Electronic Supplementary Information

Proton Coupled Electron Transfer Across Benzimidazole Bridges in Bioinspired Proton Wires

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1. Experimental Results

1.1. Materials and Methods

NMR characterization was carried out at 25 °C using a 400 MHz Bruker spectrometer, employing standard pulse techniques. Samples were dissolved in different deuterated solvents, depending on the polarity and solubility of the corresponding compounds. Chemical shifts were measured relative to internal TMS (0.05% v/v). Mass spectra were obtained with a Voyager DE STR matrix assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectrometer in positive ion mode and *trans*, *trans*-1,4-diphenyl-1,3-butadiene was used as the matrix. All chemicals were purchased from Aldrich, Acros or Alfa Aesar. Solvents were obtained from VWR. Dichloromethane (DCM) was distilled from calcium hydride and kept over molecular sieves and potassium carbonate. Tetrahydrofuran (THF) was distilled from $LiAlH_4$ in an argon atmosphere immediately prior to use. Thin layer chromatography (TLC) was performed with silica gel coated glass plates from Merck Millipore. Column chromatography was carried out using Silicycle silica gel 60 having 230–400 mesh.

Crystal Structure Determination: Crystals of **2'** were grown by the vapor diffusion technique using DCM and hexane as solvents. In the case of **4**, crystals were grown by slow evaporation technique using anhydrous acetonitrile (ACN) as a solvent. A Bruker Smart APEX diffractometer was used to obtain single crystal diffraction data. Detailed information of crystallographic structures and data collections are provided in section 1.4.

Cyclic Voltammetry: Cyclic voltammetry measurements were performed with a Biologic potentiostat in a conventional three-electrode cell, using a glassy carbon (3 mm diameter) working electrode, a Pt wire counter electrode, and a Ag wire pseudoreference electrode. All cyclic voltammograms (CVs) were collected in anhydrous ACN kept over molecular sieves and K_2CO_3. Each compound of interest was dissolved in ACN at a concentration of 1 mM, and tetrabutylammonium hexafluorophosphate ($TBAPF_6$, 0.5 M) was used as the supporting electrolyte. All experiments were conducted at room temperature under an argon atmosphere. The argon gas stream was pre-saturated by bubbling through the organic solvent in a separate Schlenk flask and let into the electrochemical cell via PEEK tubing. The working electrode was polished between measurements with an aluminum slurry on a microcloth polishing pad, followed by solvent rinses and drying under a stream of nitrogen. The cathodic to anodic peak intensity ratios

(i_c/i_a) were determined using a previous reported method.[1] The potential of the pseudoreference electrode was determined using the ferrocenium/ferrocene redox couple as an internal standard and adjusting to the saturated calomel electrode (SCE) scale (with $E_{1/2}$ taken to be 0.40 V *vs* SCE in ACN).[2]

FTIR and Infrared Spectroelectrochemistry (IRSEC): FTIR measurements were performed using a Bruker Vertex 70 spectrometer in absorption mode under a dry nitrogen purge with a 2 cm^{-1} resolution, GloBar MIR source, broadband KBr beamsplitter, and liquid nitrogen cooled MCT detector. Spectra were collected (64 scans) in anhydrous DCM (distilled over CaH_2 and kept over molecular sieves and K_2CO_3) at a concentration of 19 mM, and 0.1 M $TBAPF_6$ was used to simulate the conditions of the IRSEC measurements. Special care was taken to manipulate the molecules bearing the imine linkage (they are susceptible to hydrolysis in presence of acid traces and moisture), thus the compounds were dried under high vacuum overnight before use. The FTIR spectra were obtained using a CaF_2 liquid transmission cell (International Crystal Laboratories, Model SL-3, path length: 0.1030 mm). IRSEC measurements were conducted using a Biologic potentiostat connected to an optically transparent thin-layer electrochemical cell (Spectroelectrochemistry Reading RT OTTLE cell) equipped with CaF_2 optical windows (pathlength 0.2 mm). The cell has a Pt mesh counter electrode, a Ag wire pseudoreference electrode, and a Pt mesh working electrode that was positioned in the light path of the IR spectrophotometer. A complete and detailed description of the spectroelectrochemical technique is described in our previous report.[3]

KIE Measurements: Electrochemical experiments were conducted out at 20 ^{0}C in a conventional three electrode cell, using a Glassy Carbon as working electrode (1 mm diameter), a Pt coil counter electrode, and an Ag wire as pseudoreference electrode. Anhydrous DCM and ACN (Sigma Aldrich) were kept over K_2CO_3 and molecular sieves. These were used as solvent containing 0.5 M $TBAPF_6$ (Sigma Aldrich electrochemical grade) as supporting electrolyte. Concentrations in the 1.5 to 4.7 mM range were used for the investigated compounds. All the CVs were corrected by ohmic effect using feedback techniques. Before processing, the CVs were corrected by substracting the baseline currents, which were obtained for each scan rate in the same experimental conditions (DCM or ACN containing only supporting electrolyte). Redox potentials were calculated as ((E_{pa}+E_{pc})/2). After each electrochemical measurement, Ferrocene was added to the solution and the potential of the pseudoreference electrode was calculated. Nicholson's

method[1,4] was used to calculate the apparent standard rate constants of electron transfer (k_{app}). The different k_{app} were determined in DCM or ACN + 2% MeOH and DCM or ACN + 2% MeOD. CVs were taken at different scan rates (between 0.25 and 200 V/s) and the difference between the potential of the anodic and cathodic peaks (ΔE_p) were calculated for each scan rate. ΔE_p is related to the dimensionless parameter ψ[1,4] which is then related to k_{app} and ν according to the following equation:

$$k_{app}=\psi\left(\frac{\pi D_O F \nu}{RT}\right)^{1/2}\left(\frac{D_R}{D_O}\right)^{\alpha/2} \quad (1)$$

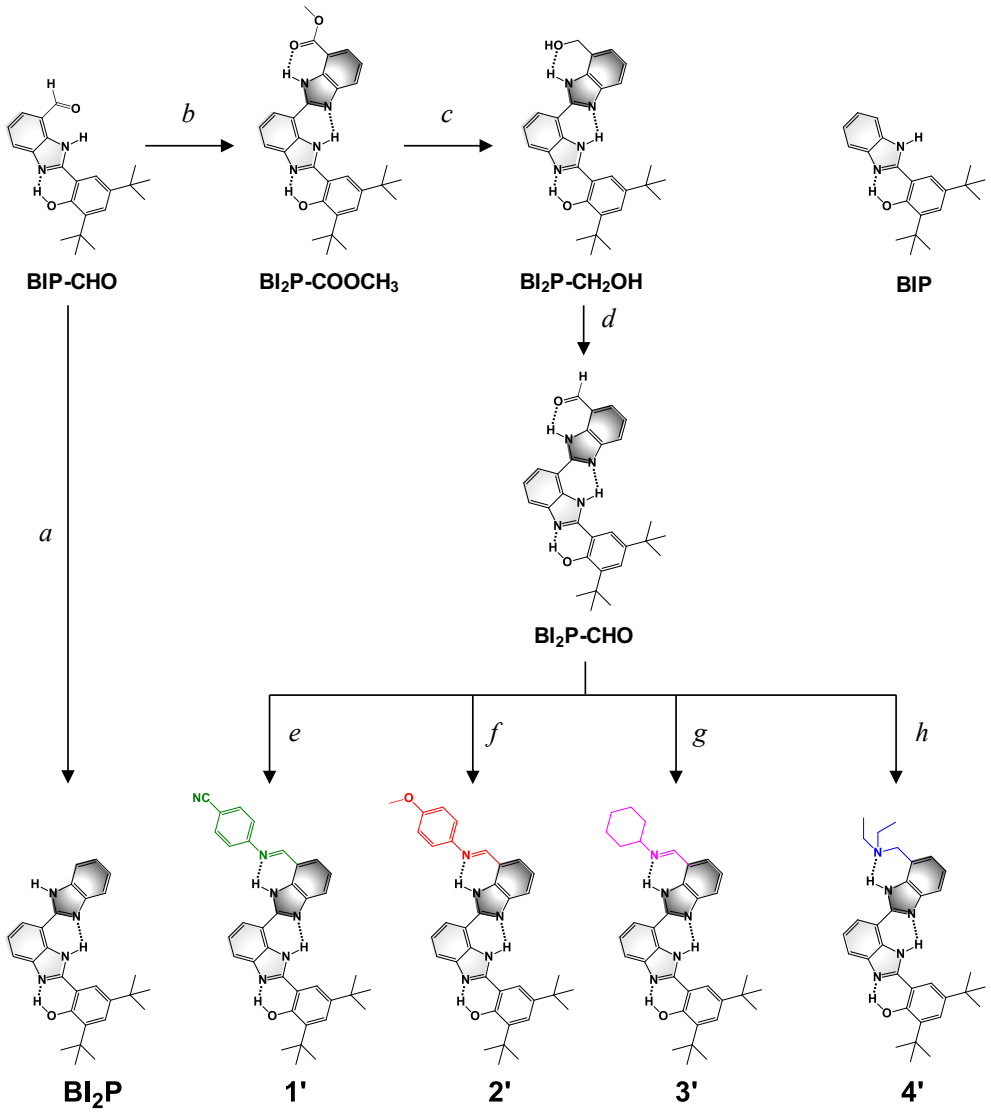
where α is the transfer coefficient (taken as 0.5), D_R and D_O are the diffusion coefficients ($cm^2\ s^{-1}$) for the oxidized and reduced forms. D_R and D_O were taken as 1×10^{-5} $cm^2\ s^{-1}$. Equation (1) can be written as follow:

$$\psi= k_{app}\left(\frac{\pi D_O F \nu}{RT}\right)^{-1/2} \quad (2)$$

k_{app} can be obtained from the slope of a plot of ψ *vs* $\nu^{-1/2}$ (Figure S14).[1,4] CVs were simulated with DigiSim 2.1 software (Figure S15 and Figure S16) using the corresponding k_{app} values shown in Table S21.

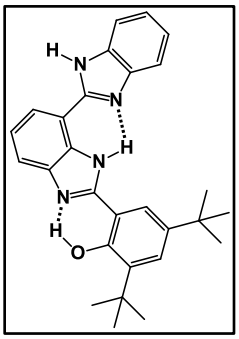
1.2. Synthesis and Structural Characterization

Scheme S1 shows the synthetic strategy for the preparation of **1'**–**4'**. Unsubstituted BI_2P was obtained by the Philipps-Ladenburg condensation reaction using BIP-CHO and *o*-phenylendiamine.[3,5] Compounds **1'**–**3'** were synthetized using the precursor BI_2P-CHO, which was obtained following a previously reported procedure,[5] and the corresponding aniline derivatives in the presence of catalytic amount of pyrrolidine (see synthetic strategy in Scheme S1).[6] Compound **4'** was prepared by reductive amination of BI_2P-CHO in presence of *N*,*N*-diethylamine.[7] The synthesis and characterization of BIP-CHO, BI_2P-$COOCH_3$, BI_2P-CH_2OH and BI_2P-CHO (see Scheme S1) were previously reported.[3,5]



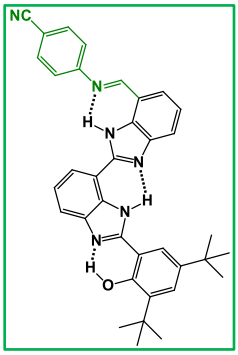
Scheme S1. Synthetic strategy for the preparation of BI_2P and compounds **1'**–**4'**. Conditions: (*a*) *o*-phenylenediamine (1 equiv.), nitrobenzene, 190 °C, overnight; (*b*) methyl 2,3-diaminobenzoate (1 equiv.), nitrobenzene, 190 °C, overnight; (*c*) excess of $LiAlH_4$, dry tetrahydrofuran, Ar, r.t; (*d*) excess of MnO_2, dry dichloromethane, Ar, r.t; (*e*, *f*, *g*) 4-aminobenzonitrile (1 equiv.), *p*-anisidine (1 equiv.) and cyclohexylamine (1 equiv.), respectively, dry dichloromethane, pyrrolidine (0.1 equiv.), 4Å molecular sieves; (*h*) *N*,*N*-diethylamine (1 equiv.), $NaBH(OAc)_3$ (2.8 equiv.), dry 1,2-dichloroethane, Ar, r.t, 18 hs. The structure of BIP is shown at the top right.

*7-(1H-Benzimidazole-2-yl)-2-(3,5-di-tert-butyl-2-hydroxyphenyl-1-yl)-1H-benzimidazole (**BI$_2$P**)*



A 5 mL solution of BIP-CHO (100 mg, 0.28 mmol) in nitrobenzene was added drop-wise to a 5 mL solution of *o*-phenylenediamine (37 mg, 0.34 mmol) in nitrobenzene. After stirring during 1 h under argon atmosphere, the mixture was refluxed overnight. The solution was cooled down to room temperature and the solvent was removed under high vacuum. The crude residue was purified by column chromatography on silica gel using DCM/MeOH (0.25–0.75%) as eluent to afford BI$_2$P (90 mg, 72%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.46 (9H, s, $C(CH_3)_3$), 1.53 (9H, s, $C(CH_3)_3$, 7.33 (1H, m, ArH), 7.34 (1H, m, ArH) 7.35 (1H, t, *J*=7.8 Hz, ArH), 7.49 (1H, d, *J*=2.2 Hz, ArH), 7.54 (1H, dd, *J*=6.1, 2.6 Hz, ArH), 7.62 (1H, d, *J*=7.5 Hz, ArH), 7.67 (1H, d, *J*=2.2 Hz, ArH), 7.81 (1H, d, *J*=8.0 Hz, ArH), 7.87 (1H, m, ArH), 9.70 (1H, s, NH), 12.14 (1H, s, NH), 13.34 (1H, s, OH). Isomers ratio, 1:0.18. ^{13}C NMR (101 MHz, $CDCl_3$): δ 156.2, 153.9, 150.1, 143.7, 142.6, 140.6, 137.7, 133.3, 132.0, 127.2, 123.8, 122.9, 122.4, 120.5, 119.6, 119.4, 118.4, 112.7, 111.1, 110.9, 35.4, 34.4, 31.6, 29.5. MALDI-TOF-MS m/z. calcd. for $C_{28}H_{30}N_4O$+(H) 439.245, experimental: 438.813.

