	

H4	-3.7012380462	-1.5974019313	3.3054135290
C5	-2.9828725115	-0.7786367640	3.3347373060
H6	1.3143681237	2.0270213630	3.4060662223
H7	3.7012380462	1.5974019313	3.3054135290
H8	-1.3143681237	-2.0270213630	3.4060662223
N9	-3.5340723799	0.4888597644	3.3300793832
H10	5.5243852305	0.1258801660	3.3467360863
C11	-1.6469538253	-0.9917050009	3.3878712516
C12	1.6469538253	0.9917050009	3.3878712516
C13	2.9828725115	0.7786367640	3.3347373060
H14	5.2728138041	-1.6284959886	3.3768554039
C15	-2.6583940438	1.5584360827	3.3429174388
C16	-0.6913416051	0.0935394900	3.3962827147
C17	-1.3160726639	1.3973490560	3.3898546607
C18	0.6913416051	-0.0935394900	3.3962827147
H19	-3.1239900984	2.5426541634	3.3407385834
H20	-0.7131887434	2.3019869681	3.4237192680
N21	3.5340723799	-0.4888597644	3.3300793832
C22	1.3160726639	-1.3973490560	3.3898546607
H23	0.7131887434	-2.3019869681	3.4237192680
C24	2.6583940438	-1.5584360827	3.3429174388
C25	-4.9270349496	0.6910225406	2.9188871628
H26	3.1239900984	-2.5426541634	3.3407385834
C27	4.9270349496	-0.6910225406	2.9188871628
C28	-5.0672697639	0.7370543119	1.4175476319
H29	-4.5423459511	2.8242641903	1.2693167940
C30	5.0672697639	-0.7370543119	1.4175476319
H31	-5.6652719251	-1.3242011335	1.2228342080
H33	5.6652719251	1.3242011335	1.2228342080
H34	4.5423459511	-2.8242641903	1.2693167940
C36	-4.7729840279	1.9105446888	0.7187172883
C37	-5.4019682433	-0.4068267575	0.6911727881
C38	5.4019682433	0.4068267575	0.6911727881



C39	4.7729840279	-1.9105446888	0.7187172883
H42	3.2698942014	2.7394702566	0.0168966616
S42	-2.1270903693	-0.5782776988	-0.0146040935
C44	2.2652947866	2.3213180846	0.0040791583
S44	2.1270903693	0.5782776988	-0.0146040935
C46	0.3623964224	0.5735303100	-0.0204987477
C48	-0.3623964224	-0.5735303100	-0.0204987477
H50	-3.2698942014	-2.7394702566	0.0168966616
H51	1.0979963562	4.1313544864	0.0140184481
C52	1.1410282919	3.0447235886	0.0028409312
C53	-2.2652947866	-2.3213180846	0.0040791583
S53	-0.3875739179	2.1817221186	-0.0173258932
S57	0.3875739179	-2.1817221186	-0.0173258932
C59	-1.1410282919	-3.0447235886	0.0028409312
H61	-1.0979963562	-4.1313544864	0.0140184481
C66	-4.7695291846	1.9276388613	-0.6699819591
C67	-5.3993333275	-0.3898162412	-0.7019117179
C68	5.3993333275	0.3898162412	-0.7019117179
C69	4.7695291846	-1.9276388613	-0.6699819591
H70	-4.5357986558	2.8544269596	-1.1971489037
H71	-5.6582532536	-1.2949917446	-1.2560187616
H72	5.6582532536	1.2949917446	-1.2560187616
C73	-5.0619746375	0.7719269719	-1.3980522132
H74	4.5357986558	-2.8544269596	-1.1971489037
C75	5.0619746375	-0.7719269719	-1.3980522132
C76	-4.9155894486	0.7624627208	-2.8988266605
H77	-3.0812971052	2.5922007039	-3.2935444454
C78	4.9155894486	-0.7624627208	-2.8988266605
C79	-2.6322739562	1.6009594328	-3.3180840827
N80	-3.5185896721	0.5469314937	-3.3016556283
H81	-5.2408151604	1.7153957201	-3.3381186828
H82	3.7253171673	1.5333006298	-3.3127921700
C83	-1.2902475589	1.4184075674	-3.3885700165

H84	-5.5188110521	-0.0353000147	-3.3527462890
C85	-2.9951096696	-0.7255538196	-3.3385854862
H86	-0.6735475634	2.3132886705	-3.4190947535
C87	2.9951096696	0.7255538196	-3.3385854862
N88	3.5185896721	-0.5469314937	-3.3016556283
H89	-3.7253171673	-1.5333006298	-3.3127921700
C90	-0.6946589329	0.1075061872	-3.4135634556
C91	1.6609466469	0.9588456936	-3.4135065648
C92	-1.6609466469	-0.9588456936	-3.4135065648
C93	0.6946589329	-0.1075061872	-3.4135634556
H94	1.3452750105	1.9987175955	-3.4510115872
C95	2.6322739562	-1.6009594328	-3.3180840827
H96	-1.3452750105	-1.9987175955	-3.4510115872
H97	3.0812971052	-2.5922007039	-3.2935444454
H98	5.5188110521	0.0353000147	-3.3527462890
C99	1.2902475589	-1.4184075674	-3.3885700165
H100	5.2408151604	-1.7153957201	-3.3381186828
H101	0.6735475634	-2.3132886705	-3.4190947535

### 8. (TTF $\subset$ CBPQT)<sup>+2</sup>

	-3432.094955	-3431.897226	-3432.417647	-3432.615375
H2	-5.2265299464	1.7089983670	3.3519096879	
H3	-5.5003583135	-0.0424216539	3.3648979946	
H4	-3.7212229556	-1.5312635982	3.3290963639	
C5	-2.9912487443	-0.7240961904	3.3554435273	
H6	1.3375930373	1.9948937818	3.5239306218	
H7	3.7212229556	1.5312635982	3.3290963639	
H8	-1.3375930373	-1.9948937818	3.5239306218	
N9	-3.4986700569	0.5431888186	3.2802434373	
H10	5.5003583135	0.0424216539	3.3648979946	
C11	-1.6533999679	-0.9570522070	3.4605103791	
C12	1.6533999679	0.9570522070	3.4605103791	
C13	2.9912487443	0.7240961904	3.3554435273	

H14	5.2265299464	-1.7089983670	3.3519096879
C15	-2.6279023544	1.5978620748	3.3260276010
C16	-0.7046065307	0.1099358333	3.4618228883
C17	-1.2815649785	1.4161458973	3.4265454812
C18	0.7046065307	-0.1099358333	3.4618228883
H19	-3.0766410722	2.5880145388	3.2875400694
H20	-0.6665754989	2.3104627424	3.4674350304
N21	3.4986700569	-0.5431888186	3.2802434373
C22	1.2815649785	-1.4161458973	3.4265454812
H23	0.6665754989	-2.3104627424	3.4674350304
C24	2.6279023544	-1.5978620748	3.3260276010
C25	-4.9096462562	0.7588261908	2.9038321795
H26	3.0766410722	-2.5880145388	3.2875400694
C27	4.9096462562	-0.7588261908	2.9038321795
C28	-5.0632866158	0.7707215132	1.4033749524
H29	-4.5398826548	2.8550580902	1.2050196684
C30	5.0632866158	-0.7707215132	1.4033749524
H31	-5.6612595636	-1.2963214403	1.2605750606
H33	5.6612595636	1.2963214403	1.2605750606
H34	4.5398826548	-2.8550580902	1.2050196684
C36	-4.7732738455	1.9283692984	0.6783890833
C37	-5.4033105646	-0.3902501094	0.7082825938
C38	5.4033105646	0.3902501094	0.7082825938
C39	4.7732738455	-1.9283692984	0.6783890833
H42	3.2680164751	2.7515017958	0.0498379723
S42	-2.1306930315	-0.5812218599	-0.0023367106
C44	2.2652042668	2.3285551024	0.0310034408
S44	2.1306930315	0.5812218599	-0.0023367106
C46	0.3613263333	0.5731362071	-0.0045672067
C48	-0.3613263333	-0.5731362071	-0.0045672067
H50	-3.2680164751	-2.7515017958	0.0498379723
H51	1.0938324148	4.1353176460	0.0452911681
C52	1.1396655444	3.0484176795	0.0291238525

C53	-2.2652042668	-2.3285551024	0.0310034408
S53	-0.3898439728	2.1837036875	-0.0094057586
S57	0.3898439728	-2.1837036875	-0.0094057586
C59	-1.1396655444	-3.0484176795	0.0291238525
H61	-1.0938324148	-4.1353176460	0.0452911681
C66	-4.7778504940	1.9129506439	-0.7105471704
C67	-5.4060175827	-0.4063237450	-0.6853242188
C68	5.4060175827	0.4063237450	-0.6853242188
C69	4.7778504940	-1.9129506439	-0.7105471704
H70	-4.5493154547	2.8283387830	-1.2586105014
H71	-5.6649301810	-1.3251637776	-1.2156696765
H72	5.6649301810	1.3251637776	-1.2156696765
C73	-5.0700367622	0.7388379657	-1.4079828348
H74	4.5493154547	-2.8283387830	-1.2586105014
C75	5.0700367622	-0.7388379657	-1.4079828348
C76	-4.9216328804	0.6928694489	-2.9083656483
H77	-3.1168848744	2.5418537801	-3.3112317222
C78	4.9216328804	-0.6928694489	-2.9083656483
C79	-2.6534290292	1.5581182859	-3.3390736508
N80	-3.5085226522	0.4910697726	-3.2847342564
H81	-5.2550496794	1.6270121717	-3.3777787904
H82	3.6986582894	1.5867655853	-3.3125557941
C83	-1.3050356670	1.3952187795	-3.4350843947
H84	-5.5011032063	-0.1284672431	-3.3477912407
C85	-2.9811953372	-0.7687513170	-3.3483360366
H86	-0.7029163463	2.2985457844	-3.4814516774
C87	2.9811953372	0.7687513170	-3.3483360366
N88	3.5085226522	-0.4910697726	-3.2847342564
H89	-3.6986582894	-1.5867655853	-3.3125557941
C90	-0.7064002327	0.0980501883	-3.4615790095
C91	1.6399000931	0.9828599111	-3.4528955207
C92	-1.6399000931	-0.9828599111	-3.4528955207
C93	0.7064002327	-0.0980501883	-3.4615790095

H94	1.3096483069	2.0164864649	-3.5098835027
C95	2.6534290292	-1.5581182859	-3.3390736508
H96	-1.3096483069	-2.0164864649	-3.5098835027
H97	3.1168848744	-2.5418537801	-3.3112317222
H98	5.5011032063	0.1284672431	-3.3477912407
C99	1.3050356670	-1.3952187795	-3.4350843947
H100	5.2550496794	-1.6270121717	-3.3777787904
H101	0.7029163463	-2.2985457844	-3.4814516774

**9. (TTF  $\subset$  CBPQT)<sup>+3</sup>**

	-3431.953464	-3431.536016	-3432.048603	-3432.466051
H2	-5.1973760007	1.7680555217	3.3469459774	
H3	-5.4942293442	0.0189364489	3.3637888156	
H4	-3.7330998557	-1.4903795038	3.3076909774	
C5	-2.9944722152	-0.6921420280	3.3482043483	
H6	1.3500922696	1.9820397434	3.4975244161	
H7	3.7330998557	1.4903795038	3.3076909774	
H8	-1.3500922696	-1.9820397434	3.4975244161	
N9	-3.4811066183	0.5794285969	3.2943791366	
H10	5.4942293442	-0.0189364489	3.3637888156	
C11	-1.6556708097	-0.9404183579	3.4506967989	
C12	1.6556708097	0.9404183579	3.4506967989	
C13	2.9944722152	0.6921420280	3.3482043483	
H14	5.1973760007	-1.7680555217	3.3469459774	
C15	-2.6096648258	1.6261466503	3.3636623663	
C16	-0.7082252680	0.1189466619	3.4736662540	
C17	-1.2614627887	1.4301319758	3.4587995399	
C18	0.7082252680	-0.1189466619	3.4736662540	
H19	-3.0509747938	2.6200653478	3.3484328291	
H20	-0.6379094865	2.3171768233	3.5243005460	
N21	3.4811066183	-0.5794285969	3.2943791366	
C22	1.2614627887	-1.4301319758	3.4587995399	
H23	0.6379094865	-2.3171768233	3.5243005460	
C24	2.6096648258	-1.6261466503	3.3636623663	

C25	-4.8898529483	0.8116390961	2.9070546806
H26	3.0509747938	-2.6200653478	3.3484328291
C27	4.8898529483	-0.8116390961	2.9070546806
C28	-5.0078809254	0.8164606817	1.4044536465
H29	-4.3916381243	2.8775541576	1.2087909625
C30	5.0078809254	-0.8164606817	1.4044536465
H31	-5.6830286604	-1.2274798790	1.2615336679
H33	5.6830286604	1.2274798790	1.2615336679
H34	4.3916381243	-2.8775541576	1.2087909625
C36	-4.6597248759	1.9603120643	0.6822774956
C37	-5.3842003878	-0.3339286361	0.7102550020
C38	5.3842003878	0.3339286361	0.7102550020
C39	4.6597248759	-1.9603120643	0.6822774956
H42	2.9370984921	3.0891263474	0.0914047842
S42	-2.0418516906	-0.8123668951	-0.0145204607
C44	1.9873506203	2.5601426695	0.0462926318
S44	2.0418516906	0.8123668951	-0.0145204607
C46	0.2954641966	0.6154646982	-0.0471610005
C48	-0.2954641966	-0.6154646982	-0.0471610005
H50	-2.9370984921	-3.0891263474	0.0914047842
H51	0.6159012699	4.2211616455	0.0635096136
C52	0.7859946076	3.1474116304	0.0303189687
C53	-1.9873506203	-2.5601426695	0.0462926318
S53	-0.6305957898	2.1178610211	-0.0556532375
S57	0.6305957898	-2.1178610211	-0.0556532375
C59	-0.7859946076	-3.1474116304	0.0303189687
H61	-0.6159012699	-4.2211616455	0.0635096136
C66	-4.6642182348	1.9463470883	-0.7058265674
C67	-5.3889666396	-0.3482693572	-0.6830722596
C68	5.3889666396	0.3482693572	-0.6830722596
C69	4.6642182348	-1.9463470883	-0.7058265674
H70	-4.4001655233	2.8533071781	-1.2518563647
H71	-5.6915312102	-1.2524518876	-1.2144722943

H72	5.6915312102	1.2524518876	-1.2144722943
C73	-5.0181164787	0.7884295665	-1.4018451737
H74	4.4001655233	-2.8533071781	-1.2518563647
C75	5.0181164787	-0.7884295665	-1.4018451737
C76	-4.9055429361	0.7510855365	-2.9036630880
H77	-3.0938378218	2.5723217358	-3.3902664559
C78	4.9055429361	-0.7510855365	-2.9036630880
C79	-2.6382502005	1.5849756328	-3.3786169975
N80	-3.4846454325	0.5289066072	-3.2785514244
H81	-5.2201815410	1.6919553683	-3.3698125795
H82	3.7083888095	1.5399883034	-3.2211831744
C83	-1.2829365969	1.4056854145	-3.4712062256
H84	-5.4935574924	-0.0619554367	-3.3444088337
C85	-2.9843560714	-0.7310367079	-3.2925985133
H86	-0.6727686527	2.2988966843	-3.5696613190
C87	2.9843560714	0.7310367079	-3.2925985133
N88	3.4846454325	-0.5289066072	-3.2785514244
H89	-3.7083888095	-1.5399883034	-3.2211831744
C90	-0.7187062348	0.1082384377	-3.4523823129
C91	1.6366811805	0.9618319271	-3.3923488016
C92	-1.6366811805	-0.9618319271	-3.3923488016
C93	0.7187062348	-0.1082384377	-3.4523823129
H94	1.3138521941	1.9991905405	-3.3958358214
C95	2.6382502005	-1.5849756328	-3.3786169975
H96	-1.3138521941	-1.9991905405	-3.3958358214
H97	3.0938378218	-2.5723217358	-3.3902664559
H98	5.4935574924	0.0619554367	-3.3444088337
C99	1.2829365969	-1.4056854145	-3.4712062256
H100	5.2201815410	-1.6919553683	-3.3698125795
H101	0.6727686527	-2.2988966843	-3.5696613190