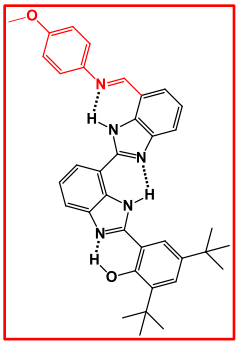
*7-(4-Cyanophenyliminomethyl-1H-benzimidazole-2-yl)-2-(3,5-di-tert-butyl-2-hydroxyphenyl-1-yl)-1H-benzimidazole (**1'**)*



Compound **1'** was synthetized following a procedure previously described.[3,5] To a solution of BI$_2$P-CHO (55 mg, 0.12 mmol) in 10 mL of dry DCM containing 4Å molecular sieves, under an argon atmosphere, an equivalent amount of 4-aminobenzonitrile (14 mg, 0.12 mmol) and pyrrolidine (1 µL, 0.016 mmol) were added. The reaction was monitored by mass spectrometry until total conversion. The crude reaction was then filtered, and the molecular sieves washed several times with dry DCM. The solvent was removed under reduced pressure and the crude solid was recrystallized from a DCM/hexanes mixture to afford **2'** (37 mg, 55%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.46 (9H, s, $C(CH_3)_3$), 1.53 (9H, s, $C(CH_3)_3$, 7.41 (2H, m, ArH), 7.42 (1H, t, *J*=7.9 Hz, ArH), 7.47 (1H, t, *J*=7.7 Hz, ArH), 7.50 (1H, d, *J*=2.3 Hz, ArH), 7.61 (1H, dd, *J*=7.6, 0.7 Hz, ArH), 7.67 (1H, d, *J*=2.3 Hz, ArH), 7.71 (1H, dd, *J*=7.6, 0.7 Hz, ArH), 7.79 (2H, m, ArH), 7.85 (1H, dd, *J*=8.0, 0.6 Hz, ArH), 8.05 (1H, d, *J*=7.8 Hz, ArH),

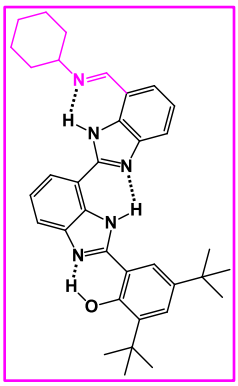
8.70 (1H, s, CH=N), 11.54 (1H, s, NH), 12.07 (1H, s, NH), 13.36 (1H, s, OH). Isomers ratio, 1:0.11. ^{13}C NMR (101 MHz, $CDCl_3$): δ 162.4, 156.2, 155.3, 153.9, 151.3, 144.4, 142.6, 140.6, 137.8, 133.6, 132.4, 132.1, 127.8, 127.2, 123.9, 122.7, 122.5, 121.9, 120.9, 119.7, 119.3, 119.0, 118.8, 112.3, 111.0, 109.8, 35.4, 34.4, 31.6, 29.5. MALDI-TOF-MS m/z. calcd. for $C_{36}H_{34}N_6O$+(H) 567.287, experimental: 567.288.

*7-(4-Methoxyphenyliminomethyl-1H-benzimidazole-2-yl)-2-(3,5-di-tert-butyl-2-hydroxyphenyl-1-yl)-1H-benzimidazole (**2'**)*



The same procedure used in the synthesis and purification of **1'** was followed, using *p*-anisidine (65%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.46 (9H, s, $C(CH_3)_3$), 1.54 (9H, s, $C(CH_3)_3$, 3.89 (3H, s, OCH_3), 7.03 (2H, m, ArH), 7.38 (2H, m, ArH) 7.43 (1H, t, *J*=7.8 Hz, ArH), 7.43 (1H, t, *J*=7.8 Hz, ArH), 7.50 (d, *J*=1.6 Hz, ArH), 7.54 (1H, d, *J*=7.2 Hz, ArH), 7.67 (1H, d, *J*=1.6 Hz, ArH), 7.67 (1H, d, *J*=2.2 Hz, ArH), 7.70 (1H, d, *J*=7.5 Hz, ArH), 7.83 (1H, d, *J*=7.9 Hz, ArH), 7.96 (1H, d, *J*=7.9 Hz, ArH), 8.74 (1H, s, CH=N), 11.83 (1H, s, NH), 12.12 (1H, s, NH), 13.40 (1H, s, OH). ^{13}C NMR (101 MHz, $CDCl_3$): δ 158.8, 157.8, 156.2, 153.8, 150.9, 144.2, 142.5, 140.5, 137.7, 132.3, 132.1, 127.1, 126.6, 122.6, 122.5, 122.4, 122.3, 120.6, 119.4, 119.0, 116.4, 114.8, 114.7, 112.6, 111.1, 55.6, 35.4, 34.4, 31.6, 29.5. MALDI-TOF-MS m/z. calcd. for $C_{36}H_{37}N_5O_2$+(H) 572.302, experimental: 572.291.

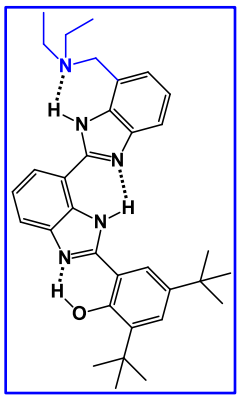
*7-(7-N-Cyclohexylimine-1H-benzimidazole-2-yl)-2-(3,5-di-tert-butyl-2-hydroxyphenyl-1-yl)-1H-benzimidazole (**3'**)*



The same procedure used in the synthesis and purification of **1'** was followed using cyclohexylamine (73%).[5] ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.46 (9H, s, $C(CH_3)_3$), 1.49 (3H, m, cy ring), 1.53 (9H, s, $C(CH_3)_3$, 1.65-1.77 (3H, m, cy ring), 1.93-1.95 (4H, m, cy ring), 3.37-3.42 (1H, m, CH-N), 7.38 (1H, t, *J*=7.6 Hz, ArH), 7.42 (1H, d, *J*=7.4 Hz, ArH), 7.44 (1H, t, *J*=7.8 Hz, ArH), 7.49 (1H, d, *J*=2.2 Hz, ArH), 7.65 (1H, d, *J*=7.4 Hz, ArH), 7.68 (1H, d, *J*=2.2 Hz, ArH), 7.84 (1H, d, *J*=8.0 Hz, ArH), 7.91 (1H, dd, *J*=7.8, 0.9 Hz, ArH), 8.58 (1H, s, CH=N), 11.90 (1H, s, NH), 12.15 (1H, s, NH) 13.42 (1H, s, OH). ^{13}C NMR (101 MHz, $CDCl_3$): δ

158.6, 156.2, 153.9, 150.8, 144.0, 142.5, 140.5, 137.7, 132.6, 132.1, 127.1, 125.4, 122.5, 122.3, 121.5, 120.6, 120.5, 119.4, 118.8, 112.8, 111.2, 69.2, 35.4, 35.0, 34.4, 31.6, 29.5, 25.7, 24.6. HRMS m/z. calcd. for $C_{35}H_{41}N_5O$+(H) 548.3384, experimental: 548.3340.[5]

*7-(7-Diethylmethyleneamine-1H-benzimidazole-2-yl)-2-(3,5-di-tert-butyl-2-hydroxyphenyl-1-yl)-1H-benzimidazole (**4'**)*



BI_2PCHO (50 mg, 0.11 mmol) and *N*,*N*-diethylamine (11 µL, 0.11 mmol) were mixed in 1,2-dichloroethane (10 mL) and stirred at room temperature under argon atmosphere for 15 minutes. The solution was then treated with $NaBH(OAc)_3$ (65 mg, 0.31 mmol) and the reaction progress was monitored by TLC until complete conversion. The reaction mixture was quenched by adding aqueous saturated $NaHCO_3$, and the product was extracted three times with 5 % MeOH/DCM. The organic extracts were combined and dried over Na_2SO_4. The solvent was evaporated, and the crude residue was purified by column chromatography on silica gel using DCM/MeOH (1–10%) as the eluent to afford **4'** (30 mg, 52 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.18 (6H, t, $NCH_2C\mathbf{H}_3$), 1.45 (9H, s, $C(CH_3)_3$), 1.53 (9H, s, $C(CH_3)_3$, 2.66 (4H, q, $NC\mathbf{H}_2CH_3$), 3.99 (2H, s, CH_2N), 7.11 (1H, d, *J*=7.2 Hz, ArH), ~7.25 (1H, t, *J*=7.8 Hz, ArH, signal under solvent peak), 7.40 (1H, t, *J*=7.8 Hz, ArH), 7.49 (1H, d, *J*=2.3 Hz, ArH), 7.57 (1H, d, *J*=7.4 Hz, ArH), 7.68 (1H, d, *J*=2.3 Hz, ArH), 7.75 (1H, d, *J*=8.0 Hz, ArH), 7.82 (1H, dd, *J*=8.0, 0.6 Hz, ArH), ~12.20 (2H, br, NH), 13.43 (1H, s, OH). ^{13}C NMR (101 MHz, $CDCl_3$): δ 156.2, 153.8, 149.5, 144.0, 142.5, 140.5, 137.7, 133.2, 132.0, 127.1, 122.5, 122.2, 120.2, 119.4, 118.4, 117.8, 113.2, 111.2, 77.1 (signal under solvent peak), 56.8, 47.1, 35.3, 34.4, 31.6, 29.5, 12.2. MALDI-TOF-MS m/z. calcd. for $C_{33}H_{41}N_5O$+(H) 524.339, experimental: 524.331.

1.3. Nuclear Magnetic Resonance Data

BI_2P

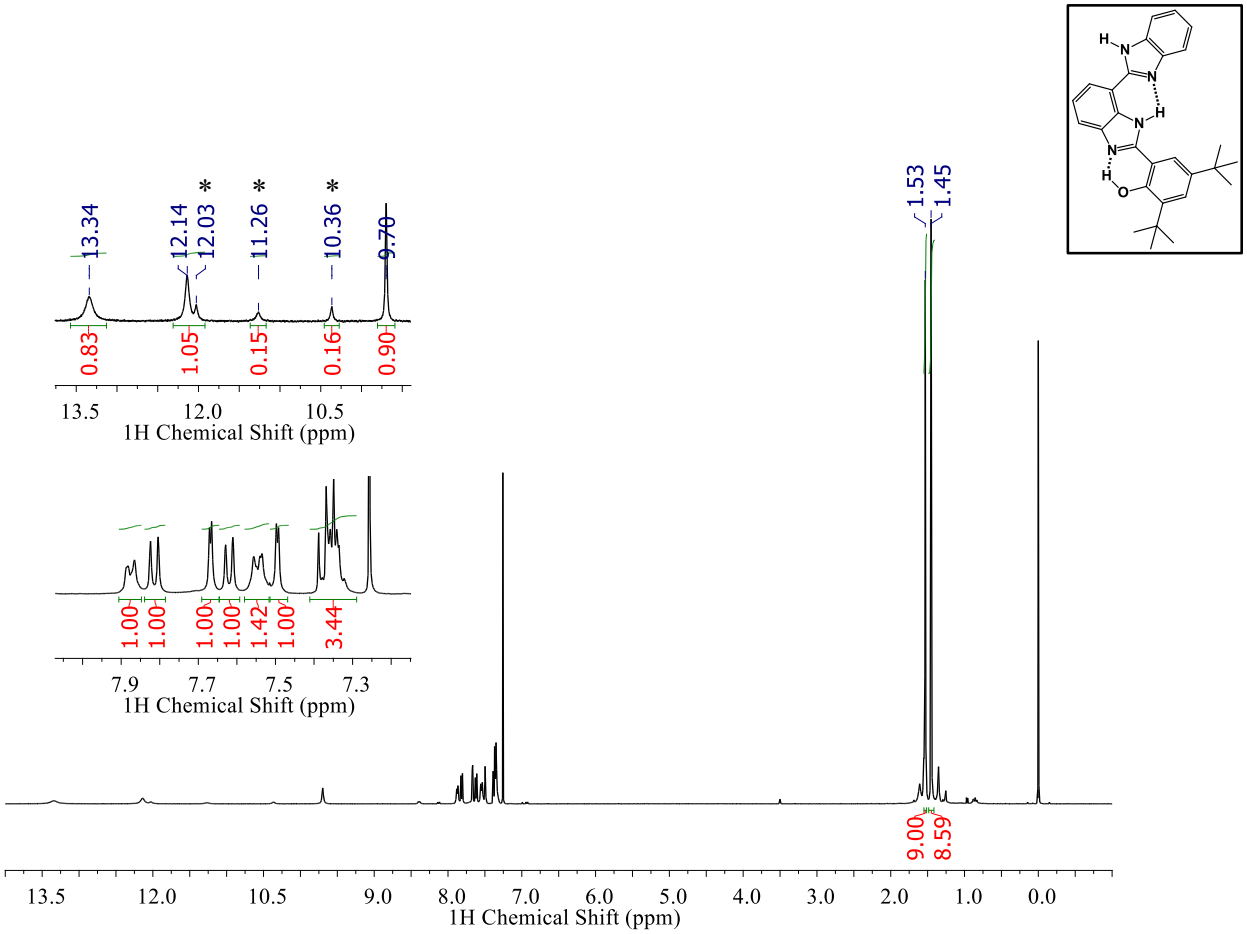


Figure S1. 400 MHz ^{1}H NMR spectrum of BI_2P in $CDCl_3$. The * denotes signals of an isomeric species (isomers ratio, 1:0.18).

BI_2P

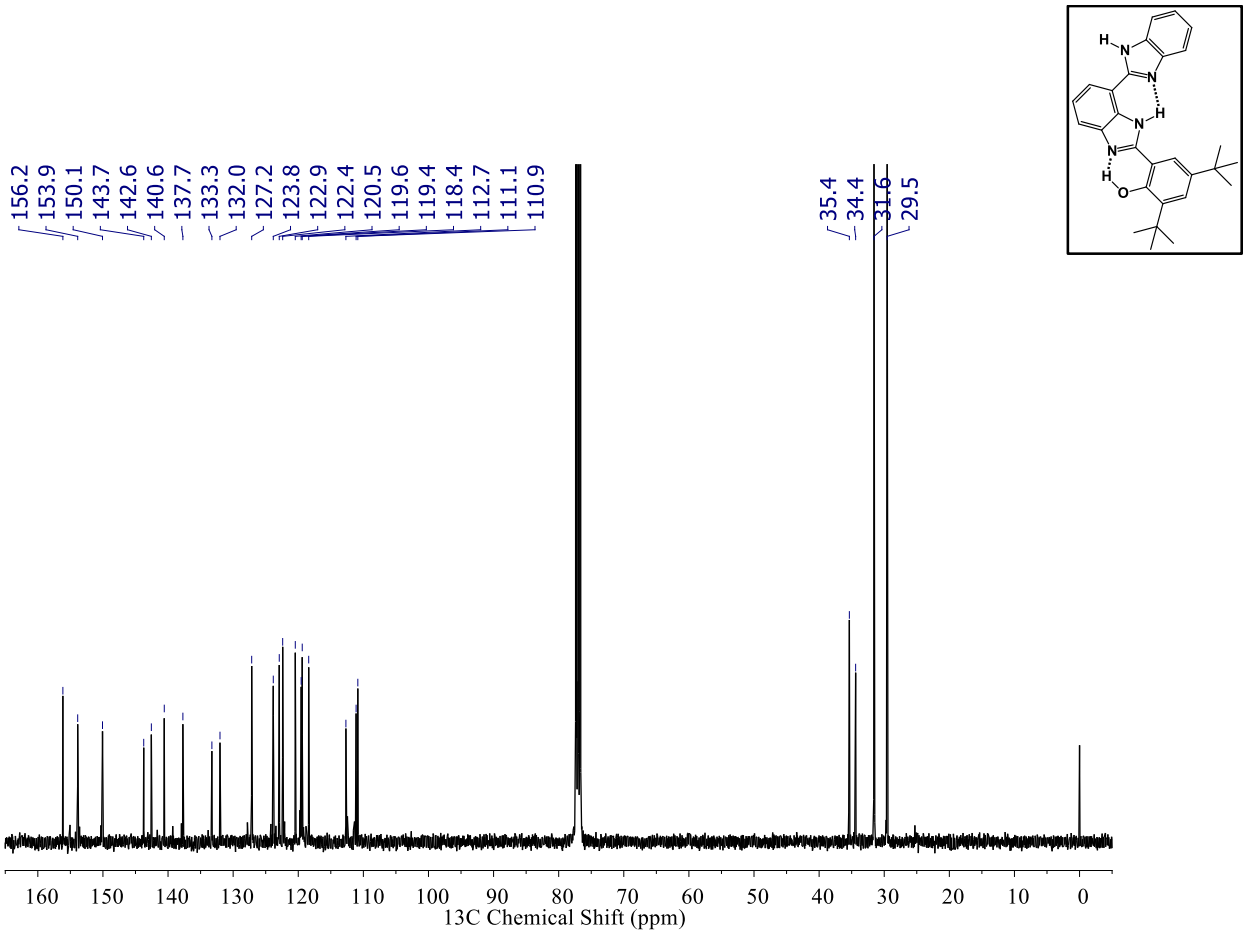


Figure S2: 101 MHz ^{13}C NMR spectrum of BI_2P in $CDCl_3$.

Compound **1'**

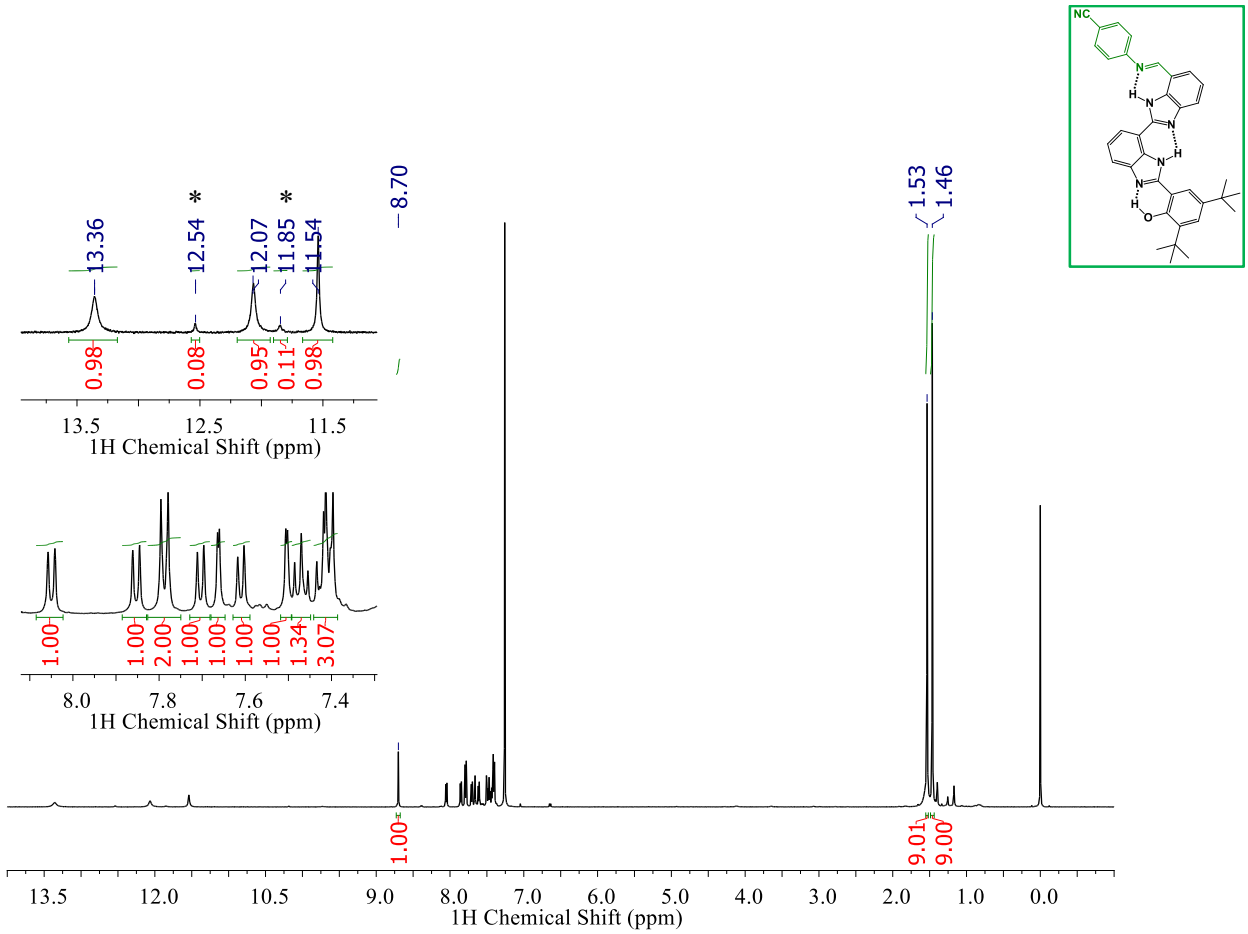


Figure S3. 400 MHz ^{1}H NMR spectrum of **1'** in $CDCl_3$. The * denotes signals of an isomeric species (isomers ratio, 1:0.11).

Compound **1'**

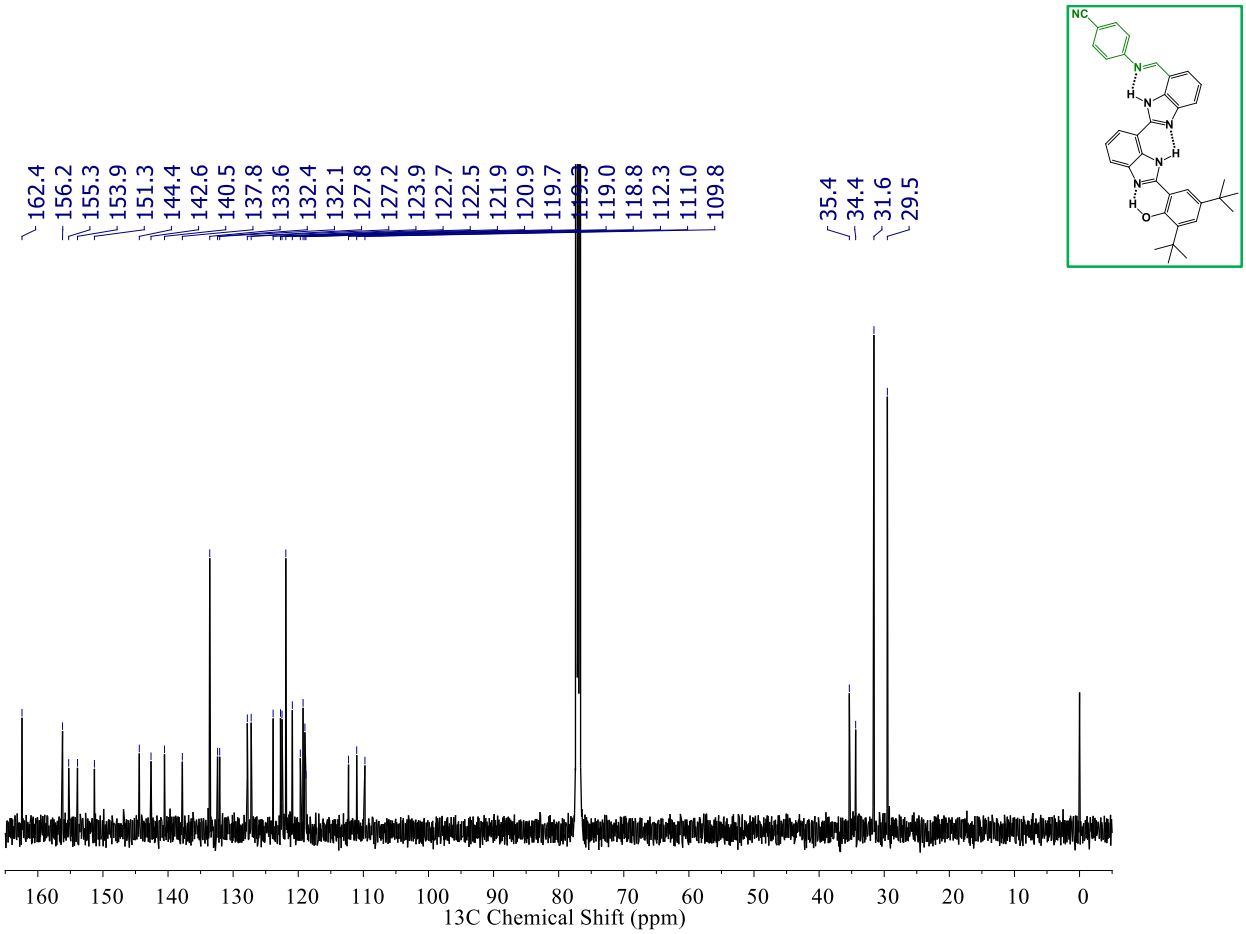


Figure S4. 101 MHz ^{13}C NMR spectrum of **1'** in $CDCl_3$.

Compound **2'**

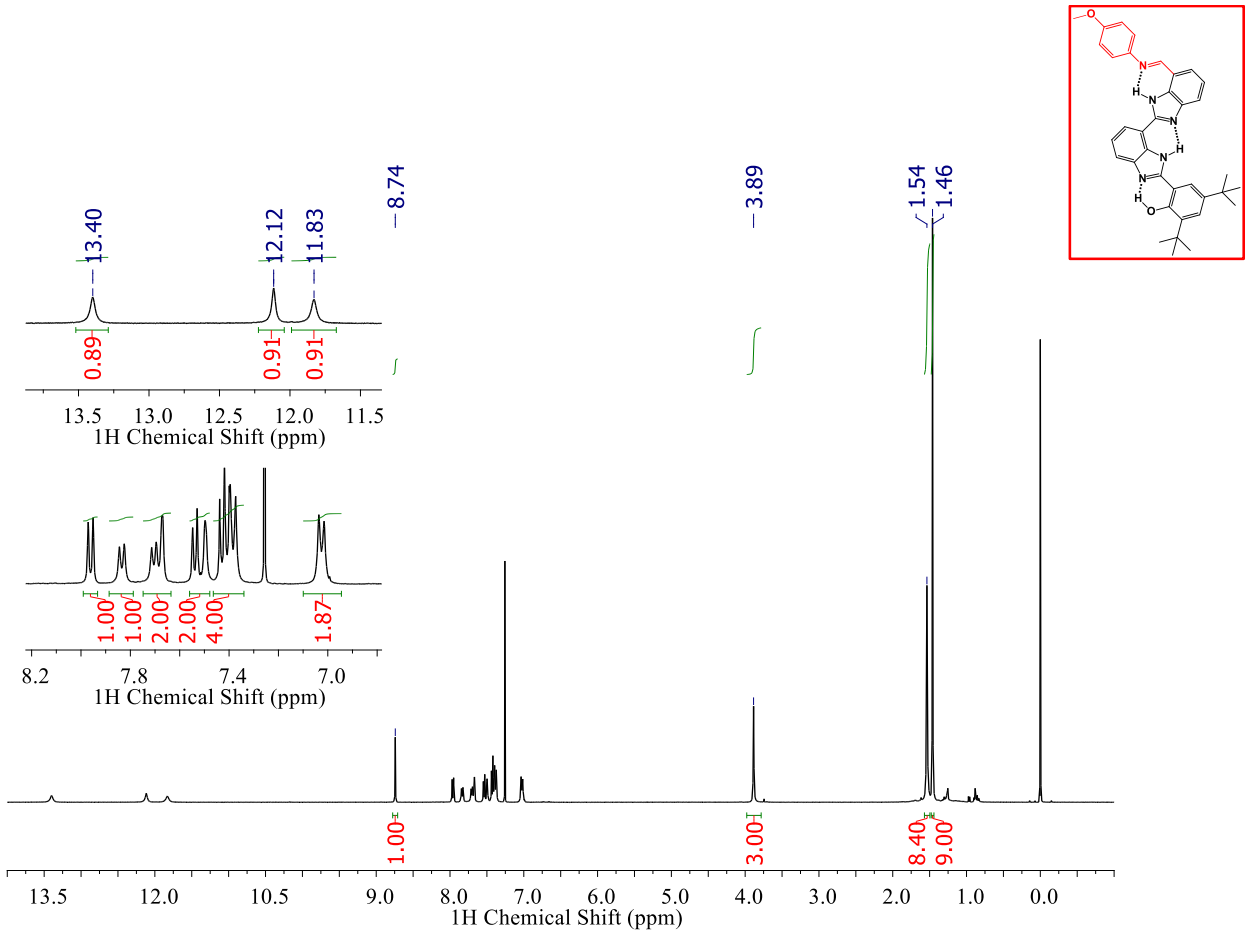


Figure S5. 400 MHz ^{1}H NMR spectrum of **2'** in $CDCl_3$.