**10. (TTF  $\subset$  CBPQT)<sup>+4</sup>**

-3431.803203      -3431.078388   -3431.583826   -3432.308641

H2      -5.1974791030      1.7203988501      3.3601260562

H3	-5.4857699580	-0.0313320920	3.3508295110
H4	-3.7125073600	-1.5219850276	3.2401803085
C5	-2.9861061255	-0.7163938453	3.3247577811
H6	1.3183352043	1.9930625910	3.4787659035
H7	3.7125073600	1.5219850276	3.2401803085
H8	-1.3183352043	-1.9930625910	3.4787659035
N9	-3.4686895537	0.5420546303	3.2868239042
H10	5.4857699580	0.0313320920	3.3508295110
C11	-1.6359541742	-0.9545603391	3.4593188132
C12	1.6359541742	0.9545603391	3.4593188132
C13	2.9861061255	0.7163938453	3.3247577811
H14	5.1974791030	-1.7203988501	3.3601260562
C15	-2.6323981173	1.5928042029	3.4167703985
C16	-0.7297343461	0.1122786719	3.5359789321
C17	-1.2746473897	1.4060244455	3.5464040060
C18	0.7297343461	-0.1122786719	3.5359789321
H19	-3.0831607252	2.5823309429	3.4156772524
H20	-0.6635564198	2.2966211791	3.6558698442
N21	3.4686895537	-0.5420546303	3.2868239042
C22	1.2746473897	-1.4060244455	3.5464040060
H23	0.6635564198	-2.2966211791	3.6558698442
C24	2.6323981173	-1.5928042029	3.4167703985
C25	-4.8930808466	0.7730340489	2.9022465443
H26	3.0831607252	-2.5823309429	3.4156772524
C27	4.8930808466	-0.7730340489	2.9022465443
C28	-4.9965391005	0.7973820210	1.3984947386
H29	-4.3571075958	2.8552887959	1.2284866393
C30	4.9965391005	-0.7973820210	1.3984947386
H31	-5.6993471398	-1.2363874939	1.2307786619
H33	5.6993471398	1.2363874939	1.2307786619
H34	4.3571075958	-2.8552887959	1.2284866393
C36	-4.6322970507	1.9457519942	0.6928769471
C37	-5.3860851876	-0.3407983981	0.6920208779



C38	5.3860851876	0.3407983981	0.6920208779
C39	4.6322970507	-1.9457519942	0.6928769471
H42	2.9488095484	3.0844914171	0.0246908647
S42	-2.0473674154	-0.8031982999	0.0005409065
C44	1.9966190013	2.5571917713	0.0170770763
S44	2.0473674154	0.8031982999	0.0005409065
C46	0.2957855467	0.6132546776	-0.0054575211
C48	-0.2957855467	-0.6132546776	-0.0054575211
H50	-2.9488095484	-3.0844914171	0.0246908647
H51	0.6341558796	4.2226184411	0.0286415347
C52	0.7979246576	3.1472121109	0.0179548397
C53	-1.9966190013	-2.5571917713	0.0170770763
S53	-0.6298518764	2.1209695728	-0.0002896993
S57	0.6298518764	-2.1209695728	-0.0002896993
C59	-0.7979246576	-3.1472121109	0.0179548397
H61	-0.6341558796	-4.2226184411	0.0286415347
C66	-4.6321252340	1.9476108970	-0.6958957514
C67	-5.3871517750	-0.3385168399	-0.7015414449
C68	5.3871517750	0.3385168399	-0.7015414449
C69	4.6321252340	-1.9476108970	-0.6958957514
H70	-4.3566089167	2.8582759764	-1.2294166672
H71	-5.7018800455	-1.2320417928	-1.2429133135
H72	5.7018800455	1.2320417928	-1.2429133135
C73	-4.9973735600	0.8015498166	-1.4047687360
H74	4.3566089167	-2.8582759764	-1.2294166672
C75	4.9973735600	-0.8015498166	-1.4047687360
C76	-4.8922198507	0.7813647855	-2.9084879309
H77	-3.0797141971	2.5879668280	-3.4275149164
C78	4.8922198507	-0.7813647855	-2.9084879309
C79	-2.6298950519	1.5981280226	-3.4247402448
N80	-3.4675898417	0.5489050003	-3.2904160471
H81	-5.1947125260	1.7302517657	-3.3644034123
H82	3.7145269811	1.5138296843	-3.2305475108

C83	-1.2721657378	1.4093001501	-3.5529578877
H84	-5.4851639954	-0.0213680056	-3.3596081745
C85	-2.9867069502	-0.7103415216	-3.3203618002
H86	-0.6591492258	2.2982060902	-3.6690239403
C87	2.9867069502	0.7103415216	-3.3203618002
N88	3.4675898417	-0.5489050003	-3.2904160471
H89	-3.7145269811	-1.5138296843	-3.2305475108
C90	-0.7294289935	0.1142790749	-3.5358795461
C91	1.6370081160	0.9509091229	-3.4527453700
C92	-1.6370081160	-0.9509091229	-3.4527453700
C93	0.7294289935	-0.1142790749	-3.5358795461
H94	1.3197889428	1.9896033628	-3.4613548476
C95	2.6298950519	-1.5981280226	-3.4247402448
H96	-1.3197889428	-1.9896033628	-3.4613548476
H97	3.0797141971	-2.5879668280	-3.4275149164
H98	5.4851639954	0.0213680056	-3.3596081745
C99	1.2721657378	-1.4093001501	-3.5529578877
H100	5.1947125260	-1.7302517657	-3.3644034123
H101	0.6591492258	-2.2982060902	-3.6690239403

**11. (DNP  $\subset$  CBPQT)<sup>0</sup>**

	-2223.377437	-2223.350398	-2223.872758	-2223.899797
H1	-5.2896753591	-1.4915916529	-3.2954575920	
H2	5.3090117358	1.7728232991	-3.4044039826	
H3	1.8897982520	-1.3773899322	-3.2771838282	
H4	-1.8654436807	1.6452829895	-3.1190608535	
H5	-4.4859435349	-3.0691493800	-3.3524626542	
H6	4.5011267723	3.3471837557	-3.3208251963	
H7	4.0209232795	-0.2340056674	-3.2372156897	
H8	-3.9949633885	0.4987138770	-3.0630324499	
C9	1.8872900554	-0.2899705051	-3.3242673739	
C10	-1.8663307794	0.5624413193	-3.2278485972	
C11	-3.0646678276	-0.0537782785	-3.1873405353	
C12	3.0871560562	0.3239085765	-3.2946850825	

C13	-0.6116097099	-0.1638593928	-3.3467247881
C14	0.6297914151	0.4412827755	-3.3546954574
H15	0.0387586787	-2.2710954102	-3.5130134013
H16	-0.0245787380	2.5548222092	-3.3854099584
C17	-0.8147297150	-1.6019073022	-3.4256017775
C18	0.8315571167	1.8821679744	-3.3644684828
N19	-3.2114538482	-1.4304393778	-3.3260856283
N20	3.2306957938	1.7060441646	-3.3591095505
C21	-2.0358101270	-2.1710735497	-3.3982197828
C22	2.0537890538	2.4495513978	-3.3489562801
H23	-2.1765361884	-3.2498866808	-3.4628309822
H24	2.1935829747	3.5306351767	-3.3589390887
C25	-4.4500686701	-2.0733399107	-2.8871879456
C26	4.4844903190	2.3213843365	-2.9250754236
C27	-4.5634124769	-2.1789615385	-1.3870413180
C28	4.6527696939	2.3221056905	-1.4265396545
H29	-5.5805520177	-0.2922775344	-1.1670812933
H30	5.6681121501	0.4222328245	-1.3735900442
H31	-3.6108201011	-4.1100457669	-1.2648651217
H32	3.7219318605	4.2454038240	-1.1340120154
C33	-5.1275084400	-1.1393265118	-0.6469083895
C34	5.2371049535	1.2319150929	-0.7804434931
C35	-4.0329631653	-3.2746919991	-0.7012165713
C36	4.1561213203	3.3695159428	-0.6461372425
H37	-1.0480548738	-3.3446988566	-0.0434353853
C38	-1.2834823196	-1.2290253514	-0.0036207581
C39	-0.6379471532	0.0269677934	0.0103290320
C40	-0.5415104656	-2.3782538614	-0.0353818669
C41	-1.3751338511	1.2477208524	0.0458089183
H42	-2.3677002642	-1.2661859304	0.0131426523
C43	0.7791510356	0.0925021231	-0.0095950437
C44	0.8680167896	-2.3422492336	-0.0594730773
C45	-0.7248050869	2.4624190370	0.0660251313

H46	1.4290968752	-3.2743878408	-0.0866179619
H47	-1.2858414035	3.3946371600	0.0945842347
C48	1.4253641575	1.3471763076	0.0113970903
C49	1.5175254840	-1.1271851571	-0.0486762575
C50	0.6847747526	2.4971955267	0.0493964519
O51	2.8675404336	-0.9839946727	-0.0715798299
C52	-5.1139455385	-1.1676110591	0.7424590880
C53	5.2678155959	1.1595148833	0.6072969307
C54	-4.0195538959	-3.3030502631	0.6893512660
C55	4.1889609152	3.2980424901	0.7429407994
H56	-5.5560655501	-0.3423427112	1.3052653635
H57	5.7208103033	0.2931132116	1.0947479373
H58	-3.5873749161	-4.1606487787	1.2103102968
H59	3.7793536260	4.1182906992	1.3370590796
C60	-4.5362543454	-2.2361902831	1.4290059130
C61	4.7169462442	2.1761824853	1.3878371871
C62	-4.3935377897	-2.1919582126	2.9297869616
C63	4.6213680229	2.0245754426	2.8855694137
H64	-2.1398804324	-3.4426209881	3.4389261702
H65	2.3741209759	3.2397530651	3.4750277794
N66	-3.1327979046	-1.5941559924	3.3680485321
N67	3.3731947425	1.3989257466	3.3213622950
C68	-1.9733178299	-2.3662625363	3.3917117524
C69	2.2119920890	2.1640944259	3.4019024465
H70	4.1211289708	-0.5432531912	3.0517482763
H71	-3.8750647458	0.3608605232	3.1778604403
H72	-5.2119670497	-1.6075136880	3.3757092223
H73	5.4508418278	1.4090699580	3.2638965683
C74	-2.9558015886	-0.2171416701	3.2671757836
C75	3.2004591199	0.0255433037	3.1815163335
H76	-4.4436034063	-3.2037850513	3.3575928894
H77	4.6893499089	3.0043267894	3.3808133722
C78	-0.7381902375	-1.8277560871	3.3992862129

C79	0.9801140982	1.6192510461	3.4257975667
H80	0.1030399420	-2.5168970929	3.4570899862
H81	0.1375881648	2.3022442141	3.5267889644
C82	1.9913586538	-0.5687125993	3.2309398337
C83	-1.7425392118	0.3689017533	3.2993632947
C84	-0.5039042939	-0.3928185107	3.3576669343
C85	0.7509967339	0.1849299799	3.3479089765
H86	1.9661077329	-1.6520330712	3.1203626036
H87	-1.7156421061	1.4544303423	3.2177424405
C88	3.6462321675	-2.1481657608	-0.1082302063
H89	4.6933015412	-1.8257400350	-0.1253322424
H90	3.4804818317	-2.7795052261	0.7801762186
H91	3.4412994366	-2.7487296818	-1.0095713495
O92	-2.7248321184	1.1050815478	0.0597387180
C93	-3.5066155360	2.2670993827	0.0785768565
H94	-4.5532786638	1.9415920481	0.0755115147
H95	-3.3218085109	2.8706690460	0.9825393346
H96	-3.3244338252	2.8976297475	-0.8071778208
H97	1.1919443085	3.4631637325	0.0665050111
H98	2.5093433495	1.3812757630	-0.0022027038

**12. (DNP  $\subset$  CBPQT)<sup>+1</sup>**

	-2223.274315	-2223.203797	-2223.711727	-2223.782246
H1	-5.2832876583	-1.5184326441	-3.3060997925	
H2	5.2995226271	1.7825448924	-3.4136341905	
H3	1.8894314544	-1.3809724659	-3.3029733527	
H4	-1.8767464989	1.6385196084	-3.1722980407	
H5	-4.4706512828	-3.0920720601	-3.3625312114	
H6	4.4838269208	3.3530642956	-3.3248576912	
H7	4.0167001148	-0.2332069635	-3.1903348510	
H8	-3.9985879532	0.4785084510	-3.0453294626	
C9	1.8849677258	-0.2928598641	-3.3356377595	
C10	-1.8718351839	0.5527074396	-3.2557671406	
C11	-3.0666892978	-0.0702774437	-3.1812020621	

C12	3.0835734639	0.3236428466	-3.2694055563
C13	-0.6138107403	-0.1714398634	-3.3671329407
C14	0.6263029254	0.4372291926	-3.3715482234
H15	0.0433304754	-2.2731180173	-3.6014016438
H16	-0.0314615640	2.5492449869	-3.4749886897
C17	-0.8097935849	-1.6105673096	-3.4556057440
C18	0.8237956356	1.8788166099	-3.3931557950
N19	-3.2029721126	-1.4493528765	-3.2811113463
N20	3.2213339842	1.7053745792	-3.3046979895
C21	-2.0290327584	-2.1861889506	-3.4074180564
C22	2.0458173883	2.4492882523	-3.3539136533
H23	-2.1674761284	-3.2636039966	-3.4962049608
H24	2.1849699129	3.5296397185	-3.3899949918
C25	-4.4488164043	-2.1004718319	-2.8877283137
C26	4.4832558075	2.3309307575	-2.9199760090
C27	-4.5840424920	-2.2173762489	-1.3890544253
C28	4.6817274441	2.3427744194	-1.4237434213
H29	-5.6634837408	-0.3654076190	-1.1731724946
H30	5.7459305110	0.4696572743	-1.3824760814
H31	-3.5760311154	-4.1203717525	-1.2644697555
H32	3.7021062969	4.2412301680	-1.1249414166
C33	-5.1826882522	-1.1954197121	-0.6515687793
C34	5.2956439432	1.2648767775	-0.7846116431
C35	-4.0225031716	-3.2971538486	-0.7025426993
C36	4.1613792946	3.3766451361	-0.6407595253
H37	-1.1076705668	-3.3104307601	-0.0424038494
C38	-1.3179438561	-1.1897069951	0.0022359863
C39	-0.6550745382	0.0579697681	0.0217764179
C40	-0.5906268932	-2.3501807044	-0.0236786162
C41	-1.3743442323	1.2906308239	0.0512644596
H42	-2.4031184867	-1.2131994643	-0.0025970828
C43	0.7639083862	0.1033686982	0.0083506206
C44	0.8198811881	-2.3340589894	-0.0391775275

C45	-0.7055112774	2.4957346373	0.0711609858
H46	1.3676942496	-3.2740306460	-0.0639208770
H47	-1.2535104149	3.4356083834	0.0897278160
C48	1.4295999375	1.3491258052	0.0280790749
C49	1.4856375670	-1.1278043489	-0.0273084564
C50	0.7048365696	2.5112170828	0.0610083294
O51	2.8353885407	-1.0003124105	-0.0343541238
C52	-5.1649557224	-1.2182522337	0.7388236988
C53	5.3275690615	1.1853827693	0.6031218351
C54	-4.0037938626	-3.3214152133	0.6876279215
C55	4.1952371612	3.3004920739	0.7474415957
H56	-5.6325552916	-0.4065985414	1.3003017313
H57	5.8016925308	0.3288050648	1.0863670233
H58	-3.5421385870	-4.1628906016	1.2090585562
H59	3.7629282636	4.1060712123	1.3451469889
C60	-4.5481661917	-2.2657227157	1.4231444575
C61	4.7500224600	2.1869549196	1.3839166814
C62	-4.3778745741	-2.2046510799	2.9177253692
C63	4.6295230828	2.0171931382	2.8747792364
H64	-2.1288265564	-3.4386295828	3.4742243310
H65	2.3933440763	3.2173452265	3.5314284286
N66	-3.0805258037	-1.5897279177	3.2670876855
N67	3.3424694445	1.3817608713	3.2248502249
C68	-1.9603252406	-2.3653159868	3.4035521273
C69	2.2253274906	2.1470125169	3.4256891950
H70	4.1089911357	-0.5408251157	2.9435303428
H71	-3.8463330308	0.3441873352	3.0695346713
H72	-5.1656646823	-1.6038635937	3.3901282804
H73	5.4293851940	1.3812365607	3.2752904697
C74	-2.9315677629	-0.2307531659	3.2026492085
C75	3.1957153178	0.0252755534	3.1189658378
H76	-4.3968867292	-3.2019621395	3.3749549008
H77	4.6701087307	2.9789155063	3.4016604719

C78	-0.7140098802	-1.8193859193	3.4711871973
C79	0.9836106753	1.5941953436	3.5118818525
H80	0.1214133054	-2.5024752553	3.6134052733
H81	0.1518606845	2.2680840840	3.7056098773
C82	1.9785344203	-0.5760396780	3.2270864728
C83	-1.7096247152	0.3628166242	3.2922592171
C84	-0.5127665898	-0.4085745923	3.3962752444
C85	0.7833540125	0.1868379260	3.3898029656
H86	1.9467544873	-1.6569396077	3.1104675984
H87	-1.6765519953	1.4471774178	3.2047083915
C88	3.6074300534	-2.1716180033	-0.1132235885
H89	4.6556913488	-1.8537953728	-0.1298475556
H90	3.4454643312	-2.8266778147	0.7582505075
H91	3.3889707246	-2.7415443223	-1.0299937788
O92	-2.7241047611	1.1681313193	0.0719939039
C93	-3.4945311783	2.3429935195	0.0480484531
H94	-4.5432402196	2.0275938433	0.0382032271
H95	-3.3144830384	2.9664498731	0.9389250722
H96	-3.2911424596	2.9453970776	-0.8519755888
H97	1.2234638993	3.4709219960	0.0673515714
H98	2.5143542457	1.3701649395	0.0059232858

**13. (DNP  $\subset$  CBPQT)<sup>+2</sup>**

	-2223.166942	-2222.97195	-2223.468458	-2223.66345
H1	-5.2655964123	-1.4801797561	-3.3298660753	
H2	5.2636126732	1.7323407278	-3.4191990121	
H3	1.8580623472	-1.3999360800	-3.3186342107	
H4	-1.8622027268	1.6400133078	-3.2390346848	
H5	-4.4721085550	-3.0652334157	-3.3833732997	
H6	4.4640092862	3.3128700813	-3.3398759044	
H7	3.9996868608	-0.2498307057	-3.1714166273	
H8	-3.9988828901	0.4808999623	-3.0813401648	
C9	1.8575763553	-0.3132846923	-3.3238585284	
C10	-1.8608336442	0.5532225132	-3.2843113272	



C11	-3.0674513231	-0.0709590028	-3.1918410843
C12	3.0673257301	0.3062989204	-3.2372006186
C13	-0.6441311444	-0.1881650397	-3.3903379236
C14	0.6414750183	0.4336061195	-3.3830867735
H15	0.0374233473	-2.2672150044	-3.6032533477
H16	-0.0400970682	2.5216050377	-3.4830883567
C17	-0.8126473815	-1.6026504534	-3.4702259316
C18	0.8112685878	1.8502922042	-3.4016825682
N19	-3.1796353779	-1.4343666065	-3.2357392088
N20	3.1828785092	1.6702771206	-3.2322978136
C21	-2.0428865936	-2.1803754637	-3.3856410186
C22	2.0444013972	2.4229212636	-3.3194050483
H23	-2.1828787784	-3.2583276514	-3.4377464297
H24	2.1848650077	3.5022119941	-3.3257216442
C25	-4.4609127149	-2.0843005484	-2.8925785254
C26	4.4784904680	2.3042490846	-2.9089859644
C27	-4.6003040232	-2.2024389886	-1.3965039667
C28	4.6886466605	2.3341136703	-1.4166582157
H29	-5.6218460872	-0.3160722603	-1.1725979601
H30	5.7277067914	0.4458407167	-1.3550582953
H31	-3.6508194194	-4.1383215085	-1.2848281025
H32	3.7420407437	4.2549152174	-1.1437670227
C33	-5.1650610753	-1.1630966790	-0.6566373223
C34	5.2891295939	1.2552112519	-0.7680294558
C35	-4.0687405474	-3.3026742024	-0.7194456664
C36	4.1854712762	3.3878245448	-0.6500011145
H37	-1.0853310887	-3.3260825685	-0.0577252150
C38	-1.3039934159	-1.2048897898	-0.0084569542
C39	-0.6438064404	0.0455587276	0.0130877287
C40	-0.5729891153	-2.3635039072	-0.0438073443
C41	-1.3682506496	1.2760073248	0.0517791406
H42	-2.3900466512	-1.2324210029	0.0038840321
C43	0.7753842411	0.0957375192	-0.0034706281

C44	0.8374821291	-2.3423541226	-0.0662347947
C45	-0.7052746112	2.4836015074	0.0802603162
H46	1.3868238177	-3.2807822065	-0.0973056923
H47	-1.2543824771	3.4222574812	0.1112395463
C48	1.4356705650	1.3451947189	0.0252375719
C49	1.5003347468	-1.1343475434	-0.0494949757
C50	0.7050747623	2.5042224415	0.0676797222
O51	2.8486136987	-1.0026824233	-0.0749525478
C52	-5.1422141939	-1.1918730962	0.7335277757
C53	5.3214868131	1.1945898826	0.6205878857
C54	-4.0462465731	-3.3316689880	0.6705949654
C55	4.2185024101	3.3274471069	0.7391454010
H56	-5.5815965268	-0.3671423356	1.2985469311
H57	5.7834026684	0.3373931862	1.1137337126
H58	-3.6111326287	-4.1900325383	1.1866874798
H59	3.7990018438	4.1470632267	1.3260769666
C60	-4.5543726223	-2.2610934603	1.4104383966
C61	4.7552157277	2.2126841501	1.3875412613
C62	-4.3709311134	-2.2102464532	2.9052918634
C63	4.6200075011	2.0570976331	2.8803065229
H64	-2.1060699202	-3.4450173398	3.3912310366
H65	2.3675181239	3.2493764524	3.4934394649
N66	-3.0698667025	-1.5967586869	3.2432411581
N67	3.3305098994	1.4171409670	3.2148138098
C68	-1.9458143965	-2.3684959752	3.3626679886
C69	2.2094426183	2.1755781594	3.4126170968
H70	4.1176035502	-0.5033791647	2.9855187682
H71	-3.8553651578	0.3367879937	3.1418477951
H72	-5.1531210718	-1.6122681893	3.3895657038
H73	5.4169730344	1.4280150077	3.2961892014
C74	-2.9336501327	-0.2348043304	3.2359341159
C75	3.1974301635	0.0576595438	3.1369653266
H76	-4.3874349358	-3.2110191049	3.3541436439

H77	4.6497800296	3.0236866512	3.3981571439
C78	-0.7038881326	-1.8152733469	3.4496296506
C79	0.9727010005	1.6129838939	3.5110953993
H80	0.1358693233	-2.4972246677	3.5638749344
H81	0.1355958741	2.2836898842	3.6894638523
C82	1.9844105493	-0.5516609753	3.2456693237
C83	-1.7150140008	0.3647858771	3.3362512962
C84	-0.5121430021	-0.4016259977	3.4088916624
C85	0.7826988504	0.2034608012	3.4017997186
H86	1.9645556426	-1.6354475059	3.1599244515
H87	-1.6935076642	1.4526184278	3.3052952162
C88	3.6246245484	-2.1765619361	-0.1349350882
H89	4.6722008929	-1.8573135482	-0.1543462391
H90	3.4586231208	-2.8168428999	0.7450718592
H91	3.4075240180	-2.7578452797	-1.0442661755
O92	-2.7154785312	1.1433319590	0.0605306112
C93	-3.4953248226	2.3163864743	0.0857494502
H94	-4.5418183380	1.9949854883	0.0740994686
H95	-3.3079818885	2.9065716400	0.9960409712
H96	-3.3020193872	2.9498130348	-0.7937325381
H97	1.2174128598	3.4666692126	0.0904397999
H98	2.5212374912	1.3714471678	0.0118844831

**14. (DNP  $\subset$  CBPQT)<sup>+3</sup>**

	-2223.023194	-2222.605495	-2223.093696	-2223.511395
H1	-5.2535800697	-1.4858976969	-3.3285024177	
H2	5.2661244645	1.7493939972	-3.4180346578	
H3	1.8723776755	-1.3770703433	-3.3687826907	
H4	-1.8566793064	1.6456372431	-3.2206607373	
H5	-4.4525862903	-3.0672092249	-3.3742526727	
H6	4.4723803353	3.3333300900	-3.3380241097	
H7	4.0113435112	-0.2276098326	-3.2192887681	
H8	-3.9926456979	0.4803182940	-3.0687095588	
C9	1.8653612444	-0.2915691547	-3.3453114088	

C10	-1.8518209176	0.5578345119	-3.2602179473
C11	-3.0580292968	-0.0690537201	-3.1698888647
C12	3.0759728749	0.3276843415	-3.2584225696
C13	-0.6356212219	-0.1781960736	-3.3697495224
C14	0.6473529906	0.4511069023	-3.3721484619
H15	0.0476155554	-2.2551117528	-3.5942698597
H16	-0.0395749832	2.5363143466	-3.4531664636
C17	-0.7991918592	-1.5913652800	-3.4538584757
C18	0.8103922504	1.8661141804	-3.3797327610
N19	-3.1659733913	-1.4310514208	-3.2140751164
N20	3.1850843138	1.6906217342	-3.2275234249
C21	-2.0295184327	-2.1739265311	-3.3681722310
C22	2.0447022753	2.4420729286	-3.3013987514
H23	-2.1689566059	-3.2511608060	-3.4285794481
H24	2.1833959402	3.5210252342	-3.3046189430
C25	-4.4494557353	-2.0861667410	-2.8848299162
C26	4.4824763581	2.3243053200	-2.9090118947
C27	-4.5989933621	-2.2022576556	-1.3887481326
C28	4.6910049617	2.3469936375	-1.4170468181
H29	-5.6486937203	-0.3303323658	-1.1796367349
H30	5.7328474008	0.4591441484	-1.3634821405
H31	-3.6345865251	-4.1311068299	-1.2660850368
H32	3.7463290750	4.2693793602	-1.1374450349
C33	-5.1822672248	-1.1672824348	-0.6572776354
C34	5.2924448975	1.2645795811	-0.7739304393
C35	-4.0602860032	-3.2960853936	-0.7060423918
C36	4.1868108069	3.3991187279	-0.6475379602
H37	-1.0743518455	-3.3564960660	-0.0528135631
C38	-1.2959085455	-1.2331141417	-0.0036146874
C39	-0.6367073557	0.0156985929	0.0192197303
C40	-0.5633074126	-2.3932633405	-0.0336417242
C41	-1.3624867016	1.2473820791	0.0666843326
H42	-2.3803396613	-1.2629050216	-0.0060040313

C43	0.7852156171	0.0672572351	-0.0024414209
C44	0.8476188872	-2.3723338042	-0.0573820373
C45	-0.6994183847	2.4563902265	0.0991669347
H46	1.3942766438	-3.3117981861	-0.0888527308
H47	-1.2488830787	3.3945581560	0.1371238246
C48	1.4446306440	1.3193119756	0.0232835304
C49	1.5109975012	-1.1638737620	-0.0498679913
C50	0.7111945871	2.4792246719	0.0781608724
O51	2.8548242745	-1.0249529945	-0.0748005242
C52	-5.1677875150	-1.1898412162	0.7325041389
C53	5.3230026859	1.1955720688	0.6140297244
C54	-4.0430442185	-3.3193938235	0.6847426195
C55	4.2142339561	3.3328324296	0.7412531986
H56	-5.6255967750	-0.3715858139	1.2909333463
H57	5.7889121362	0.3382157648	1.1030109427
H58	-3.6039341287	-4.1728714211	1.2057422547
H59	3.7961893306	4.1523869687	1.3295383077
C60	-4.5685383919	-2.2496151528	1.4136715898
C61	4.7536410630	2.2126069205	1.3828337419
C62	-4.3947059626	-2.1891435523	2.9062166901
C63	4.6222430413	2.0512791207	2.8731369929
H64	-2.1473084548	-3.4087884698	3.4387668209
H65	2.3837143540	3.2404220180	3.5004541229
N66	-3.0663097205	-1.5623266404	3.2164327800
N67	3.3030004821	1.4035238788	3.1837370551
C68	-1.9823283527	-2.3355509180	3.3865842801
C69	2.2214494273	2.1686511661	3.4109198050
H70	4.0942342491	-0.5016347073	2.9240870463
H71	-3.8618245503	0.3511624510	3.0569952807
H72	-5.1567916618	-1.5740908916	3.3989142653
H73	5.3979780081	1.4046102732	3.3003657116
C74	-2.9454531719	-0.2200161125	3.1723226059
C75	3.1812195971	0.0633897978	3.0837218511

H76	-4.3880089931	-3.1779098036	3.3777079285
H77	4.6336660918	3.0058257079	3.4106672207
C78	-0.7216881961	-1.7782550222	3.4908338513
C79	0.9652792284	1.6054152668	3.5270064267
H80	0.1095029550	-2.4595513021	3.6449768221
H81	0.1399108238	2.2793155274	3.7270258014
C82	1.9480317208	-0.5454430288	3.1950903137
C83	-1.7098045946	0.3833548285	3.2723658331
C84	-0.5536453408	-0.3938992445	3.4032439689
C85	0.7965071359	0.2247169302	3.3917286468
H86	1.9154238986	-1.6263299528	3.0937778948
H87	-1.6830550939	1.4678070391	3.2080452561
C88	3.6415759359	-2.1962591625	-0.1519716712
H89	4.6851574877	-1.8678497070	-0.1709382865
H90	3.4816401720	-2.8471381344	0.7222931554
H91	3.4206750147	-2.7642324508	-1.0676831267
O92	-2.7066429221	1.1106364391	0.0962555449
C93	-3.4957723592	2.2842041016	0.1041241699
H94	-4.5407722777	1.9564739811	0.1012095879
H95	-3.3074545932	2.8869712471	1.0053330850
H96	-3.3087508403	2.9015507619	-0.7865278199
H97	1.2198630542	3.4438896614	0.0956239849
H98	2.5300168691	1.3489953572	-0.0036818347