Compound **2'**

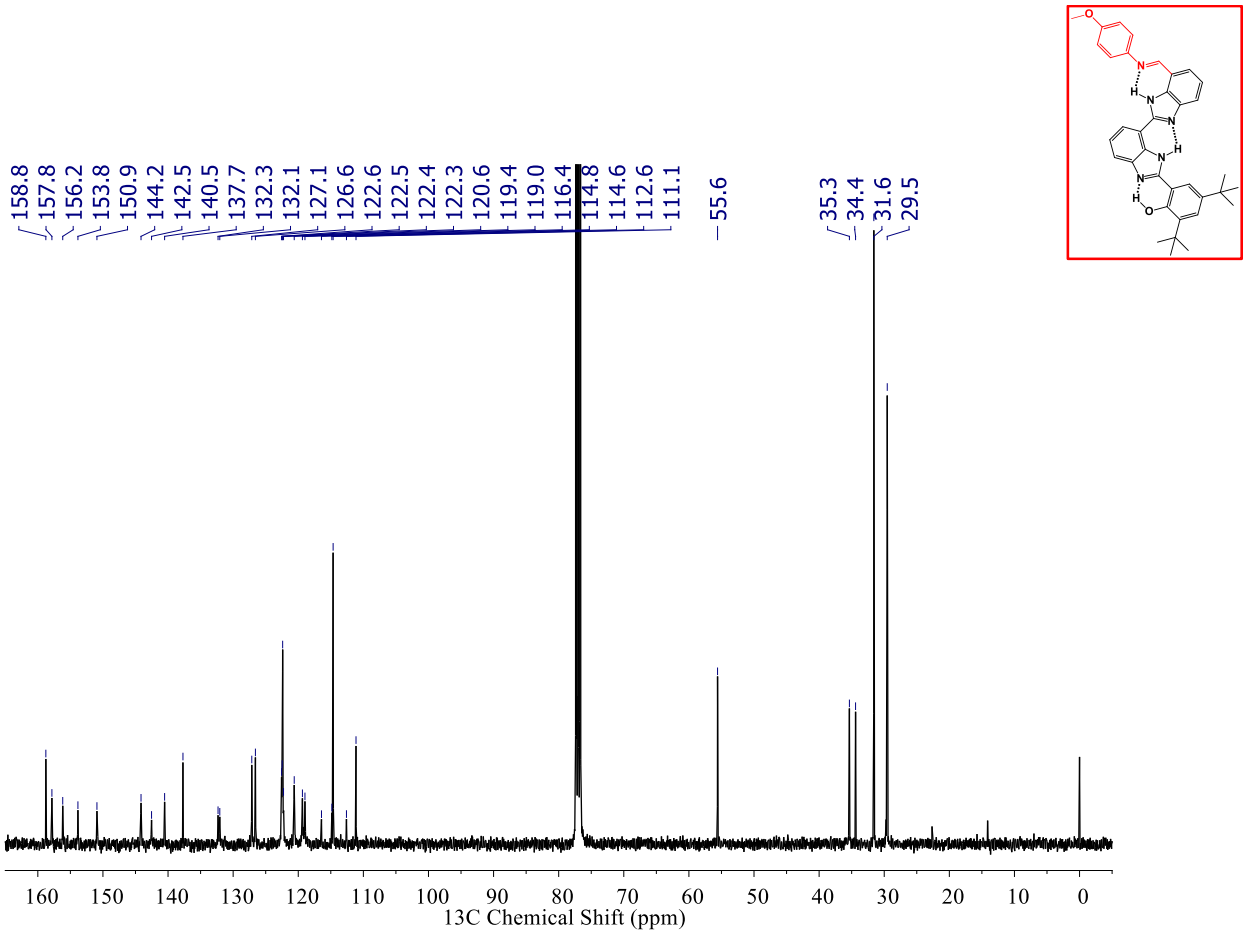


Figure S6. 101 MHz ^{13}C NMR spectrum of **2'** in $CDCl_3$.

Compound **4'**

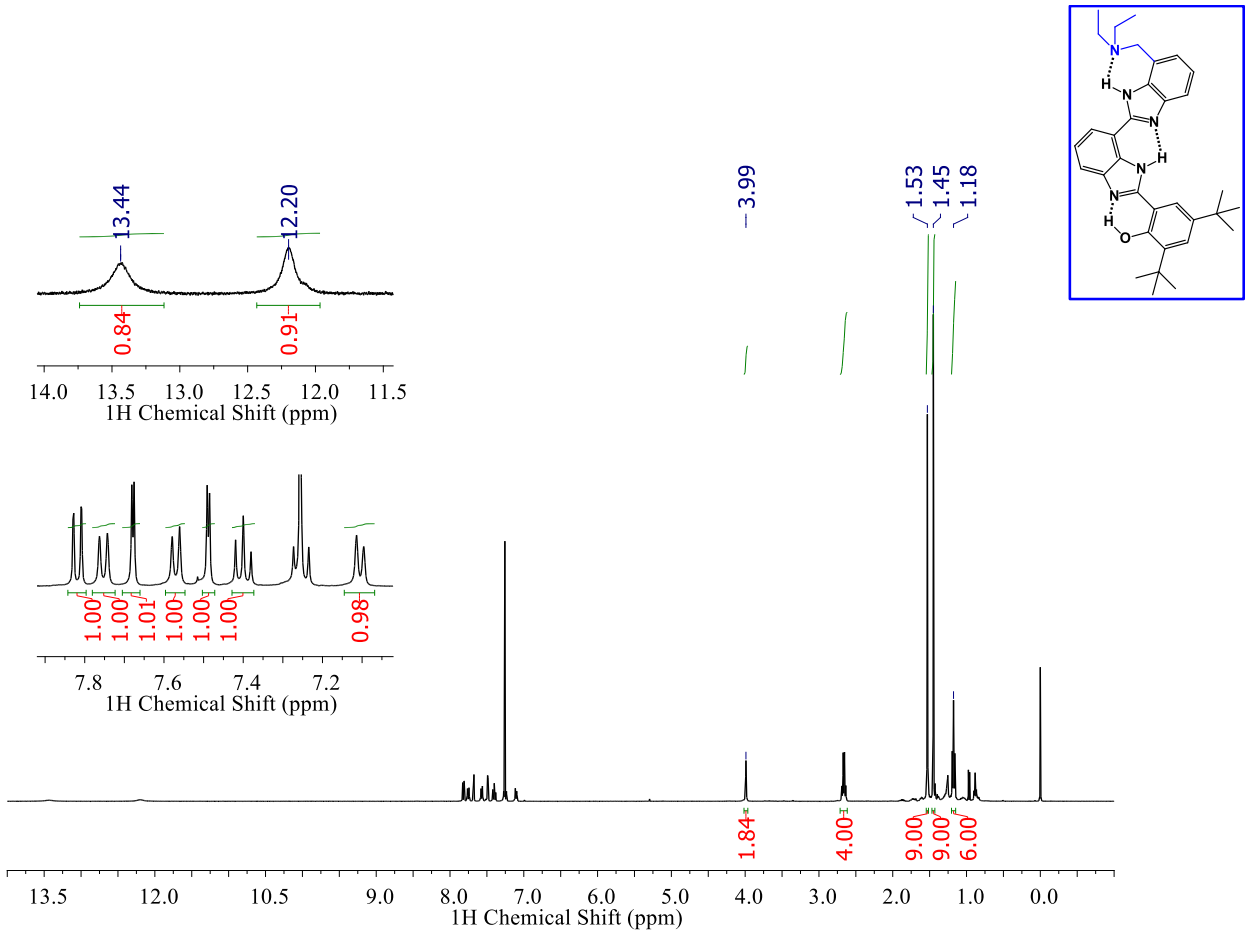


Figure S7. 400 MHz ^{1}H NMR spectrum of **4'** in $CDCl_3$.

Compound **4'**

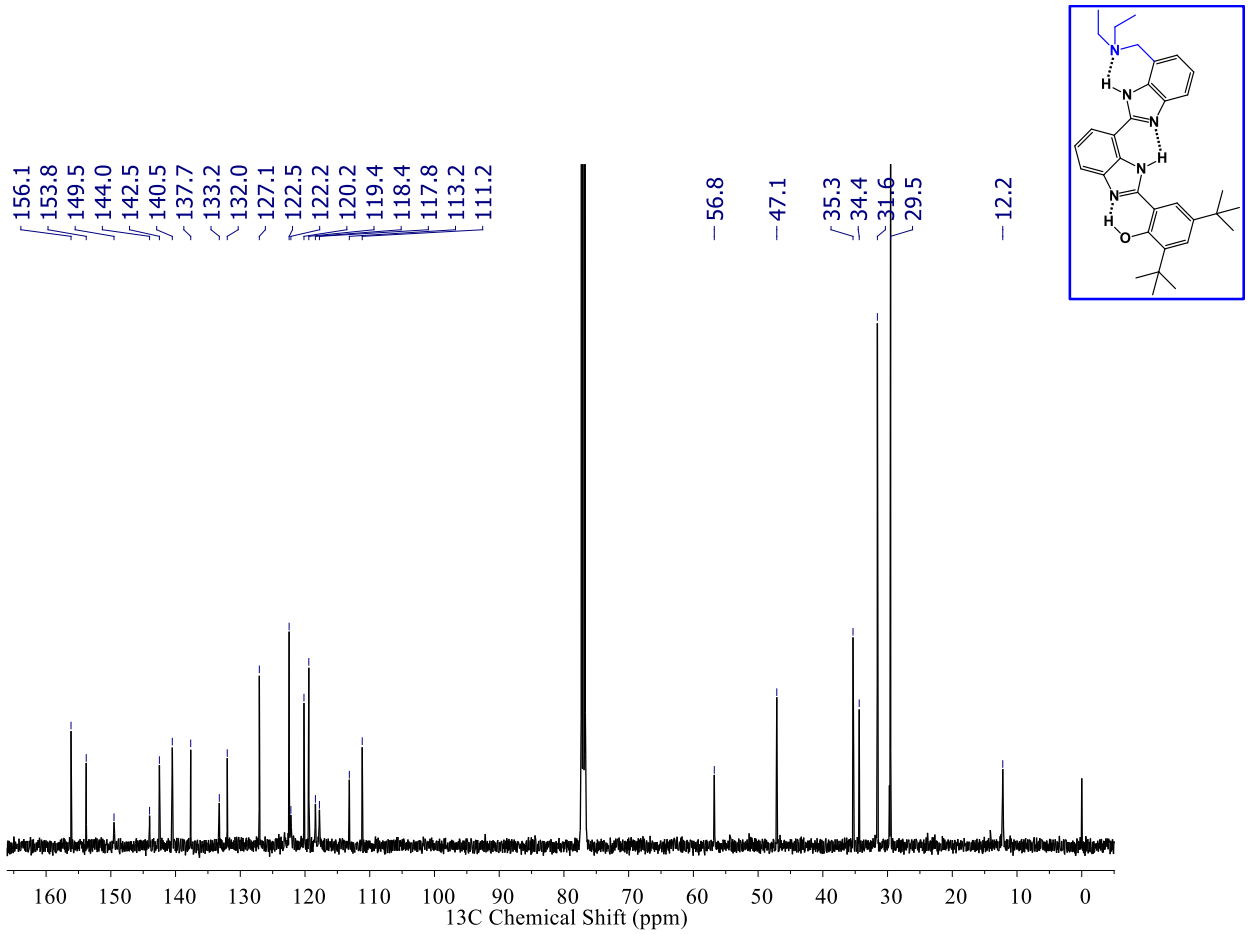


Figure S8. 101 MHz ^{13}C NMR spectrum of **4'** in $CDCl_3$.

1.4. Crystal Structure and X-Ray Data for Compounds 4 and 2'

Compound **4**

A clear pale yellow needle-like specimen of $C_{26}H_{37}N_3O$, approximate dimensions 0.253 mm x 0.264 mm x 0.468 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

Table S1. Data collection details for **4**.

Axis	dx/mm	2θ/°	ω/°	φ/°	χ/°	Width/°	Frames	Time/s	Wavelength/Å	Voltage/kV	Current/mA	Temperature/K
Omega	50.469	-34.00	-34.00	0.00	54.80	0.50	364	60.00	0.71073	50	30.0	n/a
Omega	50.469	-34.00	-34.00	120.00	54.80	0.50	364	60.00	0.71073	50	30.0	n/a
Omega	50.469	-34.00	-34.00	240.00	54.80	0.50	364	60.00	0.71073	50	30.0	n/a

A total of 1092 frames were collected. The total exposure time was 18.20 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 19785 reflections to a maximum θ angle of 25.27° (0.83 Å resolution), of which 4461 were independent (average redundancy 4.435, completeness = 100.0%, R_{int} = 3.19%, R_{sig} = 2.78%) and 3308 (74.15%) were greater than $2\sigma(F^2)$. The final cell constants of a = 9.6311(6) Å, b = 19.6619(13) Å, c = 13.5410(9) Å, β = 106.9770(10)°, volume = 2452.5(3) $Å^3$, are based upon the refinement of the XYZ-centroids of 5299 reflections above 20 σ(I) with 4.617° < 2θ < 49.93°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.862. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9690 and 0.9830. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/n 1, with Z = 4 for the formula unit, $C_{26}H_{37}N_3O$. The final anisotropic full-matrix least-squares refinement on F2 with 292 variables converged at R1 = 6.63%, for the observed data and wR2 = 20.05% for all data. The goodness-of-fit was 1.068. The largest peak in the final difference electron density synthesis was 0.466 $e^-/Å^3$ and the largest hole was -0.242 $e^-/Å^3$ with an RMS deviation of 0.058 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.104 g/cm^3 and F(000), 888 e^-.

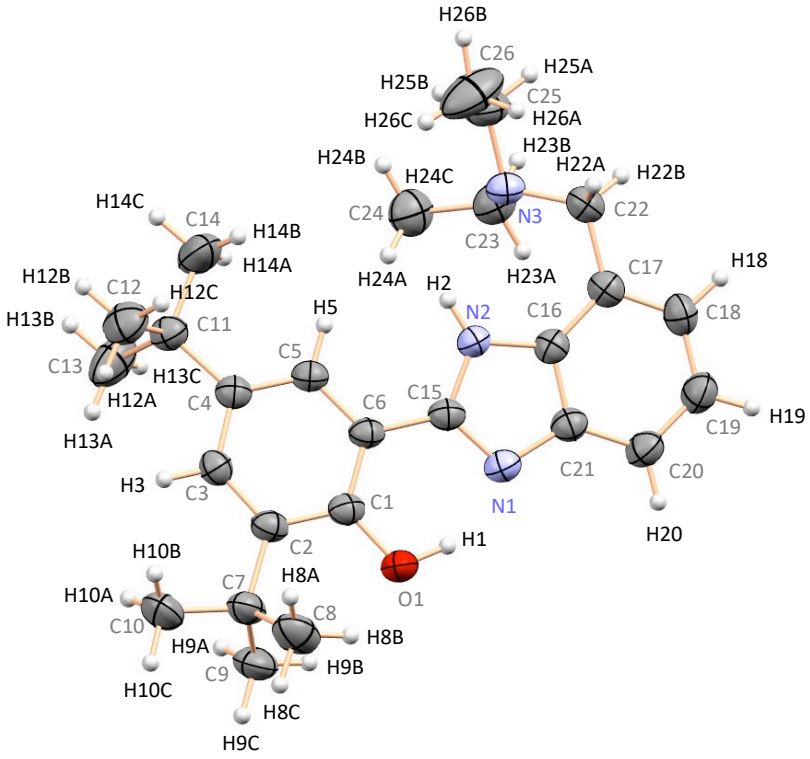


Figure S9. ORTEP representation of the crystal structure of **4**. Carbons are shown in grey, oxygens in red, nitrogens in light violet and hydrogens in white. Thermal ellipsoids are drawn at the 50% probability level.

Table S2. Sample and crystal data for **4**.

Identification code	BIP-CH_2NEt_2	
Chemical formula	$C_{26}H_{37}N_3O$	
Formula weight	407.58 g/mol	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal size	0.253 x 0.264 x 0.468 mm	
Crystal habit	clear pale yellow needle	
Crystal system	monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 9.6311(6) Å	α = 90°
	b = 19.6619(13) Å	β = 106.9770(10)°
	c = 13.5410(9) Å	γ = 90°
Volume	2452.5(3) $Å^3$	
Z	4	
Density (calculated)	1.104 g/cm^3	
Absorption coefficient	0.067 mm^{-1}	
F(000)	888	

Table S3. Data collection and structure refinement for **4**.

Theta range for data collection	1.88 to 25.27°	
Index ranges	-11<=h<=11, -23<=k<=23, -16<=l<=16	
Reflections collected	19785	
Independent reflections	4461 [R(int) = 0.0319]	
Coverage of independent reflections	100.0%	
Absorption correction	multi-scan	
Max. and min. transmission	0.9830 and 0.9690	
Structure solution technique	direct methods	
Structure solution program	SHELXTL XT-2014/4	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	4461 / 13 / 292	
Goodness-of-fit on F^2	1.068	
Δ/σ_{max}	0.001	
Final R indices	3308 data; $I>2\sigma(I)$	R1 = 0.0663, wR2 = 0.1850
	all data	R1 = 0.0831, wR2 = 0.2005
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.1334P)^2+0.1680P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.466 and -0.242 eÅ^{-3}	
R.M.S. deviation from mean	0.058 eÅ^{-3}	

Table S4. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) **4**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
O1	0.81818(14)	0.41881(8)	0.33275(11)	0.0463(4)
N1	0.71320(17)	0.51631(8)	0.41836(12)	0.0392(4)
N2	0.47826(18)	0.54182(8)	0.36188(12)	0.0355(4)
N3	0.24395(17)	0.63326(8)	0.34810(13)	0.0407(4)
C1	0.6881(2)	0.41335(10)	0.25996(15)	0.0367(5)
C2	0.6681(2)	0.36374(10)	0.18164(15)	0.0387(5)
C3	0.5374(2)	0.36357(10)	0.10444(15)	0.0383(5)
C4	0.4223(2)	0.40861(10)	0.10042(15)	0.0367(5)
C5	0.4414(2)	0.45329(9)	0.18189(15)	0.0362(5)
C6	0.57162(19)	0.45637(9)	0.26182(14)	0.0346(4)
C7	0.7900(2)	0.31275(11)	0.18130(16)	0.0463(5)
C8	0.8364(3)	0.27325(13)	0.28406(19)	0.0647(7)
C9	0.9186(2)	0.35133(13)	0.16357(19)	0.0585(7)
C10	0.7392(3)	0.25992(13)	0.0954(2)	0.0607(7)
C11	0.2864(2)	0.40753(10)	0.00775(16)	0.0432(5)
C12	0.2162(3)	0.33707(13)	0.9960(2)	0.0619(7)
C13	0.3292(3)	0.42410(17)	0.90998(19)	0.0741(8)
C14	0.1721(3)	0.45904(15)	0.0185(2)	0.0745(8)
C15	0.58904(19)	0.50400(10)	0.34647(14)	0.0356(5)
C16	0.5349(2)	0.58063(9)	0.44918(14)	0.0354(5)
C17	0.4686(2)	0.62780(10)	0.49779(16)	0.0392(5)
C18	0.5593(2)	0.65788(11)	0.58502(16)	0.0471(5)

	x/a	y/b	z/c	U(eq)
C19	0.7070(3)	0.64156(11)	0.62182(18)	0.0510(6)
C20	0.7713(2)	0.59544(11)	0.57224(17)	0.0466(5)
C21	0.6821(2)	0.56437(10)	0.48379(15)	0.0390(5)
C22	0.3074(2)	0.64173(10)	0.46020(16)	0.0423(5)
C23	0.2965(3)	0.68617(11)	0.29132(17)	0.0507(6)
C24	0.2749(3)	0.66837(15)	0.17951(18)	0.0644(7)
C25	0.0849(2)	0.63600(14)	0.3212(2)	0.0618(7)
C26	0.0201(13)	0.5726(6)	0.3473(12)	0.098(3)
C25'	0.0849(2)	0.63600(14)	0.3212(2)	0.0618(7)
C26'	0.012(6)	0.584(2)	0.368(4)	0.098(3)

Table S5. Bond lengths (Å) for **4**.

O1-C1	1.353(2)	O1-H1	0.95(3)
N1-C15	1.325(2)	N1-C21	1.387(3)
N2-C15	1.366(2)	N2-C16	1.379(2)
N2-H2	0.85(2)	N3-C25'	1.468(3)
N3-C25	1.468(3)	N3-C23	1.468(3)
N3-C22	1.471(3)	C1-C6	1.411(3)
C1-C2	1.412(3)	C2-C3	1.382(3)
C2-C7	1.545(3)	C3-C4	1.408(3)
C3-H3	0.95	C4-C5	1.380(3)
C4-C11	1.526(3)	C5-C6	1.398(3)
C5-H5	0.95	C6-C15	1.451(3)
C7-C10	1.529(3)	C7-C9	1.530(3)
C7-C8	1.541(3)	C8-H8A	0.98
C8-H8B	0.98	C8-H8C	0.98
C9-H9A	0.98	C9-H9B	0.98
C9-H9C	0.98	C10-H10A	0.98
C10-H10B	0.98	C10-H10C	0.98
C11-C12	1.529(3)	C11-C13	1.532(3)
C11-C14	1.534(3)	C12-H12A	0.98
C12-H12B	0.98	C12-H12C	0.98
C13-H13A	0.98	C13-H13B	0.98
C13-H13C	0.98	C14-H14A	0.98
C14-H14B	0.98	C14-H14C	0.98

C16-C21	1.394(3)	C16-C17	1.395(3)
C17-C18	1.381(3)	C17-C22	1.511(3)
C18-C19	1.400(3)	C18-H18	0.95
C19-C20	1.378(3)	C19-H19	0.95
C20-C21	1.395(3)	C20-H20	0.95
C22-H22A	0.99	C22-H22B	0.99
C23-C24	1.508(3)	C23-H23A	0.99
C23-H23B	0.99	C24-H24A	0.98
C24-H24B	0.98	C24-H24C	0.98
C25-C26	1.482(6)	C25-H25A	0.99
C25-H25B	0.99	C26-H26A	0.98
C26-H26B	0.98	C26-H26C	0.98
C25'-C26'	1.480(17)	C25'-H25C	0.99
C25'-H25D	0.99	C26'-H26D	0.98
C26'-H26E	0.98	C26'-H26F	0.98

Table S6. Bond angles (°) for **4**.

C1-O1-H1	109.6(17)	C15-N1-C21	106.06(16)
C15-N2-C16	107.52(16)	C15-N2-H2	126.8(14)
C16-N2-H2	125.6(14)	C25'-N3-C23	109.76(17)
C25-N3-C23	109.76(17)	C25'-N3-C22	109.92(16)
C25-N3-C22	109.92(16)	C23-N3-C22	110.94(16)
O1-C1-C6	120.74(18)	O1-C1-C2	119.74(17)
C6-C1-C2	119.52(18)	C3-C2-C1	117.65(18)
C3-C2-C7	121.44(18)	C1-C2-C7	120.89(18)
C2-C3-C4	124.14(19)	C2-C3-H3	117.9
C4-C3-H3	117.9	C5-C4-C3	116.74(18)
C5-C4-C11	123.26(17)	C3-C4-C11	119.98(18)
C4-C5-C6	121.76(18)	C4-C5-H5	119.1
C6-C5-H5	119.1	C5-C6-C1	119.89(18)
C5-C6-C15	120.66(17)	C1-C6-C15	119.45(17)
C10-C7-C9	108.15(18)	C10-C7-C8	106.8(2)
C9-C7-C8	110.93(19)	C10-C7-C2	111.61(18)
C9-C7-C2	109.23(18)	C8-C7-C2	110.14(17)
C7-C8-H8A	109.5	C7-C8-H8B	109.5
H8A-C8-H8B	109.5	C7-C8-H8C	109.5
H8A-C8-H8C	109.5	H8B-C8-H8C	109.5
C7-C9-H9A	109.5	C7-C9-H9B	109.5
H9A-C9-H9B	109.5	C7-C9-H9C	109.5
H9A-C9-H9C	109.5	H9B-C9-H9C	109.5

C7-C10-H10A	109.5	C7-C10-H10B	109.5
H10A-C10-H10B	109.5	C7-C10-H10C	109.5
H10A-C10-H10C	109.5	H10B-C10-H10C	109.5
C4-C11-C12	110.19(17)	C4-C11-C13	108.98(17)
C12-C11-C13	109.0(2)	C4-C11-C14	112.30(18)
C12-C11-C14	107.5(2)	C13-C11-C14	108.9(2)
C11-C12-H12A	109.5	C11-C12-H12B	109.5
H12A-C12-H12B	109.5	C11-C12-H12C	109.5
H12A-C12-H12C	109.5	H12B-C12-H12C	109.5
C11-C13-H13A	109.5	C11-C13-H13B	109.5
H13A-C13-H13B	109.5	C11-C13-H13C	109.5
H13A-C13-H13C	109.5	H13B-C13-H13C	109.5
C11-C14-H14A	109.5	C11-C14-H14B	109.5
H14A-C14-H14B	109.5	C11-C14-H14C	109.5
H14A-C14-H14C	109.5	H14B-C14-H14C	109.5
N1-C15-N2	111.46(17)	N1-C15-C6	124.71(17)
N2-C15-C6	123.83(17)	N2-C16-C21	105.70(17)
N2-C16-C17	130.63(18)	C21-C16-C17	123.67(18)
C18-C17-C16	115.19(19)	C18-C17-C22	122.83(19)
C16-C17-C22	121.90(18)	C17-C18-C19	122.0(2)
C17-C18-H18	119.0	C19-C18-H18	119.0
C20-C19-C18	122.1(2)	C20-C19-H19	118.9
C18-C19-H19	118.9	C19-C20-C21	117.0(2)
C19-C20-H20	121.5	C21-C20-H20	121.5

N1-C21-C16	109.26(17)	N1-C21-C20	130.77(19)
C16-C21-C20	119.97(19)	N3-C22-C17	113.80(16)
N3-C22-H22A	108.8	C17-C22-H22A	108.8
N3-C22-H22B	108.8	C17-C22-H22B	108.8
H22A-C22-H22B	107.7	N3-C23-C24	113.19(19)
N3-C23-H23A	108.9	C24-C23-H23A	108.9
N3-C23-H23B	108.9	C24-C23-H23B	108.9
H23A-C23-H23B	107.8	C23-C24-H24A	109.5
C23-C24-H24B	109.5	H24A-C24-H24B	109.5
C23-C24-H24C	109.5	H24A-C24-H24C	109.5
H24B-C24-H24C	109.5	N3-C25-C26	113.0(6)
N3-C25-H25A	109.0	C26-C25-H25A	109.0
N3-C25-H25B	109.0	C26-C25-H25B	109.0
H25A-C25-H25B	107.8	C25-C26-H26A	109.5
C25-C26-H26B	109.5	H26A-C26-H26B	109.5
C25-C26-H26C	109.5	H26A-C26-H26C	109.5
H26B-C26-H26C	109.5	N3-C25'-C26'	117.(2)
N3-C25'-H25C	107.9	C26'-C25'-H25C	107.9
N3-C25'-H25D	107.9	C26'-C25'-H25D	107.9
H25C-C25'-H25D	107.2	C25'-C26'-H26D	109.5
C25'-C26'-H26E	109.5	H26D-C26'-H26E	109.5
C25'-C26'-H26F	109.5	H26D-C26'-H26F	109.5
H26E-C26'-H26F	109.5		

Table S7. Torsion angles (°) for **4**.