**15. (DNP  $\subset$  CBPQT)<sup>+4</sup>**

	-2222.874183	-2222.15268	-2222.632653	-2223.354156
H1	-5.1982637937	-1.5450159463	-3.3421731707	
H2	5.2440036786	1.8124004071	-3.4438056425	
H3	1.8778747857	-1.3623156741	-3.3053394250	
H4	-1.8278131023	1.6217775529	-3.1504723451	
H5	-4.3737094582	-3.1173406034	-3.3541263300	
H6	4.4231360938	3.3829828727	-3.3252106496	
H7	4.0232714056	-0.1778602480	-3.1403195042	
H8	-3.9669236484	0.4250979806	-2.9667985279	

C9	1.8697467789	-0.2763793712	-3.3166199462
C10	-1.8211671612	0.5376909733	-3.2189298635
C11	-3.0318132651	-0.1101885086	-3.1089621739
C12	3.0843859952	0.3644459431	-3.2180957246
C13	-0.6405790561	-0.1967517900	-3.3954538836
C14	0.6843148360	0.4665418460	-3.4055542101
H15	0.0884303095	-2.2330277436	-3.6872279310
H16	-0.0523807491	2.5150560605	-3.5638236455
C17	-0.7632678192	-1.5851904723	-3.5048255888
C18	0.8047887913	1.8590848612	-3.4484228593
N19	-3.1079033682	-1.4561472452	-3.1717354366
N20	3.1602477114	1.7121262847	-3.2101088383
C21	-1.9979990255	-2.1884961487	-3.3808602353
C22	2.0446019321	2.4549878922	-3.3405634689
H23	-2.1254469841	-3.2662034086	-3.4454216165
H24	2.1705863624	3.5349931590	-3.3519001599
C25	-4.4083341668	-2.1370712119	-2.8674259565
C26	4.4710975083	2.3724003015	-2.9059449500
C27	-4.5738696089	-2.2343440265	-1.3734650226
C28	4.6822205166	2.3678361402	-1.4150279498
H29	-5.6785789799	-0.3877850634	-1.2049549135
H30	5.7787701002	0.5087682662	-1.4044562430
H31	-3.5739977775	-4.1426387360	-1.2112782548
H32	3.6998484338	4.2655687998	-1.0937255164
C33	-5.1936216402	-1.2036645056	-0.6670369809
C34	5.3127355651	1.2868835406	-0.7984996340
C35	-4.0230472264	-3.3083464281	-0.6697949129
C36	4.1575371592	3.3931612334	-0.6238671491
H37	-1.0844949168	-3.3324973147	-0.0198837817
C38	-1.3044305179	-1.2078345073	0.0085106414
C39	-0.6435732628	0.0428927976	0.0038295205
C40	-0.5743543735	-2.3694741312	-0.0272113500
C41	-1.3678750991	1.2759081438	0.0298825542

H42	-2.3894291730	-1.2341675385	0.0432984549
C43	0.7751193750	0.0927572963	-0.0253069264
C44	0.8354056333	-2.3502808760	-0.0791229356
C45	-0.7040106463	2.4851986781	0.0447669722
H46	1.3814112141	-3.2900489369	-0.1165172888
H47	-1.2521228743	3.4245075570	0.0639366393
C48	1.4364949742	1.3435927958	-0.0002985684
C49	1.4980802481	-1.1410181342	-0.0777283765
C50	0.7077887775	2.5070913617	0.0347697046
O51	2.8430183014	-1.0049027367	-0.1177181546
C52	-5.1956785416	-1.2066336271	0.7237891692
C53	5.3470738431	1.1906318074	0.5885269021
C54	-4.0238884134	-3.3109252493	0.7210122702
C55	4.1926219027	3.2975141438	0.7634042218
H56	-5.6821661547	-0.3933519092	1.2640485818
H57	5.8392601085	0.3377706801	1.0579528155
H58	-3.5734322792	-4.1462651318	1.2597079698
H59	3.7608343977	4.0951493883	1.3704133623
C60	-4.5777084938	-2.2403608337	1.4276405015
C61	4.7516578688	2.1742917884	1.3788288679
C62	-4.4162355789	-2.1499941932	2.9225977977
C63	4.6263049241	1.9798181908	2.8670138670
H64	-2.2129602141	-3.3771110358	3.6240861111
H65	2.4501541745	3.1596450339	3.7196631771
N66	-3.0861251068	-1.5307008546	3.2340072152
N67	3.3034524765	1.3415487388	3.1742189099
C68	-2.0233333226	-2.3124930335	3.5067054281
C69	2.2548757979	2.1039676874	3.5421808832
H70	4.0391172647	-0.5455430967	2.7029558955
H71	-3.8415774130	0.3813112134	2.9204300599
H72	-5.1802825610	-1.5196456855	3.3905535735
H73	5.4006722480	1.3184734650	3.2708786142
C74	-2.9391804167	-0.1946223806	3.1119678237



C75	3.1463088494	0.0157409546	2.9693357802
H76	-4.4302259150	-3.1297152971	3.4112023024
H77	4.6563421870	2.9236980792	3.4214059609
C78	-0.7578903250	-1.7724609726	3.6257276515
C79	0.9962272103	1.5549244673	3.6858258366
H80	0.0624894634	-2.4452554450	3.8641572752
H81	0.1913830809	2.2094412614	4.0089620080
C82	1.9081317862	-0.5784973758	3.0904891745
C83	-1.6975860090	0.3921495855	3.2179729074
C84	-0.5643940935	-0.3992812589	3.4473046060
C85	0.7906578149	0.1959394861	3.4296388747
H86	1.8310429146	-1.6441920138	2.8867420097
H87	-1.6303102687	1.4696690602	3.0806527135
C88	3.6303908215	-2.1805315127	-0.1921890282
H89	4.6727449073	-1.8504862312	-0.2354118636
H90	3.4853730700	-2.8170559670	0.6925264659
H91	3.3956035430	-2.7605826659	-1.0959111022
O92	-2.7144541102	1.1398945731	0.0383629278
C93	-3.5003431293	2.3185263948	0.0440801789
H94	-4.5455835830	1.9938737689	0.0485494918
H95	-3.3050545526	2.9253297917	0.9406314499
H96	-3.3111997081	2.9283903214	-0.8515624919
H97	1.2176216169	3.4704872170	0.0522279340
H98	2.5209430237	1.3728193962	-0.0202115640

**16. (DCB  $\subset$  CBPQT)<sup>0</sup>**

-2025.31832 -2025.281198 -2025.755646 -2025.792768

H1	0.3396412435	6.5167816315	0.5884838108
H2	-0.7654115194	6.2129892548	1.9401073525
H3	-0.6591170446	4.2107968487	3.1613467852
C4	0.1587795167	3.8294563622	2.5509065856
H5	3.9756607140	0.9795938084	0.6174350419
H6	4.9084041250	-1.2173436903	1.0145782354
H7	0.3120459316	2.0365350347	3.5955446298

N8	0.6132252398	4.7020720332	1.5663445224
H9	4.9745553308	-3.2365941776	2.1836519376
C10	0.7158227116	2.6212579988	2.7708770499
C11	3.5185342681	0.3633223063	1.3893608085
C12	4.0567778877	-0.8569097709	1.5906903737
H13	3.8331677865	-3.5773533886	3.4952063141
C14	1.6329097195	4.2321077635	0.7464002698
C15	1.8184796361	2.1060393006	1.9726735462
C16	2.2320942373	3.0379540716	0.9345480158
C17	2.3924864694	0.8644691008	2.1635397130
H18	1.9387545457	4.9141850256	-0.0461565230
H19	3.0425240558	2.7823475420	0.2536985906
N20	3.6027224259	-1.7263962644	2.5760142333
C21	1.9245656865	-0.1016814443	3.1457570669
H22	1.0732281283	0.1268610343	3.7847442083
C23	2.4907150613	-1.3172510426	3.2997331640
C24	-0.2820312297	5.7478113903	1.0690568476
H25	2.1187526679	-2.0400576984	4.0251668611
C26	3.9207631919	-3.1513366773	2.4853994091
C27	-1.3114091764	5.2141949291	0.1053866527
H28	-0.1095248867	5.5781032746	-1.6464295916
C29	3.0230102051	-3.8839077729	1.5204543691
H30	-2.7630029784	4.7547154525	1.6328652833
H31	4.2485923324	-3.4739162775	-0.2075456156
H32	1.6073327857	-4.4842563758	3.0290730971
C33	-1.0405068392	5.1567096507	-1.2622907643
C34	-2.5204400686	4.6903424475	0.5703955942
C35	3.3153936294	-3.9109112450	0.1536087706
C36	1.8425100976	-4.4806181860	1.9629878107
C37	-1.9423471339	4.5649074252	-2.1409044831
C38	-3.4216760576	4.0979934810	-0.3078474599
C39	2.4329123278	-4.4952179090	-0.7488334337
C40	0.9600666790	-5.0653664698	1.0605415529

H41	-1.7120286586	4.5274502480	-3.2073287304
H42	-4.3655447926	3.7009174064	0.0710477670
H43	2.6788633620	-4.5128062425	-1.8125438200
C44	-3.1360182923	4.0141802564	-1.6728371751
H45	0.0393284737	-5.5243653252	1.4256415185
C46	1.2365088666	-5.0675356561	-0.3066040708
C47	-4.0576085401	3.2743108340	-2.6089798633
H48	-2.3267465623	2.1519488908	-4.2245860531
C49	0.2265863669	-5.5999286974	-1.2906948441
C50	-2.6580006827	1.4371331637	-3.4720908520
N51	-3.7379394242	1.8496280500	-2.7012778077
H52	-4.0002466914	3.6944492917	-3.6233435001
H53	0.5541580178	-4.0544086207	-3.3880087987
C54	-2.0792298536	0.2260388936	-3.3308174701
H55	-5.1022377322	3.3596725885	-2.2770076673
C56	-4.1485547538	0.9852811534	-1.6935580426
H57	-1.2602770372	-0.0098293514	-4.0093559772
C58	-0.2541650641	-3.6809314129	-2.7602913460
N59	-0.6865766675	-4.5625290360	-1.7731829530
H60	-4.9740717728	1.3491421518	-1.0821051505
C61	-2.5012504608	-0.7330809199	-2.3219781718
C62	-0.8225800776	-2.4751343169	-2.9649918193
C63	-3.5999952841	-0.2332051352	-1.5083164446
C64	-1.9126225332	-1.9698574538	-2.1443360040
H65	-0.4366219390	-1.8853337130	-3.7946244592
C66	-1.6893715020	-4.0991586186	-0.9294567551
H67	-4.0213808601	-0.8464334891	-0.7138347724
H68	-1.9775755069	-4.7855862433	-0.1339725001
H69	0.7249540406	-6.0354221256	-2.1685393794
C70	-2.2953284639	-2.9058415789	-1.0988129438
H71	-0.3818521908	-6.3924989952	-0.8315489836
H72	-3.0946727442	-2.6603568931	-0.4023921732
C73	1.0043366094	-0.1515879279	-1.0765241633

C74	0.3025523475	1.0585920093	-1.0734333713
C75	-0.7084485837	1.3179525178	-0.1465226977
C76	-1.0205076490	0.3479251360	0.7867064755
C77	-0.3197779005	-0.8624459218	0.7827226545
C78	0.6924058250	-1.1210484806	-0.1427032322
H79	1.7851416159	-0.3237106965	-1.8152002426
H80	-1.2387769279	2.2703683093	-0.1616936323
H81	-1.8041221390	0.5187564829	1.5230137575
H82	1.2231063386	-2.0730238572	-0.1258548409
N84	0.9437537711	2.8187705727	-2.8586978036
C85	0.6419887099	2.0403619614	-2.0506154118
N85	-0.9713912907	-2.6207992809	2.5650539084
C86	-0.6626788266	-1.8458975312	1.7565406649

**17. (DCB  $\subset$  CBPQT)<sup>+1</sup>**

-2025.204542	-2025.116319	-2025.577904	-2025.666127
H1	0.3646198645	6.5413495027	0.5873582648
H2	-0.7387615127	6.2480894473	1.9429549548
H3	-0.6371719221	4.2489253470	3.1740789282
C4	0.1721184063	3.8585226378	2.5578542477
H5	3.9883146571	0.9932068321	0.6446108425
H6	4.9088444216	-1.2089743345	1.0436294807
H7	0.3224918651	2.0686156695	3.6098898915
N8	0.6267903338	4.7248000278	1.5672432207
H9	4.9661166716	-3.2237345460	2.2190999745
C10	0.7219704431	2.6465217237	2.7779694874
C11	3.5172406188	0.3732755793	1.4048960649
C12	4.0490302030	-0.8495734674	1.6076382517
H13	3.8130889022	-3.5631761956	3.5204521030
C14	1.6467319063	4.2504665676	0.7506847843
C15	1.8178034788	2.1217874924	1.9763807228
C16	2.2392056438	3.0526092530	0.9401202093
C17	2.3840517214	0.8756695273	2.1678585772
H18	1.9614379175	4.9331049624	-0.0380979168

H19	3.0545011065	2.7974558943	0.2654975540
N20	3.5774839941	-1.7216158000	2.5819236218
C21	1.9045606711	-0.0902418571	3.1449371901
H22	1.0542282653	0.1439038524	3.7834284608
C23	2.4644724322	-1.3089203519	3.3005087678
C24	-0.2601381142	5.7779103536	1.0722116814
H25	2.0877546034	-2.0297961266	4.0253357682
C26	3.9090474075	-3.1434774721	2.5090788726
C27	-1.2950805645	5.2448649624	0.1129969737
H28	-0.1055849809	5.6103867806	-1.6477749551
C29	3.0269647776	-3.8886359231	1.5383926628
H30	-2.7395672454	4.7911554903	1.6496017914
H31	4.2586021264	-3.4581393388	-0.1807824664
H32	1.6148386677	-4.5206457335	3.0379978712
C33	-1.0311126105	5.1845085852	-1.2562229377
C34	-2.5010424969	4.7213703591	0.5868754031
C35	3.3289053391	-3.9069315090	0.1734074633
C36	1.8544168388	-4.5059104939	1.9733827265
C37	-1.9331364388	4.5824126948	-2.1279007592
C38	-3.4037404088	4.1192513254	-0.2827173692
C39	2.4590716909	-4.4962228678	-0.7370568245
C40	0.9826104244	-5.0965031155	1.0639993587
H41	-1.7067334097	4.5400829055	-3.1946190922
H42	-4.3435261360	3.7204977297	0.1036058019
H43	2.7112772961	-4.5044436733	-1.7991034403
C44	-3.1201938124	4.0285775250	-1.6473321291
H45	0.0663149061	-5.5686704115	1.4224484907
C46	1.2677464601	-5.0829091022	-0.3009666606
C47	-4.0329125406	3.2628592090	-2.5685526655
H48	-2.3606173314	2.1209472327	-4.2237664089
C49	0.2601942920	-5.5956810946	-1.2967540919
C50	-2.6801182495	1.4058045441	-3.4685904509
N51	-3.6482810059	1.8361896761	-2.6058864732