O1-C1-C2-C3	-175.00(17)	C6-C1-C2-C3	5.5(3)
O1-C1-C2-C7	3.5(3)	C6-C1-C2-C7	-176.00(17)
C1-C2-C3-C4	-1.5(3)	C7-C2-C3-C4	179.97(18)
C2-C3-C4-C5	-2.9(3)	C2-C3-C4-C11	175.65(18)
C3-C4-C5-C6	3.4(3)	C11-C4-C5-C6	-175.11(17)
C4-C5-C6-C1	0.5(3)	C4-C5-C6-C15	179.80(17)
O1-C1-C6-C5	175.42(17)	C2-C1-C6-C5	-5.1(3)
O1-C1-C6-C15	-3.9(3)	C2-C1-C6-C15	175.60(17)
C3-C2-C7-C10	-6.8(3)	C1-C2-C7-C10	174.72(19)
C3-C2-C7-C9	112.7(2)	C1-C2-C7-C9	-65.7(2)
C3-C2-C7-C8	-125.2(2)	C1-C2-C7-C8	56.3(3)
C5-C4-C11-C12	-122.5(2)	C3-C4-C11-C12	59.0(2)
C5-C4-C11-C13	117.9(2)	C3-C4-C11-C13	-60.5(3)
C5-C4-C11-C14	-2.8(3)	C3-C4-C11-C14	178.8(2)
C21-N1-C15-N2	0.0(2)	C21-N1-C15-C6	-179.86(17)
C16-N2-C15-N1	-0.2(2)	C16-N2-C15-C6	179.74(16)
C5-C6-C15-N1	-171.34(17)	C1-C6-C15-N1	8.0(3)
C5-C6-C15-N2	8.8(3)	C1-C6-C15-N2	-171.89(17)
C15-N2-C16-C21	0.2(2)	C15-N2-C16-C17	179.63(19)
N2-C16-C17-C18	-179.86(19)	C21-C16-C17-C18	-0.5(3)
N2-C16-C17-C22	3.3(3)	C21-C16-C17-C22	-177.39(18)
C16-C17-C18-C19	-0.4(3)	C22-C17-C18-C19	176.5(2)
C17-C18-C19-C20	1.2(3)	C18-C19-C20-C21	-1.0(3)

C15-N1-C21-C16	0.1(2)	C15-N1-C21-C20	179.8(2)
N2-C16-C21-N1	-0.2(2)	C17-C16-C21-N1	-179.67(17)
N2-C16-C21-C20	-179.89(18)	C17-C16-C21-C20	0.6(3)
C19-C20-C21-N1	-179.5(2)	C19-C20-C21-C16	0.2(3)
C25'-N3-C22-C17	170.17(17)	C25-N3-C22-C17	170.17(17)
C23-N3-C22-C17	-68.3(2)	C18-C17-C22-N3	152.36(19)
C16-C17-C22-N3	-31.0(3)	C25'-N3-C23-C24	-76.5(2)
C25-N3-C23-C24	-76.5(2)	C22-N3-C23-C24	161.79(19)
C23-N3-C25-C26	161.6(8)	C22-N3-C25-C26	-76.2(8)
C23-N3-C25'-C26'	178.(3)	C22-N3-C25'-C26'	-60.(3)

Table S8. Anisotropic atomic displacement parameters ($Å^2$) for **4**.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.0333(8)	0.0604(10)	0.0435(9)	-0.0025(7)	0.0082(7)	0.0085(6)
N1	0.0322(9)	0.0416(10)	0.0421(10)	0.0007(7)	0.0082(7)	-0.0008(7)
N2	0.0293(9)	0.0388(9)	0.0370(9)	-0.0023(7)	0.0074(7)	0.0000(7)
N3	0.0345(9)	0.0428(10)	0.0458(10)	0.0031(8)	0.0134(8)	0.0006(7)
C1	0.0327(10)	0.0421(11)	0.0366(10)	0.0077(9)	0.0123(8)	0.0026(8)
C2	0.0370(11)	0.0434(12)	0.0389(11)	0.0065(9)	0.0161(9)	0.0068(8)
C3	0.0419(11)	0.0380(11)	0.0369(11)	0.0002(8)	0.0144(9)	-0.0001(8)
C4	0.0362(11)	0.0360(10)	0.0394(11)	0.0031(8)	0.0135(9)	-0.0012(8)
C5	0.0320(10)	0.0364(10)	0.0416(11)	0.0029(8)	0.0130(8)	0.0015(8)
C6	0.0307(10)	0.0378(10)	0.0372(10)	0.0049(8)	0.0130(8)	0.0019(8)
C7	0.0424(12)	0.0539(13)	0.0442(12)	0.0036(10)	0.0150(10)	0.0152(10)
C8	0.0732(17)	0.0648(16)	0.0590(15)	0.0143(12)	0.0237(13)	0.0310(13)
C9	0.0429(13)	0.0751(17)	0.0628(15)	-0.0003(12)	0.0235(11)	0.0146(11)
C10	0.0604(15)	0.0593(15)	0.0640(15)	-0.0084(12)	0.0205(12)	0.0185(12)
C11	0.0378(11)	0.0426(12)	0.0474(12)	0.0004(9)	0.0097(9)	-0.0010(9)
C12	0.0515(14)	0.0616(15)	0.0690(17)	-0.0039(13)	0.0121(12)	-0.0114(12)
C13	0.0638(17)	0.102(2)	0.0478(15)	0.0190(14)	0.0031(12)	-0.0162(15)
C14	0.0542(15)	0.0771(19)	0.0744(18)	-0.0134(14)	-0.0090(13)	0.0160(13)
C15	0.0330(10)	0.0353(10)	0.0399(11)	0.0053(8)	0.0129(8)	0.0001(8)
C16	0.0362(10)	0.0342(10)	0.0361(10)	0.0024(8)	0.0112(8)	-0.0044(8)
C17	0.0425(12)	0.0346(11)	0.0421(11)	0.0022(8)	0.0149(9)	-0.0001(8)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C18	0.0573(14)	0.0413(12)	0.0433(12)	-0.0060(9)	0.0157(10)	-0.0005(10)
C19	0.0500(13)	0.0513(13)	0.0459(13)	-0.0067(10)	0.0048(10)	-0.0051(10)
C20	0.0385(11)	0.0473(13)	0.0491(13)	-0.0018(10)	0.0052(10)	-0.0033(9)
C21	0.0360(11)	0.0393(11)	0.0419(11)	0.0018(9)	0.0118(9)	-0.0026(8)
C22	0.0448(12)	0.0399(11)	0.0454(12)	0.0008(9)	0.0183(10)	0.0034(9)
C23	0.0533(13)	0.0470(13)	0.0509(13)	0.0097(10)	0.0139(10)	0.0006(10)
C24	0.0688(17)	0.0735(17)	0.0530(15)	0.0104(13)	0.0209(12)	0.0001(13)
C25	0.0394(13)	0.0828(19)	0.0635(16)	0.0084(13)	0.0157(11)	0.0043(11)
C26	0.052(2)	0.138(5)	0.093(6)	0.039(4)	0.006(3)	-0.025(3)
C25'	0.0394(13)	0.0828(19)	0.0635(16)	0.0084(13)	0.0157(11)	0.0043(11)
C26'	0.052(2)	0.138(5)	0.093(6)	0.039(4)	0.006(3)	-0.025(3)

Table S9. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for **4**.

	x/a	y/b	z/c	U(eq)
H1	0.815(3)	0.4550(14)	0.378(2)	0.076(8)
H2	0.390(2)	0.5415(10)	0.3253(16)	0.039(6)
H3	0.5244	0.3310	0.0507	0.046
H5	0.3640	0.4827	0.1837	0.043
H8A	0.8755	0.3051	0.3411	0.097
H8B	0.9111	0.2399	0.2820	0.097
H8C	0.7520	0.2497	0.2944	0.097
H9A	0.8879	0.3741	0.0963	0.088
H9B	0.9971	0.3193	0.1650	0.088
H9C	0.9532	0.3854	0.2181	0.088
H10A	0.6532	0.2364	0.1030	0.091
H10B	0.8169	0.2268	0.1000	0.091
H10C	0.7149	0.2827	0.0281	0.091
H12A	0.2864	0.3029	-0.0119	0.093
H12B	0.1311	0.3365	-0.0651	0.093
H12C	0.1861	0.3266	0.0575	0.093
H13A	0.3708	0.4699	-0.0843	0.111
H13B	0.2430	0.4219	-0.1502	0.111
H13C	0.4012	0.3910	-0.0981	0.111
H14A	0.1480	0.4504	0.0829	0.112
H14B	0.0845	0.4544	-0.0401	0.112
H14C	0.2108	0.5052	0.0197	0.112
H18	0.5204	0.6906	0.6212	0.057

	x/a	y/b	z/c	U(eq)
H19	0.7648	0.6630	0.6829	0.061
H20	0.8720	0.5853	0.5972	0.056
H22A	0.2574	0.6106	0.4961	0.051
H22B	0.2895	0.6888	0.4792	0.051
H23A	0.4012	0.6938	0.3253	0.061
H23B	0.2448	0.7292	0.2950	0.061
H24A	0.3270	0.6262	0.1752	0.097
H24B	0.3125	0.7053	0.1459	0.097
H24C	0.1711	0.6621	0.1448	0.097
H25A	0.0450	0.6447	0.2462	0.074
H25B	0.0565	0.6745	0.3582	0.074
H26A	0.0392	0.5350	0.3055	0.147
H26B	-0.0849	0.5786	0.3329	0.147
H26C	0.0632	0.5623	0.4207	0.147
H25C	0.0458	0.6320	0.2452	0.074
H25D	0.0574	0.6815	0.3406	0.074
H26D	0.0655	0.5414	0.3758	0.147
H26E	-0.0875	0.5774	0.3237	0.147
H26F	0.0091	0.6002	0.4363	0.147

Table S10. Hydrogen bond distances (Å) and angles (°) for **4**.

	Donor-H	**Acceptor-H**	**Donor-Acceptor**	**Angle**
N2-H2···N3	0.85(2)	2.36(2)	2.848(2)	116.8(17)
O1-H1···N1	0.95(3)	1.74(3)	2.593(2)	148.(3)

Compound **2'**

A clear pale yellow long thin plate-like specimen of $C_{73}H_{76}Cl_2N_{10}O_4$, approximate dimensions 0.063 mm x 0.199 mm x 0.514 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

Table S11. Data collection details for **2'**.

Axis	dx/mm	2θ/°	ω/°	φ/°	χ/°	Width/°	Frames	Time/s	Wavelength/Å	Voltage/kV	Current/mA	Temperature/K
Omega	50.518	-34.00	-34.00	0.00	54.80	0.50	364	120.00	0.71073	50	30.0	n/a
Omega	50.518	-34.00	-34.00	120.00	54.80	0.50	364	120.00	0.71073	50	30.0	n/a
Omega	50.518	-34.00	-34.00	240.00	54.80	0.50	364	120.00	0.71073	50	30.0	n/a

A total of 1092 frames were collected. The total exposure time was 36.40 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 27063 reflections to a maximum θ angle of 25.38° (0.83 Å resolution), of which 6369 were independent (average redundancy 4.249, completeness = 99.8%, R_{int} = 5.87%, R_{sig} = 7.32%) and 4424 (69.46%) were greater than $2\sigma(F^2)$. The final cell constants of a = 33.136(4) Å, b = 6.8671(8) Å, c = 30.967(4) Å, β = 100.031(2)°, volume = 6938.8(14) $Å^3$, are based upon the refinement of the XYZ-centroids of 3568 reflections above 20 σ(I) with 4.993° < 2θ < 49.83°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.830. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9280 and 0.9910. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group C 1 2/c 1, with Z = 4 for the formula unit, $C_{73}H_{76}Cl_2N_{10}O_4$. The final anisotropic full-matrix least-squares refinement on F^2 with 410 variables converged at R1 = 6.67%, for the observed data and wR2 = 16.07% for all data. The

goodness-of-fit was 1.054. The largest peak in the final difference electron density synthesis was 0.318 $e^-/Å^3$ and the largest hole was -0.262 $e^-/Å^3$ with an RMS deviation of 0.057 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.176 g/cm^3 and F(000), 2600 e^-.

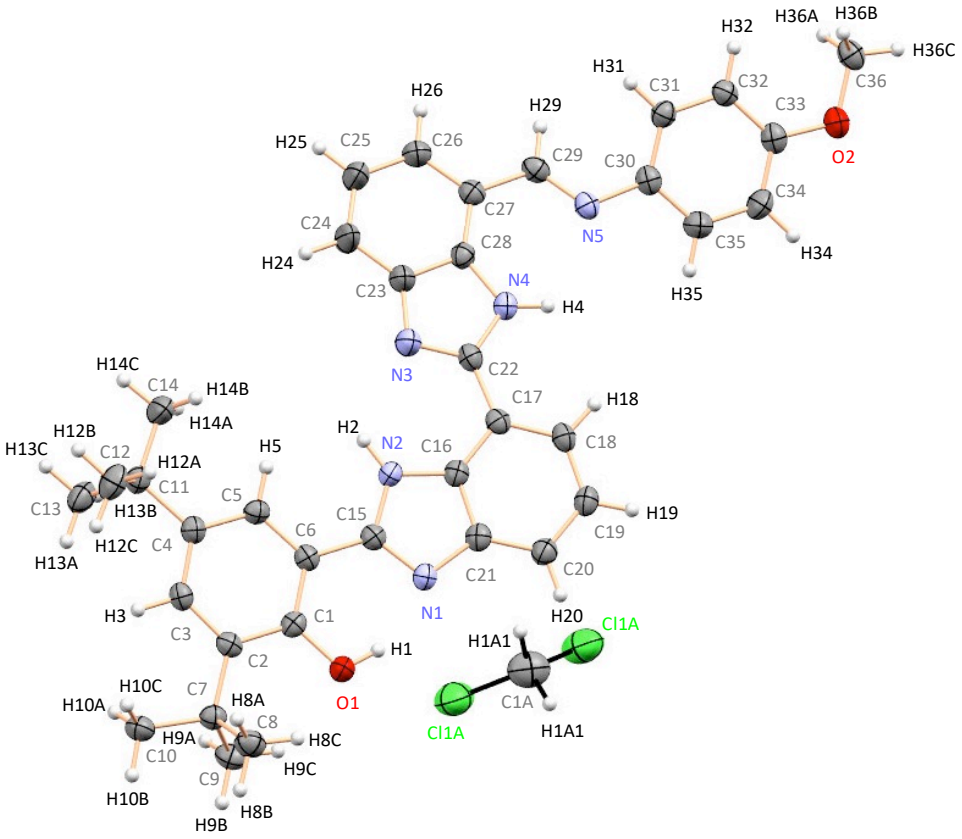


Figure S10. ORTEP representation of the crystal structure of **2'**. A molecule of CH_2Cl_2 has been found in the crystal unit cell. Carbons are shown in grey, oxygens in red, nitrogens in light violet, chlorines in green, and hydrogens in white. Thermal ellipsoids are drawn at the 50% probability level.

Table S12. Sample and crystal data for **2'**.

Identification code	BI_2P-Ph^{OMe}imine	
Chemical formula	$C_{73}H_{76}Cl_2N_{10}O_4$	
Formula weight	1228.33 g/mol	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal size	0.063 x 0.199 x 0.514 mm	
Crystal habit	clear pale yellow long thin plate	
Crystal system	monoclinic	
Space group	C 1 2/c 1	
Unit cell dimensions	a = 33.136(4) Å	α = 90°
	b = 6.8671(8) Å	β = 100.031(2)°
	c = 30.967(4) Å	γ = 90°
Volume	6938.8(14) $Å^3$	
Z	4	
Density (calculated)	1.176 g/cm^3	
Absorption coefficient	0.148 mm^{-1}	
F(000)	2600	

Table S13. Data collection and structure refinement for **2'**.

Theta range for data collection	1.98 to 25.38°
Index ranges	-39<=h<=39, -8<=k<=8, -36<=l<=37
Reflections collected	27063
Independent reflections	6369 [R(int) = 0.0587]
Coverage of independent reflections	99.8%
Absorption correction	multi-scan
Max. and min. transmission	0.9910 and 0.9280
Structure solution technique	direct methods
Structure solution program	SHELXTL XT-2014/4
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	6369 / 0 / 410
Goodness-of-fit on F^2	1.054
Δ/σ_{max}	0.001
Final R indices	4424 data; I>2σ(I) R1 = 0.0667, wR2 = 0.1470
	all data R1 = 0.0977, wR2 = 0.1607
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0302P)^2+15.7348P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.318 and -0.262 eÅ^{-3}
R.M.S. deviation from mean	0.057 eÅ^{-3}

Table S14. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) **2'**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
O1	0.59098(6)	0.3754(3)	0.25925(6)	0.0329(5)
O2	0.32507(6)	0.1421(3)	0.63246(7)	0.0366(5)
N1	0.54807(7)	0.3693(3)	0.32171(7)	0.0274(5)
N2	0.57880(7)	0.3313(3)	0.39143(7)	0.0272(5)
N3	0.57878(7)	0.2759(4)	0.48095(8)	0.0387(6)
N4	0.51987(7)	0.2484(3)	0.50630(7)	0.0284(5)
N5	0.47566(7)	0.1745(3)	0.57535(8)	0.0297(6)
C1	0.62566(8)	0.3597(4)	0.28953(9)	0.0260(6)
C2	0.66393(8)	0.3553(4)	0.27578(9)	0.0265(6)
C3	0.69892(8)	0.3467(4)	0.30816(9)	0.0265(6)
C4	0.69780(8)	0.3408(4)	0.35318(9)	0.0276(6)
C5	0.65966(8)	0.3393(4)	0.36546(9)	0.0269(6)
C6	0.62361(8)	0.3476(4)	0.33462(9)	0.0256(6)
C7	0.66700(8)	0.3612(4)	0.22673(9)	0.0290(6)
C8	0.64907(10)	0.5537(5)	0.20608(10)	0.0392(8)
C9	0.64402(10)	0.1865(4)	0.20295(10)	0.0379(8)
C10	0.71141(9)	0.3483(5)	0.21913(9)	0.0358(7)
C11	0.73797(8)	0.3379(4)	0.38684(9)	0.0319(7)
C12	0.76137(10)	0.5271(5)	0.38220(12)	0.0463(9)
C13	0.76421(9)	0.1646(5)	0.37757(11)	0.0428(8)
C14	0.73015(10)	0.3227(6)	0.43388(10)	0.0503(9)
C15	0.58376(8)	0.3480(4)	0.34865(9)	0.0264(6)

	x/a	y/b	z/c	U(eq)
C16	0.53760(8)	0.3430(4)	0.39212(9)	0.0275(6)
C17	0.51612(8)	0.3305(4)	0.42727(9)	0.0277(6)
C18	0.47379(8)	0.3500(4)	0.41629(10)	0.0303(7)
C19	0.45427(9)	0.3796(4)	0.37310(10)	0.0330(7)
C20	0.47596(9)	0.3880(4)	0.33876(10)	0.0328(7)
C21	0.51832(8)	0.3680(4)	0.34860(9)	0.0284(6)
C22	0.53847(9)	0.2891(4)	0.47088(9)	0.0288(6)
C23	0.58670(9)	0.2204(5)	0.52485(10)	0.0383(8)
C24	0.62391(10)	0.1821(7)	0.55250(11)	0.0593(11)
C25	0.62262(10)	0.1299(6)	0.59524(11)	0.0559(10)
C26	0.58585(9)	0.1143(5)	0.61067(10)	0.0389(8)
C27	0.54848(9)	0.1504(4)	0.58421(9)	0.0298(6)
C28	0.55011(8)	0.2034(4)	0.54088(9)	0.0286(6)
C29	0.50985(9)	0.1348(4)	0.60002(9)	0.0310(7)
C30	0.43882(9)	0.1650(4)	0.59272(9)	0.0296(6)
C31	0.43656(9)	0.1733(4)	0.63707(9)	0.0300(7)
C32	0.39957(9)	0.1648(4)	0.65165(9)	0.0301(7)
C33	0.36327(9)	0.1483(4)	0.62165(10)	0.0311(7)
C34	0.36505(9)	0.1414(5)	0.57714(10)	0.0412(8)
C35	0.40226(9)	0.1504(5)	0.56296(10)	0.0394(8)
C36	0.32307(9)	0.1481(4)	0.67814(10)	0.0360(7)
Cl1A	0.53785(3)	0.86035(17)	0.23211(3)	0.0682(3)
C1A	0.5	0.0034(7)	0.25	0.0570(14)

Table S15. Bond lengths (Å) for **2'**.

O1-C1	1.355(3)	O1-H1	0.84
O2-C33	1.365(3)	O2-C36	1.428(3)
N1-C15	1.331(3)	N1-C21	1.397(3)
N2-C15	1.368(3)	N2-C16	1.371(3)
N2-H2	0.88	N3-C22	1.321(4)
N3-C23	1.392(4)	N4-C28	1.368(3)
N4-C22	1.377(3)	N4-H4	0.88
N5-C29	1.281(4)	N5-C30	1.419(4)
C1-C2	1.407(4)	C1-C6	1.412(4)
C2-C3	1.396(4)	C2-C7	1.540(4)
C3-C4	1.402(4)	C3-H3	0.95
C4-C5	1.382(4)	C4-C11	1.541(4)
C5-C6	1.395(4)	C5-H5	0.95
C6-C15	1.460(4)	C7-C10	1.533(4)
C7-C9	1.538(4)	C7-C8	1.542(4)
C8-H8A	0.98	C8-H8B	0.98
C8-H8C	0.98	C9-H9A	0.98
C9-H9B	0.98	C9-H9C	0.98
C10-H10A	0.98	C10-H10B	0.98
C10-H10C	0.98	C11-C14	1.527(4)
C11-C13	1.530(4)	C11-C12	1.533(4)
C12-H12A	0.98	C12-H12B	0.98
C12-H12C	0.98	C13-H13A	0.98

C13-H13B	0.98	C13-H13C	0.98
C14-H14A	0.98	C14-H14B	0.98
C14-H14C	0.98	C16-C21	1.398(4)
C16-C17	1.403(4)	C17-C18	1.391(4)
C17-C22	1.451(4)	C18-C19	1.395(4)
C18-H18	0.95	C19-C20	1.385(4)
C19-H19	0.95	C20-C21	1.390(4)
C20-H20	0.95	C23-C28	1.393(4)
C23-C24	1.398(4)	C24-C25	1.379(5)
C24-H24	0.95	C25-C26	1.388(4)
C25-H25	0.95	C26-C27	1.383(4)
C26-H26	0.95	C27-C28	1.401(4)
C27-C29	1.452(4)	C29-H29	0.95
C30-C31	1.390(4)	C30-C35	1.392(4)
C31-C32	1.379(4)	C31-H31	0.95
C32-C33	1.390(4)	C32-H32	0.95
C33-C34	1.391(4)	C34-C35	1.381(4)
C34-H34	0.95	C35-H35	0.95
C36-H36A	0.98	C36-H36B	0.98
C36-H36C	0.98	Cl1A-C1A	1.757(3)
C1A-Cl1A	1.757(3)	C1A-H1A1	0.99
C1A-H1A2	0.99		

Table S16. Bond angles (°) for **2'**.

C1-O1-H1	109.5	C33-O2-C36	116.6(2)
C15-N1-C21	105.5(2)	C15-N2-C16	107.3(2)
C15-N2-H2	126.3	C16-N2-H2	126.3
C22-N3-C23	105.1(2)	C28-N4-C22	107.5(2)
C28-N4-H4	126.3	C22-N4-H4	126.3
C29-N5-C30	119.6(2)	O1-C1-C2	119.5(2)
O1-C1-C6	120.5(2)	C2-C1-C6	120.0(2)
C3-C2-C1	117.6(2)	C3-C2-C7	121.4(2)
C1-C2-C7	121.1(2)	C2-C3-C4	123.6(2)
C2-C3-H3	118.2	C4-C3-H3	118.2
C5-C4-C3	117.3(3)	C5-C4-C11	122.5(2)
C3-C4-C11	120.2(2)	C4-C5-C6	121.8(3)
C4-C5-H5	119.1	C6-C5-H5	119.1
C5-C6-C1	119.8(2)	C5-C6-C15	120.5(2)
C1-C6-C15	119.7(2)	C10-C7-C9	106.9(2)
C10-C7-C2	112.3(2)	C9-C7-C2	109.9(2)
C10-C7-C8	107.2(2)	C9-C7-C8	110.3(2)
C2-C7-C8	110.1(2)	C7-C8-H8A	109.5
C7-C8-H8B	109.5	H8A-C8-H8B	109.5
C7-C8-H8C	109.5	H8A-C8-H8C	109.5
H8B-C8-H8C	109.5	C7-C9-H9A	109.5
C7-C9-H9B	109.5	H9A-C9-H9B	109.5
C7-C9-H9C	109.5	H9A-C9-H9C	109.5

H9B-C9-H9C	109.5	C7-C10-H10A	109.5
C7-C10-H10B	109.5	H10A-C10-H10B	109.5
C7-C10-H10C	109.5	H10A-C10-H10C	109.5
H10B-C10-H10C	109.5	C14-C11-C13	108.8(3)
C14-C11-C12	108.7(3)	C13-C11-C12	109.2(2)
C14-C11-C4	112.1(2)	C13-C11-C4	109.6(2)
C12-C11-C4	108.5(2)	C11-C12-H12A	109.5
C11-C12-H12B	109.5	H12A-C12-H12B	109.5
C11-C12-H12C	109.5	H12A-C12-H12C	109.5
H12B-C12-H12C	109.5	C11-C13-H13A	109.5
C11-C13-H13B	109.5	H13A-C13-H13B	109.5
C11-C13-H13C	109.5	H13A-C13-H13C	109.5
H13B-C13-H13C	109.5	C11-C14-H14A	109.5
C11-C14-H14B	109.5	H14A-C14-H14B	109.5
C11-C14-H14C	109.5	H14A-C14-H14C	109.5
H14B-C14-H14C	109.5	N1-C15-N2	111.9(2)
N1-C15-C6	124.4(2)	N2-C15-C6	123.7(2)
N2-C16-C21	106.3(2)	N2-C16-C17	130.5(3)
C21-C16-C17	123.2(3)	C18-C17-C16	115.5(3)
C18-C17-C22	125.2(3)	C16-C17-C22	119.2(2)
C17-C18-C19	121.8(3)	C17-C18-H18	119.1
C19-C18-H18	119.1	C20-C19-C18	121.7(3)
C20-C19-H19	119.1	C18-C19-H19	119.1
C19-C20-C21	117.8(3)	C19-C20-H20	121.1