H52	-3.9844102493	3.6415315899	-3.5968903538
H53	0.5678402900	-4.0471304952	-3.3900307080
C54	-2.1559322625	0.1504927863	-3.3875801745
H55	-5.0787902123	3.3112749530	-2.2411556315
C56	-4.1034859310	0.9749240467	-1.6462614706
H57	-1.3980214577	-0.1139507790	-4.1200600860
C58	-0.2597556350	-3.6915732691	-2.7796337204
N59	-0.6225016045	-4.4941003500	-1.7338553095
H60	-4.8873223572	1.3578395073	-0.9960612894
C61	-2.5726990041	-0.7701202232	-2.3791286571
C62	-0.9025885625	-2.5189076205	-3.0393961063
C63	-3.6070031430	-0.2878673231	-1.5205266686
C64	-1.9693447023	-2.0538518643	-2.2120151234
H65	-0.5541047514	-1.9461427366	-3.8942979708
C66	-1.6766873009	-4.1154315376	-0.9511722982
H67	-4.0316564562	-0.9070042886	-0.7354635881
H68	-1.9434835828	-4.7976971237	-0.1469000637
H69	0.7394176820	-6.0072978873	-2.1934054404
C70	-2.3517117131	-2.9529291128	-1.1713402483
H71	-0.3775817162	-6.3768851071	-0.8650880130
H72	-3.1834824527	-2.7340115981	-0.5073541948
C73	1.0053796224	-0.1535943739	-1.0766691717
C74	0.3169451898	1.0639218448	-1.0810376168
C75	-0.6933798808	1.3374673157	-0.1564360934
C76	-1.0280123552	0.3751345353	0.7789936288
C77	-0.3461929671	-0.8453639962	0.7781538293
C78	0.6726132233	-1.1143562826	-0.1400772781
H79	1.7975079051	-0.3329548088	-1.8015663831
H80	-1.1975399263	2.3034678320	-0.1665535068
H81	-1.8069129709	0.5640525641	1.5156793481
H82	1.2025887749	-2.0664154998	-0.1038200917
N84	0.9436846534	2.8322994777	-2.8628547802
C85	0.6639895017	2.0472123804	-2.0538291819

N85	-1.0145285705	-2.6531175733	2.5049291517
C86	-0.7021444206	-1.8394447086	1.7367635224

**18. (DCB  $\subset$  CBPQT)<sup>+2</sup>**

	-2025.088238	-2024.873604	-2025.32141	-2025.536045
H1	0.3755917710	6.4727147835	0.5877564558	
H2	-0.7222570055	6.1570065238	1.9445979894	
H3	-0.5682048097	4.2273955528	3.1858597527	
C4	0.2343161637	3.8352937568	2.5650098355	
H5	4.0993052117	1.0364015203	0.7058811571	
H6	4.9360136823	-1.2312329690	1.0118185892	
H7	0.5367534581	2.1245500066	3.7335882456	
N8	0.5886329948	4.5998559293	1.4877360187	
H9	4.9949040591	-3.2184040992	2.1936161036	
C10	0.8642523681	2.6605426726	2.8470550833	
C11	3.6088642145	0.4044705472	1.4427097077	
C12	4.0983958371	-0.8577841038	1.5980158372	
H13	3.8532210528	-3.5413470601	3.5116527880	
C14	1.6228835049	4.1823032276	0.6983020711	
C15	1.9157424966	2.1605031181	2.0216594348	
C16	2.2914783305	3.0209787479	0.9466948506	
C17	2.5142392978	0.8802277208	2.2286143258	
H18	1.8800802617	4.8337124768	-0.1349538548	
H19	3.1024575348	2.7653310260	0.2700239417	
N20	3.5716287870	-1.7264513438	2.5161145292	
C21	2.0352028158	-0.0407344108	3.2099305589	
H22	1.2247586626	0.2192862803	3.8873271202	
C23	2.5485058005	-1.2988616502	3.3154006251	
C24	-0.2720036729	5.7155944705	1.0469354321	
H25	2.1741197105	-2.0199645106	4.0406204419	
C26	3.9402611909	-3.1564907966	2.4883231204	
C27	-1.3147117919	5.2141069313	0.0806484682	
H28	-0.1764486470	5.7153735182	-1.6799997114	
C29	3.0455221541	-3.9040147600	1.5324632077	

H30	-2.7072999023	4.6287174811	1.6250582333
H31	4.2705394583	-3.4882235682	-0.1964994129
H32	1.6415776388	-4.5233939080	3.0471748151
C33	-1.0809013995	5.2435443025	-1.2933846554
C34	-2.4929274233	4.6297550901	0.5548520312
C35	3.3379665894	-3.9234785332	0.1660620790
C36	1.8716107899	-4.5080860676	1.9809958904
C37	-1.9866202118	4.6637927966	-2.1774300552
C38	-3.3977722527	4.0513435543	-0.3276639812
C39	2.4503789174	-4.4968794213	-0.7369419365
C40	0.9817442504	-5.0815971323	1.0766656810
H41	-1.7845674725	4.6867910681	-3.2492133320
H42	-4.3146932012	3.6013060817	0.0570414168
H43	2.6939863850	-4.5075827951	-1.8006487209
C44	-3.1420934500	4.0451583658	-1.7023185404
H45	0.0628329110	-5.5419240653	1.4429423329
C46	1.2521022225	-5.0621369805	-0.2913082044
C47	-4.0549954333	3.2983711969	-2.6419422032
H48	-2.2923138372	2.1938790452	-4.2203439512
C49	0.2289917425	-5.5533071559	-1.2839685385
C50	-2.6555984191	1.4616522028	-3.5021552574
N51	-3.6783610413	1.8710759460	-2.6935534347
H52	-3.9964497997	3.6935438932	-3.6635049227
H53	0.5893296468	-3.9935133662	-3.3582204805
C54	-2.1301040117	0.2072313383	-3.4140605999
H55	-5.1026617605	3.3495597241	-2.3210133188
C56	-4.1965784713	0.9847544496	-1.7906164515
H57	-1.3240033932	-0.0371212619	-4.1009840008
C58	-0.2486396950	-3.6354524214	-2.7635562964
N59	-0.6320108967	-4.4359330721	-1.7231124247
H60	-5.0315413376	1.3444790360	-1.1929361764
C61	-2.5980119575	-0.7317930240	-2.4457247010
C62	-0.8896005747	-2.4656849113	-3.0414838627



C63	-3.6999394588	-0.2773295129	-1.6602324160
C64	-1.9828344017	-2.0059304259	-2.2467907758
H65	-0.5299344803	-1.8972865216	-3.8947518892
C66	-1.7044954582	-4.0575795946	-0.9647407238
H67	-4.1802361660	-0.9219691899	-0.9296513127
H68	-1.9855374608	-4.7375174103	-0.1629484087
H69	0.6999630024	-5.9771162057	-2.1795137044
C70	-2.3822369174	-2.9001284141	-1.2078299552
H71	-0.4224211839	-6.3220398677	-0.8503907720
H72	-3.2282261663	-2.6805336652	-0.5618434792
C73	0.9773990983	-0.1716603036	-0.9825401104
C74	0.2487009008	1.0224879538	-1.0089181012
C75	-0.7858088000	1.2720579654	-0.1015036801
C76	-1.0984566859	0.3132712086	0.8459904116
C77	-0.3714534400	-0.8813128497	0.8702564943
C78	0.6641972168	-1.1314430545	-0.0364691150
H79	1.7777097923	-0.3376919542	-1.7014432261
H80	-1.3343163697	2.2133042788	-0.1475291435
H81	-1.8982013984	0.4785361213	1.5656789020
H82	1.2137839561	-2.0727717675	0.0067689744
N84	0.8217958435	2.7975251779	-2.8041809288
C85	0.5652701252	2.0058958149	-1.9936430726
N85	-0.9618749688	-2.6844583305	2.6280184172
C86	-0.6963166006	-1.8739107119	1.8411034233

**19. (DCB  $\subset$  CBPQT)<sup>+3</sup>**

	-2024.932932	-2024.487602	-2024.929062	-2025.374392
H1	0.4201911197	6.4578832359	0.5655150344	
H2	-0.6688592640	6.1589097768	1.9369033200	
H3	-0.3849954240	4.3836427353	3.2818883092	
C4	0.3686203553	3.9419630556	2.6335919572	
H5	4.3188007871	1.1698571933	1.0336767786	
H6	5.0675767796	-1.1680624383	1.2623677308	
H7	0.7937911644	2.3130650765	3.9180709220	

N8	0.6245932172	4.5763465918	1.4732635100
H9	4.9520784193	-3.1917793431	2.2430468571
C10	1.0305377886	2.7763010161	2.9636310089
C11	3.7357370526	0.4935910681	1.6533783175
C12	4.1805703879	-0.8078873206	1.7790789737
H13	3.7882810711	-3.5209574006	3.5438370288
C14	1.5765712486	4.1163482996	0.6356506612
C15	1.9679627206	2.2307394291	2.0804156476
C16	2.2590821546	2.9527053130	0.9151233594
C17	2.5712941304	0.8995149594	2.3138477081
H18	1.7603690921	4.6960059120	-0.2666818213
H19	2.9947851611	2.6121192790	0.1903563431
N20	3.5156233773	-1.6954192373	2.5438814396
C21	1.9400360734	-0.0317215446	3.1497437186
H22	1.0443620963	0.2109707994	3.7164760069
C23	2.4288961322	-1.3160544373	3.2469272109
C24	-0.2407824398	5.7183119849	1.0303973151
H25	1.9587015149	-2.0716565578	3.8732160023
C26	3.8934786154	-3.1467905019	2.5195810924
C27	-1.2885238271	5.1993046995	0.0815987893
H28	-0.2101476444	5.7616672562	-1.7011510209
C29	3.0050476961	-3.8741560375	1.5459188383
H30	-2.6279805345	4.5590157819	1.6541623384
H31	4.2130292855	-3.3758711610	-0.1765624686
H32	1.6271839190	-4.5782968665	3.0505151131
C33	-1.0898665156	5.2589049422	-1.2968359488
C34	-2.4411884215	4.5822460235	0.5793885620
C35	3.2961999767	-3.8491189040	0.1780647046
C36	1.8526680126	-4.5248089248	1.9845307970
C37	-2.0068831111	4.6732786300	-2.1659824808
C38	-3.3557402418	4.0001099381	-0.2896788908
C39	2.4269679550	-4.4336035396	-0.7350380902
C40	0.9815389193	-5.1074923219	1.0679619800

H41	-1.8336218098	4.7206665376	-3.2418693497
H42	-4.2524512303	3.5253904468	0.1115785934
H43	2.6697318655	-4.4138544076	-1.7985149762
C44	-3.1344111660	4.0203929504	-1.6710677133
H45	0.0802085729	-5.6070398372	1.4255351020
C46	1.2492599454	-5.0501857012	-0.2988879643
C47	-4.0590926555	3.2715795639	-2.5990789757
H48	-2.3055939024	2.1752763747	-4.1924520648
C49	0.2445821528	-5.5631206841	-1.3010740726
C50	-2.6678813444	1.4376934435	-3.4782796797
N51	-3.6814999525	1.8449843869	-2.6554495583
H52	-4.0131893119	3.6684619624	-3.6204812483
H53	0.5468041756	-4.0347489362	-3.4142847015
C54	-2.1507466819	0.1783420091	-3.4078293654
H55	-5.1022664348	3.3234149855	-2.2650075881
C56	-4.2035099675	0.9496657538	-1.7616192761
H57	-1.3513466827	-0.0649932281	-4.1042243403
C58	-0.2786228741	-3.6736715083	-2.8042903967
N59	-0.6338127139	-4.4621626813	-1.7440387312
H60	-5.0380111657	1.3052085105	-1.1605888907
C61	-2.6178097396	-0.7670548926	-2.4443844384
C62	-0.9311223882	-2.5094791853	-3.0797007486
C63	-3.7108740726	-0.3158956781	-1.6440658021
C64	-2.0067078609	-2.0459245684	-2.2629822787
H65	-0.5982223499	-1.9517861273	-3.9514382729
C66	-1.7013087117	-4.0892336143	-0.9752942508
H67	-4.1974606885	-0.9680994241	-0.9238046591
H68	-1.9665331795	-4.7660809659	-0.1651768903
H69	0.7315069880	-5.9766529019	-2.1922658099
C70	-2.3910405111	-2.9386013505	-1.2166948493
H71	-0.3926375723	-6.3453943412	-0.8712424239
H72	-3.2306791527	-2.7204950659	-0.5608927631
C73	0.9575372091	-0.1721201243	-1.0681717718

C74	0.2389928709	1.0277835195	-1.0815332930
C75	-0.7909446590	1.2772475371	-0.1672627662
C76	-1.1151615230	0.3144101974	0.7728070988
C77	-0.3955857713	-0.8851838551	0.7878135750
C78	0.6374715256	-1.1324832590	-0.1238355837
H79	1.7483049500	-0.3444748186	-1.7957167424
H80	-1.3381050785	2.2204696663	-0.2099162395
H81	-1.9193762976	0.4786966961	1.4874586905
H82	1.1722769137	-2.0830437925	-0.0968930446
N84	0.8045295165	2.8896915172	-2.7877094180
C85	0.5565065119	2.0382673851	-2.0377329069
N85	-0.9162556079	-2.7058167244	2.5524623595
C86	-0.7037866118	-1.8854008202	1.7581145009

**20. (DCB  $\subset$  CBPQT)<sup>+4</sup>**

-2024.774139	-2024.022816	-2024.457727	-2025.20905
H1	0.3882341272	6.4424259058	0.5936943708
H2	-0.7042123595	6.1196885571	1.9558978195
H3	-0.3744324512	4.3687982354	3.3145651582
C4	0.3801706859	3.9323221032	2.6638490201
H5	4.3720148355	1.2063164941	1.0801826651
H6	5.1215569904	-1.1347799601	1.2739419825
H7	0.8345650197	2.3183215094	3.9570316939
N8	0.6195477404	4.5614624085	1.4965902567
H9	4.9864746808	-3.1823844597	2.1907212274
C10	1.0609671623	2.7780919140	2.9986828338
C11	3.7860469828	0.5195324123	1.6846751868
C12	4.2313583023	-0.7837767680	1.7913265037
H13	3.8480228101	-3.5206885491	3.5110936764
C14	1.5757868617	4.1107452928	0.6582283487
C15	2.0001336212	2.2396089576	2.1129224399
C16	2.2758805203	2.9580600902	0.9414099946
C17	2.6166607691	0.9131318845	2.3437308167
H18	1.7487466318	4.6893822915	-0.2471711590

H19	3.0151735745	2.6259738017	0.2169357964
N20	3.5624837190	-1.6837385286	2.5380876312
C21	1.9881864770	-0.0283449562	3.1698853897
H22	1.0934668978	0.2063458000	3.7403934697
C23	2.4770476540	-1.3137411985	3.2488403610
C24	-0.2619117162	5.6891860552	1.0516414067
H25	2.0079338839	-2.0778710969	3.8656964824
C26	3.9342128335	-3.1347091076	2.4895121829
C27	-1.2983709994	5.1613729361	0.0919414858
H28	-0.2426368416	5.7979470718	-1.6793822563
C29	3.0226641198	-3.8496134478	1.5248021514
H30	-2.6228006332	4.4588727922	1.6506677003
H31	4.1654959763	-3.2909395602	-0.2238440999
H32	1.7099067467	-4.6196240144	3.0553791930
C33	-1.1071430212	5.2626141435	-1.2851649901
C34	-2.4376037952	4.5097331526	0.5769876785
C35	3.2681499133	-3.7863385675	0.1488937234
C36	1.8973402762	-4.5319636350	1.9847215566
C37	-2.0165689538	4.6833703993	-2.1679885903
C38	-3.3443956896	3.9315892710	-0.3032951443
C39	2.3779530846	-4.3607655939	-0.7504219230
C40	1.0047302441	-5.1072903168	1.0831141756
H41	-1.8533384652	4.7738938474	-3.2424698953
H42	-4.2320675035	3.4329983727	0.0881255052
H43	2.5858881558	-4.3102773086	-1.8198185898
C44	-3.1279512089	3.9947574141	-1.6839995617
H45	0.1294503672	-5.6378013170	1.4594153564
C46	1.2265958840	-5.0080453163	-0.2893831588
C47	-4.0548007403	3.2720336498	-2.6279417067
H48	-2.1389420485	2.2340972812	-4.0333567156
C49	0.2101376137	-5.5355094466	-1.2698421216
C50	-2.5949456635	1.4634865960	-3.4146227213
N51	-3.6724657965	1.8236842548	-2.6866140918

H52	-3.9964434739	3.6597877483	-3.6508291992
H53	0.3656980055	-4.1529063558	-3.4933751149
C54	-2.0992557555	0.1798248954	-3.3525411041
H55	-5.1002065608	3.3102648509	-2.3044657969
C56	-4.3251801134	0.9144635931	-1.9367184245
H57	-1.2133456594	-0.0444668140	-3.9404696987
C58	-0.4174624106	-3.7496751720	-2.8552377898
N59	-0.6796388111	-4.4137283669	-1.7130747209
H60	-5.2111882213	1.2551898078	-1.4049019000
C61	-2.7103657593	-0.7726819624	-2.5254998523
C62	-1.1089583927	-2.5995878547	-3.1805973237
C63	-3.8713776341	-0.3874120958	-1.8466618153
C64	-2.0845414261	-2.0988148333	-2.3124540231
H65	-0.8613362791	-2.1130528956	-4.1198767917
C66	-1.6708802833	-4.0026422943	-0.8955024269
H67	-4.4461341447	-1.0786413614	-1.2368433082
H68	-1.8624925463	-4.6066637180	-0.0107734316
H69	0.6701362298	-5.9501853776	-2.1727356624
C70	-2.3844401256	-2.8567192151	-1.1724546583
H71	-0.4366130996	-6.3022246822	-0.8297231898
H72	-3.1515697069	-2.5599907574	-0.4620366894
C73	1.0268985314	-0.1786471555	-1.0063282005
C74	0.3133468170	1.0231637499	-1.0511502396
C75	-0.7430494760	1.2856526559	-0.1703233817
C76	-1.1008775263	0.3363623780	0.7709553706
C77	-0.3887874499	-0.8667468049	0.8147138117
C78	0.6695880190	-1.1280870770	-0.0638196129
H79	1.8452894583	-0.3564350360	-1.7003993047
H80	-1.2771234431	2.2353375127	-0.2290963149
H81	-1.9174605981	0.5152740188	1.4668694499
H82	1.2071171536	-2.0758863964	-0.0005856974
N84	0.9085297959	2.8611335730	-2.7712903513
C85	0.6568837510	2.0225721450	-2.0089973517

N85	-0.9938390950	-2.6903678162	2.5474464225
C86	-0.7347442116	-1.8623024687	1.7760526850

**21. (DCFB  $\subset$  CBPQT)<sup>0</sup>**

	-2422.13745	-2422.104001	-2422.683109	-2422.716558
H1	0.3379124329	6.5228443025	0.6052753614	
H2	-0.7720269488	6.2032937806	1.9494415679	
H3	-0.7811005856	4.1183389453	3.0341926426	
C4	0.0431117186	3.7493780347	2.4247437248	
H5	3.8502385841	0.9007489491	0.4314177268	
H6	4.8157560369	-1.2798599679	0.8381940046	
H7	0.2006155093	1.9475423572	3.4542355705	
N8	0.4950143281	4.6291366724	1.4491475349	
H9	5.0328429327	-3.2187490995	2.1508048470	
C10	0.6087631470	2.5416526989	2.6380565862	
C11	3.4250110856	0.2968190815	1.2313157931	
C12	3.9821659999	-0.9160202287	1.4377933205	
H13	3.9063052085	-3.5456480314	3.4792752988	
C14	1.5049888368	4.1693996968	0.6221834032	
C15	1.7134339573	2.0351483445	1.8350317614	
C16	2.1064132949	2.9697724292	0.7930923193	
C17	2.3118982426	0.7989970044	2.0253883425	
H18	1.8100860869	4.8561835403	-0.1664714035	
H19	2.9152911682	2.7267239587	0.1058990491	
N20	3.5699352752	-1.7691928938	2.4534758163	
C21	1.8836306301	-0.1569479948	3.0333202125	
H22	1.0540127227	0.0739059923	3.6995762869	
C23	2.4779921882	-1.3608910134	3.1987989116	
C24	-0.3340128701	5.7689239362	1.0396816674	
H25	2.1408961139	-2.0668407062	3.9567529784	
C26	3.9745093423	-3.1796748458	2.4449547930	
C27	-1.4045723322	5.3654128674	0.0578502411	
H28	-0.1266463101	5.5836416688	-1.6667052091	
C29	3.1196060620	-4.0070089648	1.5187696700	

H30	-2.9467339538	5.1131967353	1.5417715618
H31	4.4744778000	-3.8939778746	-0.1530907978
H32	1.5886116894	-4.3635478056	2.9963321349
C33	-1.0977853525	5.2459833672	-1.2990004075
C34	-2.6744871968	4.9841062575	0.4920580513
C35	3.4879511146	-4.2139638443	0.1891931132
C36	1.8757561597	-4.4735015950	1.9485737770
C37	-2.0028359670	4.6701528360	-2.1810789218
C38	-3.5810493066	4.4066285439	-0.3918773112
C39	2.5952505692	-4.7862645509	-0.7119323056
C40	0.9850060830	-5.0449384088	1.0493766617
H41	-1.7350824583	4.5611007168	-3.2339016977
H42	-4.5600103968	4.0835228267	-0.0312950490
H43	2.8849350389	-4.9118959470	-1.7574948935
C44	-3.2365382056	4.1992149732	-1.7278124011
H45	0.0060821807	-5.3793545068	1.3986370619
C46	1.3164180827	-5.1638437346	-0.3018101372
C47	-4.1053637417	3.3682004597	-2.6375359543
H48	-2.2821934644	2.2734277475	-4.1752267999
C49	0.2625387514	-5.5627368271	-1.3036167700
C50	-2.6028714566	1.5641417876	-3.4131848612
N51	-3.6936890810	1.9601139784	-2.6568530024
H52	-4.0608045592	3.7363247831	-3.6724914529
H53	0.7236230674	-3.8794673737	-3.2679678804
C54	-1.9951052463	0.3663290806	-3.2556665564
H55	-5.1574941962	3.4010073831	-2.3214620402
C56	-4.0845779569	1.1025188898	-1.6366023055
H57	-1.1708965394	0.1436961452	-3.9319293582
C58	-0.1126759673	-3.5266903270	-2.6652557609
N59	-0.5702664015	-4.4246428029	-1.7091109462
H60	-4.9111350648	1.4598859686	-1.0230823051
C61	-2.4078445614	-0.5982687863	-2.2486929297
C62	-0.6858685196	-2.3207216641	-2.8692893396



C63	-3.5160332833	-0.1064853044	-1.4403116445
C64	-1.8021737888	-1.8320413986	-2.0704344628
H65	-0.2703643501	-1.7108503769	-3.6698445724
C66	-1.5922393541	-3.9824671806	-0.8857999258
H67	-3.9239386723	-0.7135047600	-0.6335847474
H68	-1.9039686301	-4.6842420750	-0.1132202436
H69	0.7169336876	-5.9809980101	-2.2129142585
C70	-2.1976051906	-2.7835205364	-1.0443983649
H71	-0.4089008878	-6.3282673488	-0.8889820157
H72	-3.0159129848	-2.5560001936	-0.3632902213
C73	0.9840774697	-0.0945845507	-1.0197438309
C74	0.2601990977	1.0981580481	-1.0551780985
C75	-0.7673391950	1.2713280021	-0.1291516702
C76	-1.0597934205	0.2902465001	0.7947716945
C77	-0.3398098800	-0.9047247253	0.8269397293
C78	0.6895415495	-1.0776394224	-0.0980696581
F79	1.9685706345	-0.2943214822	-1.8816366512
F81	-1.4762690289	2.3785216837	-0.1264155436
F82	-2.0419136577	0.4917420150	1.6589117023
F84	1.3986230228	-2.1855182439	-0.1034550719
N84	0.8810674209	2.8625389826	-2.8291419467
C85	0.5818158713	2.0862062335	-2.0179748981
N85	-0.9896999251	-2.6732566044	2.5853735662
C86	-0.6723358438	-1.8943917676	1.7838466386

**22. (DCFB  $\subset$  CBPQT)<sup>+1</sup>**

	-2422.019985	-2421.936344	-2422.504023	-2422.587663
H1	0.4320535709	6.5130866380	0.4790012270	
H2	-0.6439345483	6.2637412033	1.8652739481	
H3	-0.6745122892	4.2325930570	3.0191884699	
C4	0.1126409423	3.8139654615	2.3939514372	
H5	3.9403576949	0.9085905829	0.5582157800	
H6	4.8530795874	-1.2937465617	0.9972075545	
H7	0.2799203244	2.0563984991	3.4996262698	

N8	0.5447317755	4.6295595975	1.3598379767
H9	4.9709345523	-3.2291789191	2.2974470349
C10	0.6609928751	2.6025811331	2.6389079704
C11	3.4507977245	0.2935595137	1.3107318838
C12	3.9803267806	-0.9298066590	1.5368788378
H13	3.7757267337	-3.5547858204	3.5652524077
C14	1.5372785000	4.1373528208	0.5432845738
C15	1.7237541663	2.0473064563	1.8225797759
C16	2.1278107645	2.9332484825	0.7511326906
C17	2.3010382900	0.7938123625	2.0404313149
H18	1.8410110508	4.7910098942	-0.2732139435
H19	2.9284188304	2.6562629802	0.0678692240
N20	3.4807664884	-1.7882663931	2.5035252252
C21	1.8103285668	-0.1473618522	3.0246480567
H22	0.9595181974	0.0980295056	3.6575540983
C23	2.3743049870	-1.3684536265	3.2057706308
C24	-0.2516364747	5.7954607528	0.9524292814
H25	1.9898205887	-2.0729565051	3.9418075939
C26	3.8987669948	-3.1967797431	2.5340907258
C27	-1.3631677980	5.3951317240	0.0152967522
H28	-0.1429011251	5.5670780881	-1.7557507850
C29	3.0939757852	-4.0264257217	1.5657997653
H30	-2.8554859895	5.1893653497	1.5575493511
H31	4.5077164537	-3.8625937046	-0.0532112441
H32	1.5181003616	-4.4350056821	2.9819990089
C33	-1.1029688984	5.2447488979	-1.3481976602
C34	-2.6201391778	5.0352412745	0.5026973332
C35	3.5137096102	-4.1999265725	0.2466897850
C36	1.8427347790	-4.5179122971	1.9430292115
C37	-2.0390633657	4.6516842083	-2.1847872866
C38	-3.5586677609	4.4398049424	-0.3346803886
C39	2.6587370844	-4.7565563241	-0.6994892555
C40	0.9891299052	-5.0758484729	1.0002827427

H41	-1.8064792835	4.5146561725	-3.2422476479
H42	-4.5251195807	4.1296275479	0.0671242066
H43	2.9853573914	-4.8517291401	-1.7368236069
C44	-3.2561826148	4.1974948581	-1.6743273897
H45	0.0024125491	-5.4275413079	1.3070079218
C46	1.3709434394	-5.1539708834	-0.3402242093
C47	-4.1529441432	3.3392640868	-2.5271282786
H48	-2.4919427427	2.2167319234	-4.2174340375
C49	0.3547551090	-5.5247121031	-1.3879483214
C50	-2.7364956359	1.5173862295	-3.4211613553
N51	-3.6776811989	1.9345927666	-2.5222813743
H52	-4.1672748541	3.6684667824	-3.5734664668
H53	0.8599613466	-3.7261482035	-3.2190378007
C54	-2.1518344722	0.2876281042	-3.3337350694
H55	-5.1870405685	3.3345585324	-2.1614044396
C56	-4.0390783179	1.0847218239	-1.5152750587
H57	-1.4302029205	0.0279158907	-4.1048582499
C58	-0.0343199972	-3.4445579655	-2.6666060161
N59	-0.4729313970	-4.3454791911	-1.7378960674
H60	-4.7892043728	1.4591705828	-0.8213954190
C61	-2.4892211773	-0.6292931287	-2.2925342265
C62	-0.6861596719	-2.2679026623	-2.8922774701
C63	-3.4968891547	-0.1610910504	-1.3939950663
C64	-1.8411813296	-1.8944742801	-2.1383978153
H65	-0.2688578101	-1.6122337120	-3.6524823378
C66	-1.5921768396	-4.0431157554	-1.0138969306
H67	-3.8447741718	-0.7720346189	-0.5639149081
H68	-1.9177311472	-4.7966266044	-0.3004321546
H69	0.8268719639	-5.8775475747	-2.3131018335
C70	-2.2699043893	-2.8718379065	-1.1898982656
H71	-0.3320956337	-6.3061301258	-1.0400527905
H72	-3.1635503110	-2.7229235327	-0.5883936917
C73	1.0105709570	-0.0835902366	-0.9822405537

C74	0.2797331304	1.1080250623	-1.0517689012
C75	-0.7345904866	1.2996986798	-0.1075122168
C76	-1.0339159650	0.3355857980	0.8279356037
C77	-0.3497441286	-0.8853387328	0.8517353609
C78	0.6944430090	-1.0581767920	-0.0636155914
F79	2.0066937858	-0.2933678617	-1.8292723410
F81	-1.4330399505	2.4176092219	-0.1112411350
F82	-2.0044758850	0.5615910204	1.6999340407
F84	1.3920058991	-2.1771852040	-0.0621936985
N84	0.7772320832	2.8085992280	-2.9195199511
C85	0.5568419813	2.0580912539	-2.0578820927
N85	-1.0793182661	-2.7386487141	2.4837359845
C86	-0.7268077168	-1.9008260087	1.7571097079

**23. (DCFB  $\subset$  CBPQT)<sup>+2</sup>**

	-2421.895148	-2421.684635	-2422.240488	-2422.451001
H1	0.3133394518	6.4922643592	0.7158689558	
H2	-0.8311408989	6.1236411874	2.0200604455	
H3	-0.9120291920	3.9765228920	2.9607628737	
C4	-0.0212877252	3.6736136190	2.4149346372	
H5	3.8310155678	0.9624736397	0.4258961842	
H6	4.7376977271	-1.2799813219	0.7032308080	
H7	0.1978549660	1.8669908124	3.4489781708	
N8	0.4270862996	4.5486803152	1.4666804090	
H9	5.0660118701	-3.1674685134	2.0493650195	
C10	0.6202010051	2.4967192638	2.6703898403	
C11	3.4413779631	0.3511255526	1.2378847025	
C12	3.9652385461	-0.9015451753	1.3715946885	
H13	3.9928340073	-3.4930609093	3.4238205015	
C14	1.5526779975	4.2270099063	0.7628721599	
C15	1.7775206655	2.0992268118	1.9325952093	
C16	2.2229797582	3.0563129169	0.9717009255	
C17	2.4124301387	0.8292684347	2.1089515653	
H18	1.8926173698	4.9653282682	0.0400715370	

H19	3.1253311835	2.8936538041	0.3876834639
N20	3.5599082452	-1.7508927366	2.3631765834
C21	2.0387462846	-0.0831837242	3.1433678642
H22	1.3064106812	0.1865777789	3.9019381515
C23	2.6030056270	-1.3219556230	3.2415848096
C24	-0.3823716813	5.7355031377	1.0975793141
H25	2.3300915886	-2.0183804194	4.0323530269
C26	4.0201826472	-3.1601957257	2.3792265610
C27	-1.4258317551	5.3563002162	0.0787744533
H28	-0.0850160521	5.5502547570	-1.6030717224
C29	3.1406383729	-4.0018849704	1.4916514692
H30	-3.0219970550	5.1426204429	1.5122456706
H31	4.4787171131	-3.9605216517	-0.1987595909
H32	1.6260517219	-4.2966403127	3.0032256846
C33	-1.0717829876	5.2278965857	-1.2659587217
C34	-2.7156207223	5.0036472315	0.4741698315
C35	3.4919836720	-4.2517983822	0.1654240014
C36	1.8965567973	-4.4354018946	1.9548446644
C37	-1.9550300171	4.6598103943	-2.1747650371
C38	-3.6013612572	4.4356718535	-0.4372385680
C39	2.5770865971	-4.8331579169	-0.7080759361
C40	0.9835809815	-5.0138639592	1.0828388127
H41	-1.6537380217	4.5405833028	-3.2170667722
H42	-4.5970838626	4.1341546252	-0.1083384934
H43	2.8524933067	-4.9946405409	-1.7516674693
C44	-3.2091928278	4.2107127150	-1.7564273711
H45	0.0053202310	-5.3238509075	1.4546747773
C46	1.2975510968	-5.1711527999	-0.2685925404
C47	-4.0548100158	3.3739898974	-2.6813850990
H48	-2.3347082089	2.1967086225	-4.2788670128
C49	0.2227459903	-5.5661978572	-1.2482246563
C50	-2.6375656772	1.5103531923	-3.4908662347
N51	-3.6085560382	1.9595340851	-2.6417787928

H52	-3.9787931647	3.7051848197	-3.7240221993
H53	0.7290506970	-3.8803872509	-3.1841889984
C54	-2.0943266553	0.2634348286	-3.3689998063
H55	-5.1143219213	3.3900829308	-2.3984680123
C56	-4.0492329406	1.1235909938	-1.6546156020
H57	-1.3453824480	-0.0193771605	-4.1050857993
C58	-0.1380055390	-3.5412622019	-2.6206092457
N59	-0.5778702546	-4.3784507077	-1.6344846151
H60	-4.8343715964	1.5156562675	-1.0112659446
C61	-2.5031690625	-0.6357001774	-2.3368262132
C62	-0.7604319477	-2.3578889409	-2.8917372868
C63	-3.5439532117	-0.1338248592	-1.4953924557
C64	-1.8902880170	-1.9139323576	-2.1368019537
H65	-0.3487512749	-1.7646405902	-3.7048356476
C66	-1.6763773786	-4.0117477410	-0.9098098250
H67	-3.9658038704	-0.7319258723	-0.6910607931
H68	-2.0098446299	-4.7190895222	-0.1534363069
H69	0.6415730492	-5.9901469029	-2.1689462506
C70	-2.3295752621	-2.8342439953	-1.1365551722
H71	-0.4736490992	-6.3001396588	-0.8250274740
H72	-3.2098770930	-2.6366176620	-0.5293442290
C73	0.9876568500	-0.0987650502	-1.0386510010
C74	0.2642341390	1.0925951391	-1.0672893232
C75	-0.7678619341	1.2779205484	-0.1488902147
C76	-1.0697249367	0.3032962131	0.7813593552
C77	-0.3439658624	-0.8862444464	0.8131124049
C78	0.6855515074	-1.0750806206	-0.1083944575
F79	1.9661981755	-0.3046157556	-1.8954353175
F81	-1.4712867973	2.3871395265	-0.1555317804
F82	-2.0470042070	0.5090448883	1.6393326016
F84	1.3871897142	-2.1861736206	-0.1086209025
N84	0.8835822795	2.8919702025	-2.8096547789
C85	0.5928437745	2.0911283154	-2.0223569773

N85	-0.9561545892	-2.6552438647	2.5890577228
C86	-0.6681333392	-1.8720770422	1.7827280136

**24. (DCFB  $\subset$  CBPQT)<sup>+3</sup>**

-2421.735503	-2421.295023	-2421.843062	-2422.283541
H1	0.3432770650	6.4981427619	0.7083231603
H2	-0.8019383879	6.1435590217	2.0195751968
H3	-0.9702912800	3.9503040100	2.8693657844
C4	-0.0410457041	3.6748788974	2.3749306285
H5	3.7202100454	0.9504997737	0.3763364024
H6	4.6100481020	-1.3256977514	0.6424459961
H7	0.1585664960	1.8263303304	3.3775894027
N8	0.4497546086	4.5485094408	1.4727904510
H9	5.0428236800	-3.1323884745	2.0852326062
C10	0.6139386966	2.4908830757	2.6465318670
C11	3.3837289237	0.3609897930	1.2261854561
C12	3.8940698223	-0.9149757247	1.3516940822
H13	3.9585922582	-3.4555344804	3.4551996461
C14	1.6128142024	4.2909719790	0.8420986334
C15	1.8054802187	2.1712334962	1.9780129472
C16	2.3076637181	3.1203111334	1.0787578450
C17	2.4591272088	0.8499282868	2.1617192236
H18	1.9763194919	5.0479265941	0.1503955317
H19	3.2514739839	2.9856395848	0.5564278930
N20	3.5217388048	-1.7142259404	2.3721965646
C21	2.1276106122	0.0082082862	3.2307817190
H22	1.4646157996	0.3213615565	4.0329982772
C23	2.6650490375	-1.2622189866	3.3097791368
C24	-0.3654484197	5.7566820285	1.0922546493
H25	2.4277712933	-1.9387591682	4.1279528296
C26	3.9954117422	-3.1446262041	2.4057033229
C27	-1.4047625454	5.3538510086	0.0815621411
H28	-0.0601869766	5.5094275311	-1.6035446016
C29	3.1207937353	-3.9812265702	1.5117962083

H30	-3.0056525474	5.1836166507	1.5187896511
H31	4.4784723467	-3.9500215859	-0.1658393485
H32	1.5917128841	-4.2711086191	3.0116557345
C33	-1.0490733022	5.2003919047	-1.2603332916
C34	-2.6978172266	5.0194284877	0.4851503461
C35	3.4875947058	-4.2361920016	0.1897669681
C36	1.8737779004	-4.4144617116	1.9671803525
C37	-1.9403480539	4.6314152010	-2.1605864859
C38	-3.5897086599	4.4488109096	-0.4188754212
C39	2.5807530355	-4.8206951182	-0.6896330763
C40	0.9706703648	-4.9985977626	1.0882395972
H41	-1.6419346158	4.4984969605	-3.2018405491
H42	-4.5897403278	4.1670207139	-0.0861687892
H43	2.8666961685	-4.9854987932	-1.7295658314
C44	-3.1999761064	4.2026971891	-1.7354975038
H45	-0.0105986186	-5.3061088117	1.4533476305
C46	1.2959888296	-5.1557907520	-0.2609063944
C47	-4.0610898315	3.3721136496	-2.6536772122
H48	-2.4004367871	2.1807620199	-4.3061029480
C49	0.2287048669	-5.5523520547	-1.2506985071
C50	-2.6834657050	1.4972541455	-3.5080193965
N51	-3.6204552914	1.9559878827	-2.6257961675
H52	-3.9963382275	3.7083617489	-3.6952291165
H53	0.7302787032	-3.8642560690	-3.1903395801
C54	-2.1505431004	0.2438441849	-3.4062124543
H55	-5.1166984051	3.3931350808	-2.3574331181
C56	-4.0505127789	1.1180003126	-1.6351893139
H57	-1.4345308173	-0.0502406946	-4.1699236795
C58	-0.1462825948	-3.5346405621	-2.6359837712
N59	-0.5757236453	-4.3679851472	-1.6402813999
H60	-4.8132811694	1.5165068991	-0.9688256178
C61	-2.5398906414	-0.6523208252	-2.3651259277
C62	-0.7862980465	-2.3636264354	-2.9217386733



C63	-3.5579073415	-0.1472501092	-1.4977683097
C64	-1.9238892959	-1.9307529927	-2.1725075544
H65	-0.3799121460	-1.7675827949	-3.7360651762
C66	-1.6942311422	-4.0212255164	-0.9375473083
H67	-3.9652353911	-0.7474927636	-0.6863215120
H68	-2.0291042275	-4.7335338215	-0.1862784635
H69	0.6558346018	-5.9733638184	-2.1686755652
C70	-2.3631331336	-2.8550141946	-1.1769472748
H71	-0.4664421208	-6.2903172479	-0.8329547725
H72	-3.2612829078	-2.6733628440	-0.5914081358
C73	0.9831195785	-0.1134734479	-1.0701727335
C74	0.2578504257	1.0766777627	-1.0837235854
C75	-0.7720452771	1.2504875439	-0.1602964613
C76	-1.0832818954	0.2574146830	0.7490404802
C77	-0.3483406142	-0.9272918318	0.7725855197
C78	0.6881034596	-1.0955982747	-0.1444305757
F79	1.9651286275	-0.3041732438	-1.9228530186
F81	-1.4588340914	2.3717113677	-0.1316517292
F82	-2.0678335312	0.4474231690	1.5987578550
F84	1.4153481644	-2.1911728508	-0.1344094025
N84	0.8860505458	2.9087983410	-2.7872750575
C85	0.5904963410	2.0877996898	-2.0232532366
N85	-0.9098304548	-2.7429009049	2.5188979924
C86	-0.6594081329	-1.9321255087	1.7276387937

**25. (DCFB  $\subset$  CBPQT)<sup>+4</sup>**

	-2421.571029	-2420.821188	-2421.362738	-2422.112579
H1	0.3342149756	6.4724474284	0.7041215394	
H2	-0.8018686288	6.1228679738	2.0241991573	
H3	-0.9805325441	3.9149427180	2.8654069672	
C4	-0.0447216983	3.6475521385	2.3776663094	
H5	3.7642851911	0.9526188669	0.4278487563	
H6	4.6385621867	-1.3316765625	0.6877902173	
H7	0.1607156816	1.8033897043	3.3868345863	

N8	0.4472661627	4.5255652458	1.4782030798
H9	5.0322775110	-3.1648936945	2.1051383181
C10	0.6177296686	2.4693671870	2.6575331968
C11	3.4196893639	0.3610204196	1.2735540953
C12	3.9215280098	-0.9192192766	1.3954102959
H13	3.9489966158	-3.4794441817	3.4773325277
C14	1.6259663257	4.2844852896	0.8686084546
C15	1.8291341845	2.1680415211	2.0133918340
C16	2.3352298751	3.1247412560	1.1230935238
C17	2.4926173931	0.8512237966	2.2066931491
H18	1.9906462059	5.0433041079	0.1779891740
H19	3.2942803360	3.0061460066	0.6239155210
N20	3.5366872355	-1.7218203484	2.4096729820
C21	2.1611732768	0.0119916643	3.2776558127
H22	1.5027772974	0.3284528356	4.0823523528
C23	2.6893668873	-1.2636978336	3.3527908782
C24	-0.3713869813	5.7321809751	1.0958277155
H25	2.4463349758	-1.9403481567	4.1693979085
C26	3.9865782182	-3.1596664986	2.4306910134
C27	-1.4186145282	5.3280403244	0.0918167840
H28	-0.1126961241	5.5572268155	-1.6160316019
C29	3.0936286183	-3.9770388270	1.5335944764
H30	-2.9914381946	5.0981688361	1.5541154162
H31	4.4651294276	-3.9946355818	-0.1332844214
H32	1.5516493491	-4.2294863778	3.0279034192
C33	-1.0867305777	5.2159158739	-1.2607044030
C34	-2.6976647694	4.9602154742	0.5125551353
C35	3.4657857411	-4.2544335368	0.2177978347
C36	1.8354232802	-4.3821916842	1.9853827642
C37	-1.9829071471	4.6450156604	-2.1571094421
C38	-3.5941237930	4.3875312677	-0.3844316758
C39	2.5549602027	-4.8318984172	-0.6625769422
C40	0.9261907096	-4.9579598323	1.1066056155

H41	-1.7031086052	4.5435121787	-3.2073080332
H42	-4.5816995928	4.0805932020	-0.0370837132
H43	2.8495336575	-5.0219457794	-1.6953689580
C44	-3.2223958268	4.1767228522	-1.7131555881
H45	-0.0601139064	-5.2515286561	1.4690627649
C46	1.2612388421	-5.1369732087	-0.2376678857
C47	-4.0941087077	3.3595274885	-2.6296326464
H48	-2.5222924313	2.1362532505	-4.3406277571
C49	0.2028824758	-5.5527382997	-1.2259754150
C50	-2.7842237399	1.4592609235	-3.5290554747
N51	-3.6449267613	1.9211068690	-2.5990375605
H52	-4.0325825455	3.6799089491	-3.6748647037
H53	0.8112389358	-3.7740532068	-3.0300041333
C54	-2.2680664268	0.1790888014	-3.4495199643
H55	-5.1473083123	3.3626773608	-2.3284202194
C56	-4.0513345968	1.1189555870	-1.5936228793
H57	-1.6001604428	-0.1407072464	-4.2459820132
C58	-0.1193325201	-3.4892963829	-2.5429650243
N59	-0.6120883815	-4.3488111445	-1.6260899289
H60	-4.7768699583	1.5317031462	-0.8950263650
C61	-2.6243543443	-0.6618700798	-2.3865043641
C62	-0.7737825075	-2.3096044968	-2.8367546269
C63	-3.5606500464	-0.1651893659	-1.4662374531
C64	-1.9758242102	-1.9856639295	-2.1868029181
H65	-0.3180193138	-1.6607865716	-3.5812910588
C66	-1.7869551663	-4.0901868946	-1.0176819451
H67	-3.9240706124	-0.7533345064	-0.6263631833
H68	-2.1564445882	-4.8368329283	-0.3169284651
H69	0.6230851269	-5.9656477779	-2.1493872788
C70	-2.4866035751	-2.9271686042	-1.2842030112
H71	-0.5043018792	-6.2796681409	-0.8128643058
H72	-3.4389422955	-2.7920998621	-0.7778873274
C73	1.0753783067	-0.0809154087	-1.0993876043

C74	0.3403582749	1.1033235258	-1.1328271030
C75	-0.7038754579	1.2752082681	-0.2233204602
C76	-1.0147485752	0.2948997021	0.6998824047
C77	-0.2796215070	-0.8902979242	0.7324219402
C78	0.7648248369	-1.0627704006	-0.1750831849
F79	2.0657943645	-0.2778492066	-1.9373304819
F81	-1.4120371037	2.3843814555	-0.2267031250
F82	-2.0056084512	0.4880881560	1.5396185663
F84	1.4741075257	-2.1704455328	-0.1715204480
N84	0.9248729891	2.9528616478	-2.8350504671
C85	0.6585133187	2.1209780854	-2.0719951851
N85	-0.9527198145	-2.6880671449	2.4557960518
C86	-0.6289838661	-1.8901684596	1.6788237871

**26. TTF<sup>-1</sup>**

-1823.509931	-1823.424468	-1823.602554	-1823.688017
C1	0.4690862844	0.4830358856	0.0090028766
C2	-0.4690862844	-0.4830358856	0.0090028766
S3	-2.2199777337	-0.0768679618	0.0058972894
S4	2.2199777337	0.0768679618	0.0058972894
S5	0.0115782615	2.2212230616	0.0028722871
S6	-0.0115782615	-2.2212230616	0.0028722871
C7	1.7562532898	2.7569093114	-0.0145714570
C8	-1.7562532898	-2.7569093114	-0.0145714570
C9	2.7037816322	1.8366805183	-0.0134195052
C10	-2.7037816322	-1.8366805183	-0.0134195052
H11	3.7754350782	2.0203844891	-0.0249233401
H12	-3.7754350782	-2.0203844891	-0.0249233401
H13	1.9082178713	3.8334542941	-0.0271933403
H14	-1.9082178713	-3.8334542941	-0.0271933403

**27. TTF<sup>0</sup>**

-1823.509931	-1823.424468	-1823.602554	-1823.688017
C1	0.4705030373	0.4844479389	0.0632892002
C2	-0.4705030373	-0.4844479389	0.0632892002

S3	-2.2163560130	-0.1399924834	0.0621079721
S4	2.2163560130	0.1399924834	0.0621079721
S5	0.0751932548	2.2194583631	0.0668381612
S6	-0.0751932548	-2.2194583631	0.0668381612
C7	1.7368694287	2.7466173670	-0.1767308464
C8	-1.7368694287	-2.7466173670	-0.1767308464
C9	2.6937895725	1.8169069089	-0.1797542254
C10	-2.6937895725	-1.8169069089	-0.1797542254
H11	3.7555549045	2.0177301512	-0.3034725257
H12	-3.7555549045	-2.0177301512	-0.3034725257
H13	1.9063967079	3.8143748587	-0.2961597647
H14	-1.9063967079	-3.8143748587	-0.2961597647

**28. TTF<sup>+1</sup>**

-1823.291935	-1823.216041	-1823.385364	-1823.461258
C1	0.4860196483	0.5005599952	0.0219659288
C2	-0.4860196483	-0.5005599952	0.0219659288
S3	-2.1894697306	-0.1488039058	0.0091340566
S4	2.1894697306	0.1488039058	0.0091340566
S5	0.0842592945	2.1929598997	0.0121585271
S6	-0.0842592945	-2.1929598997	0.0121585271
C7	1.7285685587	2.7444782555	-0.0333472983
C8	-1.7285685587	-2.7444782555	-0.0333472983
C9	2.6922255391	1.8086937698	-0.0346335052
C10	-2.6922255391	-1.8086937698	-0.0346335052
H11	3.7607024480	2.0088133471	-0.0654205149
H12	-3.7607024480	-2.0088133471	-0.0654205149
H13	1.8971986101	3.8184372910	-0.0621705767
H14	-1.8971986101	-3.8184372910	-0.0621705767

**29. DNP<sup>-1</sup>**

-614.5665893	-614.4762544	-614.6414593	-614.7317943
H1	-1.4098662996	-3.2449802378	-0.1689602965
C2	-1.4411961143	-1.0802449565	-0.0090212157
C3	-0.6784344449	0.1094973524	0.0341621523

C4	-0.8118882119	-2.3333758455	-0.1363803506
C5	-1.2673605605	1.4010119042	0.1625735100
H6	-2.5250197788	-1.0107287150	0.0579745214
C7	0.7563194571	0.0408093488	-0.0533544552
C8	0.5713447491	-2.4202366467	-0.2213646398
C9	-0.4945667347	2.5704771767	0.2029322715
H10	1.0482264069	-3.3942248351	-0.3189268091
H11	-0.9718395956	3.5442817108	0.3009896603
C12	1.5185456008	1.2310660243	-0.0110015498
C13	1.3448546682	-1.2511391015	-0.1807029261
C14	0.8886562023	2.4840370943	0.1163563348
O15	2.7331301463	-1.2459683220	-0.2585940951
C16	3.3769804404	-2.4858548516	-0.3897082234
H17	4.4526888088	-2.2845105800	-0.4397713689
H18	3.1820985759	-3.1490338869	0.4692246392
H19	3.0748820395	-3.0170810431	-1.3072926249
O20	-2.6551433076	1.3940189033	0.2436777945
C21	-3.3006622851	2.6330289795	0.3709392799
H22	-4.3757334669	2.4284173856	0.4212391730
H23	-3.0005065404	3.1671921835	1.2874668290
H24	-3.1066990882	3.2941903969	-0.4897582296
H25	1.4861873556	3.3959787617	0.1478488177
H26	2.6023840906	1.1622989336	-0.0786108438

### 30. DNP<sup>0</sup>

-614.5250462	-614.5133756	-614.6607499	-614.6724205
H1	-1.4152982114	-3.2055181402	-0.1652456868
C2	-1.4434888304	-1.0753110293	-0.0066831664
C3	-0.6702346812	0.1114564657	0.0361609292
C4	-0.8230831102	-2.2919162512	-0.1319286951
C5	-1.2760823027	1.4005374039	0.1635121225
H6	-2.5265490119	-1.0072475526	0.0604620322
C7	0.7476523492	0.0377875778	-0.0513793810
C8	0.5818166746	-2.3916406545	-0.2200644877

C9	-0.5045626315	2.5411415149	0.2010801451
H10	1.0407475597	-3.3725751940	-0.3194182769
H11	-0.9635751743	3.5222643569	0.2977645985
C12	1.5210439434	1.2244308828	-0.0080624502
C13	1.3532594662	-1.2510622383	-0.1812618858
C14	0.9004764024	2.4412087648	0.1154295481
O15	2.7068113513	-1.2422515569	-0.2608007113
C16	3.3746787708	-2.4832358522	-0.3937898986
H17	4.4424121640	-2.2531207569	-0.4462771788
H18	3.1844209295	-3.1341330896	0.4714108204
H19	3.0707149589	-3.0046632339	-1.3124477541
O20	-2.6295061290	1.3921690327	0.2405483417
C21	-3.2971994425	2.6343704188	0.3656172688
H22	-4.3652636950	2.4061203734	0.4182839783
H23	-2.9935613972	3.1609186986	1.2813866467
H24	-3.1056244517	3.2796785968	-0.5032626145
H25	1.4927271126	3.3550001369	0.1486619792
H26	2.6041029725	1.1561549456	-0.0729949379

### 31. DNP<sup>+1</sup>

	-614.3373078	-614.2660845	-614.4020566	-614.47328
H1	-1.4115266143	-3.2077844648	-0.1600696184	
C2	-1.4348340264	-1.0589004552	-0.0046125376	
C3	-0.6716868121	0.1103879451	0.0366324456	
C4	-0.8055298840	-2.3043558893	-0.1302997884	
C5	-1.2849309984	1.4020407951	0.1643370243	
H6	-2.5188024734	-1.0029981991	0.0617010477	
C7	0.7502476574	0.0394217768	-0.0492627135	
C8	0.5708237175	-2.4110824978	-0.2181075265	
C9	-0.4937305171	2.5616550330	0.2043013276	
H10	1.0303226922	-3.3912465804	-0.3152945806	
H11	-0.9548746921	3.5411126330	0.3002897629	
C12	1.5126737478	1.2096350434	-0.0052174309	
C13	1.3624876577	-1.2522124879	-0.1807931405	
C14	0.8829341506	2.4554899220	0.1210764862	

O15	2.6818266629	-1.2612191977	-0.2615626444
C16	3.3825194486	-2.5023426281	-0.4017715082
H17	4.4400060716	-2.2369603689	-0.4564237148
H18	3.2027126159	-3.1435595333	0.4691508384
H19	3.0802359392	-3.0138813343	-1.3234560223
O20	-2.6036331280	1.4088321970	0.2394582138
C21	-3.3083432260	2.6499592711	0.3621508637
H22	-4.3663066015	2.3837641766	0.4081503603
H23	-3.0140682735	3.1662945770	1.2833728012
H24	-3.1202523308	3.2841278196	-0.5122795123
H25	1.4888464317	3.3585850631	0.1541426899
H26	2.5967750882	1.1539165400	-0.0686079764

### 32. DCB<sup>-1</sup>

-416.5513978	-416.4630504	-416.5767337	-416.6650812
C73	1.0127155483	-0.1758076772	-1.0757235752
C74	0.3201894206	1.0775793510	-1.1055988353
C75	-0.7137231747	1.3185930402	-0.1443063939
C76	-1.0330637479	0.3718579764	0.7835766657
C77	-0.3399856568	-0.8813363607	0.8138577277
C78	0.6934581815	-1.1225847691	-0.1478789707
H79	1.7997328372	-0.3648620973	-1.8057924900
H80	-1.2438404615	2.2709139540	-0.1628839836
H81	-1.8205760458	0.5607078359	1.5131455626
H82	1.2234436661	-2.0749566062	-0.1295349271
N84	0.9245293935	2.8570060284	-2.8562576998
C85	0.6465008208	2.0433086893	-2.0534284050
N85	-0.9434276143	-2.6598846571	2.5658868153
C86	-0.6658655763	-1.8467173830	1.7623010706

### 33. DCB<sup>0</sup>

-416.4525477	-416.432225	-416.5289353	-416.549258
C73	1.0085856030	-0.1632889330	-1.0781664538
C74	0.3123503199	1.0502541386	-1.0801860236
C75	-0.7025382587	1.3192370297	-0.1553390019
C76	-1.0275239710	0.3597685801	0.7871790952
C77	-0.3314315020	-0.8538780004	0.7888627419
C78	0.6834499370	-1.1226505214	-0.1357200274



H79	1.7940685960	-0.3471746174	-1.8081095696
H80	-1.2269470528	2.2721486238	-0.1801428522
H81	-1.8123032999	0.5432952779	1.5177875956
H82	1.2084469455	-2.0752025046	-0.1107386341
N84	0.9168359103	2.8463527735	-2.8436468313
C85	0.6448796543	2.0416744181	-2.0513851141
N85	-0.9381846224	-2.6502629750	2.5510886797
C86	-0.6650648033	-1.8451262107	1.7597820562

### 34. DCB<sup>+1</sup>

-416.1784585	-416.0584171	-416.1480773	-416.2681187
C73	0.9994350127	-0.1339401602	-1.0865545105
C74	0.3144157962	1.0873205370	-1.1054361102
C75	-0.6866138401	1.3315035077	-0.1787548530
C76	-1.0174454875	0.3297245164	0.7948352346
C77	-0.3326599141	-0.8916474570	0.8138333351
C78	0.6697104225	-1.1350770329	-0.1117664193
H79	1.7891358066	-0.3431587827	-1.8072636413
H80	-1.2328557198	2.2733174650	-0.1707631298
H81	-1.8084308534	0.5392218732	1.5142869352
H82	1.2191406577	-2.0752836136	-0.1184803461
N84	0.9367323606	2.8669150330	-2.8781931567
C85	0.6526913544	2.0746651396	-2.0811476059
N85	-0.9613258463	-2.6691786212	2.5864282679
C86	-0.6733527849	-1.8785665390	1.7891779148

### 35. DCFB<sup>-1</sup>

-813.3799938	-813.3037818	-813.5329298	-813.6091418
C73	0.9953568325	-0.1275103432	-1.0162192005
C74	0.2769790716	1.1024304545	-1.0757215870
C75	-0.7751747380	1.2774652022	-0.1299620913
C76	-1.0778655334	0.3201323325	0.7852693307
C77	-0.3580318643	-0.9086032199	0.8464396954
C78	0.6926105289	-1.0850141145	-0.1008747554
F79	1.9862654330	-0.3209203290	-1.8917701909
F81	-1.4673861980	2.4203860252	-0.1633338742
F82	-2.0699266214	0.5127304275	1.6596661000
F84	1.3836530906	-2.2287043357	-0.0682183511

N84	0.8455270401	2.9102056123	-2.8001012873
C85	0.5852006451	2.0825591708	-2.0108143524
N85	-0.9283982523	-2.7115766671	2.5749533494
C86	-0.6668079110	-1.8867928505	1.7831056324

### 36. DCFB<sup>0</sup>

-813.2612647	-813.2465488	-813.4564169	-813.4711328
C73	0.9931674500	-0.1162700687	-1.0214239388
C74	0.2687746257	1.0758978921	-1.0517907974
C75	-0.7677896274	1.2826274697	-0.1412543793
C76	-1.0761575685	0.3089646553	0.7904604815
C77	-0.3508939725	-0.8826328630	0.8218360683
C78	0.6847238359	-1.0900661091	-0.0897364212
F79	1.9717955252	-0.3142005339	-1.8805092337
F81	-1.4534194216	2.4067689923	-0.1686287974
F82	-2.0549033398	0.5069026102	1.6494940555
F84	1.3697275646	-2.2145434805	-0.0631641628
N84	0.8400598278	2.8984522933	-2.7866446051
C85	0.5840313798	2.0784167581	-2.0076469690
N85	-0.9218730067	-2.7007382977	2.5614320017
C86	-0.6657651442	-1.8834765860	1.7795112524

### 37. DCFB<sup>+1</sup>

-812.9904506	-812.8813099	-813.079011	-813.1881517
C73	0.9861891007	-0.0840132467	-1.0313636532
C74	0.2798811909	1.1125802389	-1.0865880461
C75	-0.7489645722	1.2909575152	-0.1685286862
C76	-1.0665735518	0.2794342625	0.8041072593
C77	-0.3625365107	-0.9185359812	0.8570026497
C78	0.6630989985	-1.0989091103	-0.0641820335
F79	1.9509781269	-0.3278064235	-1.8425226444
F81	-1.4521046959	2.3654060655	-0.1535561671
F82	-2.0263057258	0.5263312198	1.6203989112
F84	1.3604078767	-2.1770227305	-0.0842692300
N84	0.8534195884	2.9319786985	-2.8228732125
C85	0.5962278494	2.1141949614	-2.0441487475
N85	-0.9338839309	-2.7384750731	2.5932910431
C86	-0.6784496951	-1.9204699109	1.8142291180

## E. References

- (S1) Odell, B.; Reddington, M. V.; Slawin, A. M.; Spencer, N.; Stoddart, J. F.; Williams, D. J. *Angew. Chem., Int. Ed. Eng.* **1988**, *27*, 1547–1550.
- (S2) Ashton, P. R.; Menzer, S.; Raymo, F. M.; Shimizu, G. K. H.; Stoddart, J. F.; Williams, D. *J. Chem. Commun.* **1996**, 487–490.
- (S3) Monk, P. M. S. *The Viologens: Physicochemical Properties, Synthesis and Applications of the Salts of 4,4'-Bipyridine*; Wiley: New York, 1998.
- (S4) Fulmer, G. R.; Miller, A. J. M.; Sherden, N. H.; Gottlieb, H. E.; Nudelman, A.; Stoltz, B. M.; Bercaw, J. E.; Goldberg, K. I. *Organometallics* **2010**, *29*, 2176–2179.
- (S5) Trabolsi, A.; Khashab, N.; Fahrenbach, A. C.; Friedman, D. C.; Colvin, M. T.; Cotí, K. K.; Benítez, D.; Tkatchouk, E.; Olsen, J.-C.; Belowich, M. E.; Carmielli, R.; Khatib, H. A.; Goddard, W. A., III; Wasielewski, M. R.; Stoddart, J. F. *Nature Chem.* **2010**, *2*, 42–49.
- (S6) Johnson, C. S.; Gutowsky, H. S. *J. Chem. Phys.* **1963**, *39*, 58–62.
- (S7) Gaudiello, J. G.; Ghosh, P. K.; Jones, C. C. *J. Am. Chem. Soc.* **1985**, *107*, 3027–3032.
- (S8) Thorn, A.; Dittrich, B.; Sheldrick, G. M. *Acta Cryst.* **2012**, *A68*, 448–451.
- (S9) Jaguar, version 7.0. Schrödinger, LLC. New York, NY (2007).
- (S10) Tannor, D. J.; Marten, B.; Murphy, R.; Friesner, R. A.; Sitkoff, D.; Nicholls, A.; Honig, B.; Ringnalda, M.; Goddard III, W. A. *J. Am. Chem. Soc.* **1994**, *116*, 11875–11882.