C21-C20-H20	121.1	C20-C21-N1	131.2(3)
C20-C21-C16	119.9(3)	N1-C21-C16	108.9(2)
N3-C22-N4	111.9(3)	N3-C22-C17	124.4(3)
N4-C22-C17	123.7(2)	N3-C23-C28	110.1(3)
N3-C23-C24	130.2(3)	C28-C23-C24	119.7(3)
C25-C24-C23	117.7(3)	C25-C24-H24	121.1
C23-C24-H24	121.1	C24-C25-C26	121.8(3)
C24-C25-H25	119.1	C26-C25-H25	119.1
C27-C26-C25	122.1(3)	C27-C26-H26	119.0
C25-C26-H26	119.0	C26-C27-C28	115.7(3)
C26-C27-C29	122.6(3)	C28-C27-C29	121.7(3)
N4-C28-C23	105.5(2)	N4-C28-C27	131.5(3)
C23-C28-C27	123.0(3)	N5-C29-C27	121.6(3)
N5-C29-H29	119.2	C27-C29-H29	119.2
C31-C30-C35	117.8(3)	C31-C30-N5	124.8(3)
C35-C30-N5	117.3(3)	C32-C31-C30	121.7(3)
C32-C31-H31	119.1	C30-C31-H31	119.1
C31-C32-C33	120.0(3)	C31-C32-H32	120.0
C33-C32-H32	120.0	O2-C33-C32	124.7(3)
O2-C33-C34	116.3(3)	C32-C33-C34	118.9(3)
C35-C34-C33	120.5(3)	C35-C34-H34	119.7
C33-C34-H34	119.7	C34-C35-C30	121.0(3)
C34-C35-H35	119.5	C30-C35-H35	119.5
O2-C36-H36A	109.5	O2-C36-H36B	109.5

H36A-C36-H36B	109.5	O2-C36-H36C	109.5
H36A-C36-H36C	109.5	H36B-C36-H36C	109.5
Cl1A-C1A-Cl1A	112.0(3)	Cl1A-C1A-H1A1	109.2
Cl1A-C1A-H1A1	109.2	Cl1A-C1A-H1A2	109.2
Cl1A-C1A-H1A2	109.2	H1A1-C1A-H1A2	107.9

Table S17. Torsion angles (°) for **2'**.

O1-C1-C2-C3	177.5(2)	C6-C1-C2-C3	-2.5(4)
O1-C1-C2-C7	-2.1(4)	C6-C1-C2-C7	177.9(2)
C1-C2-C3-C4	0.5(4)	C7-C2-C3-C4	-179.9(2)
C2-C3-C4-C5	1.4(4)	C2-C3-C4-C11	-178.1(2)
C3-C4-C5-C6	-1.4(4)	C11-C4-C5-C6	178.1(3)
C4-C5-C6-C1	-0.6(4)	C4-C5-C6-C15	-179.3(3)
O1-C1-C6-C5	-177.4(2)	C2-C1-C6-C5	2.5(4)
O1-C1-C6-C15	1.3(4)	C2-C1-C6-C15	-178.7(2)
C3-C2-C7-C10	2.2(4)	C1-C2-C7-C10	-178.1(3)
C3-C2-C7-C9	121.0(3)	C1-C2-C7-C9	-59.3(3)
C3-C2-C7-C8	-117.2(3)	C1-C2-C7-C8	62.4(3)
C5-C4-C11-C14	2.9(4)	C3-C4-C11-C14	-177.6(3)
C5-C4-C11-C13	123.9(3)	C3-C4-C11-C13	-56.7(3)
C5-C4-C11-C12	-117.0(3)	C3-C4-C11-C12	62.4(3)
C21-N1-C15-N2	0.6(3)	C21-N1-C15-C6	-177.9(3)
C16-N2-C15-N1	-0.2(3)	C16-N2-C15-C6	178.3(3)
C5-C6-C15-N1	175.1(3)	C1-C6-C15-N1	-3.6(4)
C5-C6-C15-N2	-3.2(4)	C1-C6-C15-N2	178.0(2)
C15-N2-C16-C21	-0.3(3)	C15-N2-C16-C17	178.6(3)
N2-C16-C17-C18	179.6(3)	C21-C16-C17-C18	-1.7(4)
N2-C16-C17-C22	-3.5(5)	C21-C16-C17-C22	175.1(3)
C16-C17-C18-C19	0.1(4)	C22-C17-C18-C19	-176.5(3)
C17-C18-C19-C20	1.1(4)	C18-C19-C20-C21	-0.8(4)

C19-C20-C21-N1	179.8(3)	C19-C20-C21-C16	-0.8(4)
C15-N1-C21-C20	178.8(3)	C15-N1-C21-C16	-0.7(3)
N2-C16-C21-C20	-179.0(3)	C17-C16-C21-C20	2.1(4)
N2-C16-C21-N1	0.6(3)	C17-C16-C21-N1	-178.4(2)
C23-N3-C22-N4	1.1(3)	C23-N3-C22-C17	-175.6(3)
C28-N4-C22-N3	-1.0(3)	C28-N4-C22-C17	175.7(3)
C18-C17-C22-N3	-178.2(3)	C16-C17-C22-N3	5.3(4)
C18-C17-C22-N4	5.4(4)	C16-C17-C22-N4	-171.1(3)
C22-N3-C23-C28	-0.8(4)	C22-N3-C23-C24	179.0(4)
N3-C23-C24-C25	179.7(4)	C28-C23-C24-C25	-0.5(6)
C23-C24-C25-C26	0.3(6)	C24-C25-C26-C27	-0.1(6)
C25-C26-C27-C28	0.1(5)	C25-C26-C27-C29	-179.9(3)
C22-N4-C28-C23	0.5(3)	C22-N4-C28-C27	-179.7(3)
N3-C23-C28-N4	0.2(3)	C24-C23-C28-N4	-179.6(3)
N3-C23-C28-C27	-179.7(3)	C24-C23-C28-C27	0.5(5)
C26-C27-C28-N4	179.8(3)	C29-C27-C28-N4	-0.1(5)
C26-C27-C28-C23	-0.3(4)	C29-C27-C28-C23	179.7(3)
C30-N5-C29-C27	-177.4(2)	C26-C27-C29-N5	177.9(3)
C28-C27-C29-N5	-2.2(4)	C29-N5-C30-C31	20.4(4)
C29-N5-C30-C35	-160.9(3)	C35-C30-C31-C32	0.9(4)
N5-C30-C31-C32	179.5(3)	C30-C31-C32-C33	-0.3(4)
C36-O2-C33-C32	-1.7(4)	C36-O2-C33-C34	179.7(3)
C31-C32-C33-O2	-178.8(3)	C31-C32-C33-C34	-0.2(4)
O2-C33-C34-C35	178.8(3)	C32-C33-C34-C35	0.1(5)

C33-C34-C35-C30	0.5(5)	C31-C30-C35-C34	-1.0(5)
N5-C30-C35-C34	-179.7(3)		

Table S18. Anisotropic atomic displacement parameters (Å^2) for **2'**.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.0267(11)	0.0424(12)	0.0292(11)	0.0015(9)	0.0036(9)	0.0014(10)
O2	0.0305(11)	0.0383(12)	0.0423(12)	0.0001(10)	0.0101(9)	-0.0006(10)
N1	0.0248(12)	0.0266(13)	0.0306(13)	0.0004(10)	0.0043(10)	-0.0002(10)
N2	0.0229(12)	0.0309(13)	0.0267(12)	-0.0002(10)	0.0014(10)	0.0014(10)
N3	0.0287(14)	0.0551(17)	0.0321(14)	0.0020(12)	0.0048(11)	-0.0025(12)
N4	0.0241(12)	0.0282(13)	0.0332(13)	0.0003(11)	0.0055(11)	0.0002(10)
N5	0.0290(13)	0.0280(13)	0.0331(13)	-0.0006(11)	0.0086(11)	-0.0010(11)
C1	0.0270(15)	0.0207(14)	0.0291(15)	-0.0009(12)	0.0015(12)	-0.0013(12)
C2	0.0334(16)	0.0195(14)	0.0276(15)	0.0000(12)	0.0082(12)	0.0018(12)
C3	0.0256(15)	0.0218(14)	0.0334(15)	0.0010(12)	0.0087(12)	-0.0008(12)
C4	0.0282(15)	0.0226(14)	0.0324(15)	0.0008(12)	0.0059(12)	0.0008(12)
C5	0.0306(16)	0.0236(15)	0.0264(14)	0.0023(12)	0.0048(12)	0.0010(12)
C6	0.0274(15)	0.0209(14)	0.0292(15)	0.0001(12)	0.0074(12)	-0.0002(12)
C7	0.0319(16)	0.0269(15)	0.0280(15)	0.0014(12)	0.0051(12)	0.0002(13)
C8	0.0460(19)	0.0392(18)	0.0332(17)	0.0050(14)	0.0094(15)	0.0031(15)
C9	0.0469(19)	0.0353(18)	0.0328(17)	-0.0051(14)	0.0100(14)	-0.0018(15)
C10	0.0396(18)	0.0403(18)	0.0287(16)	0.0009(14)	0.0091(13)	0.0001(15)
C11	0.0266(15)	0.0342(17)	0.0344(16)	0.0017(13)	0.0042(13)	0.0000(13)
C12	0.0324(18)	0.046(2)	0.057(2)	0.0011(17)	-0.0034(16)	-0.0050(15)
C13	0.0354(18)	0.0429(19)	0.0459(19)	-0.0025(16)	-0.0044(15)	0.0086(15)
C14	0.0314(18)	0.083(3)	0.0351(18)	0.0009(18)	0.0010(14)	-0.0011(18)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C15	0.0285(15)	0.0223(14)	0.0285(15)	-0.0006(12)	0.0052(12)	0.0000(12)
C16	0.0261(15)	0.0231(14)	0.0325(15)	-0.0021(12)	0.0033(12)	-0.0002(12)
C17	0.0298(16)	0.0240(15)	0.0299(15)	-0.0025(12)	0.0067(12)	0.0005(12)
C18	0.0262(15)	0.0285(15)	0.0375(17)	-0.0019(13)	0.0094(13)	-0.0018(13)
C19	0.0262(15)	0.0314(16)	0.0408(18)	-0.0020(14)	0.0042(13)	0.0025(13)
C20	0.0304(16)	0.0335(17)	0.0336(16)	-0.0009(13)	0.0033(13)	0.0016(13)
C21	0.0284(15)	0.0228(14)	0.0340(16)	-0.0014(12)	0.0052(12)	-0.0030(12)
C22	0.0288(16)	0.0263(15)	0.0329(16)	-0.0017(13)	0.0094(13)	-0.0006(12)
C23	0.0295(17)	0.054(2)	0.0317(17)	0.0020(15)	0.0057(13)	0.0015(15)
C24	0.0263(17)	0.115(4)	0.0378(19)	0.013(2)	0.0079(15)	0.001(2)
C25	0.0291(18)	0.100(3)	0.0371(19)	0.010(2)	0.0024(15)	0.005(2)
C26	0.0370(18)	0.049(2)	0.0303(16)	0.0032(15)	0.0050(14)	0.0032(15)
C27	0.0317(16)	0.0278(15)	0.0302(15)	-0.0013(13)	0.0066(13)	-0.0007(13)

Table S19. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for **2'**.

	x/a	y/b	z/c	U(eq)
H1	0.5706	0.3795	0.2720	0.049
H2	0.5984	0.3159	0.4143	0.033
H4	0.4934	0.2508	0.5066	0.034
H3	0.7249	0.3447	0.2992	0.032
H5	0.6580	0.3325	0.3957	0.032
H8A	0.6203	0.5649	0.2096	0.059
H8B	0.6508	0.5551	0.1748	0.059
H8C	0.6647	0.6635	0.2207	0.059
H9A	0.6567	0.0652	0.2152	0.057
H9B	0.6454	0.1932	0.1716	0.057
H9C	0.6153	0.1898	0.2068	0.057
H10A	0.7270	0.4594	0.2332	0.054
H10B	0.7118	0.3505	0.1876	0.054
H10C	0.7238	0.2269	0.2318	0.054
H12A	0.7868	0.5286	0.4038	0.069
H12B	0.7443	0.6387	0.3872	0.069
H12C	0.7680	0.5350	0.3526	0.069
H13A	0.7697	0.1739	0.3476	0.064
H13B	0.7495	0.0431	0.3809	0.064
H13C	0.7902	0.1658	0.3983	0.064
H14A	0.7564	0.3203	0.4541	0.075
H14B	0.7149	0.2028	0.4372	0.075

	x/a	y/b	z/c	U(eq)
H14C	0.7141	0.4353	0.4405	0.075
H18	0.4577	0.3428	0.4388	0.036
H19	0.4253	0.3945	0.3671	0.04
H20	0.4623	0.4067	0.3094	0.039
H24	0.6492	0.1918	0.5422	0.071
H25	0.6476	0.1039	0.6146	0.067
H26	0.5864	0.0777	0.6403	0.047
H29	0.5099	0.0940	0.6294	0.037
H31	0.4611	0.1851	0.6579	0.036
H32	0.3989	0.1701	0.6822	0.036
H34	0.3405	0.1304	0.5563	0.049

Table S20. Hydrogen bond distances (Å) and angles (°) for **2'**.

	Donor-H	**Acceptor-H**	**Donor-Acceptor**	**Angle**
O1-H1···N1	0.84	1.83	2.593(3)	151.0
N2-H2···N3	0.88	2.29	2.798(3)	117.0
N4-H4···N5	0.88	2.36	2.840(3)	114.3
C20-H20···O1	0.95	2.53	3.434(3)	160.0

1.5. UV-Visible Spectroscopy Data

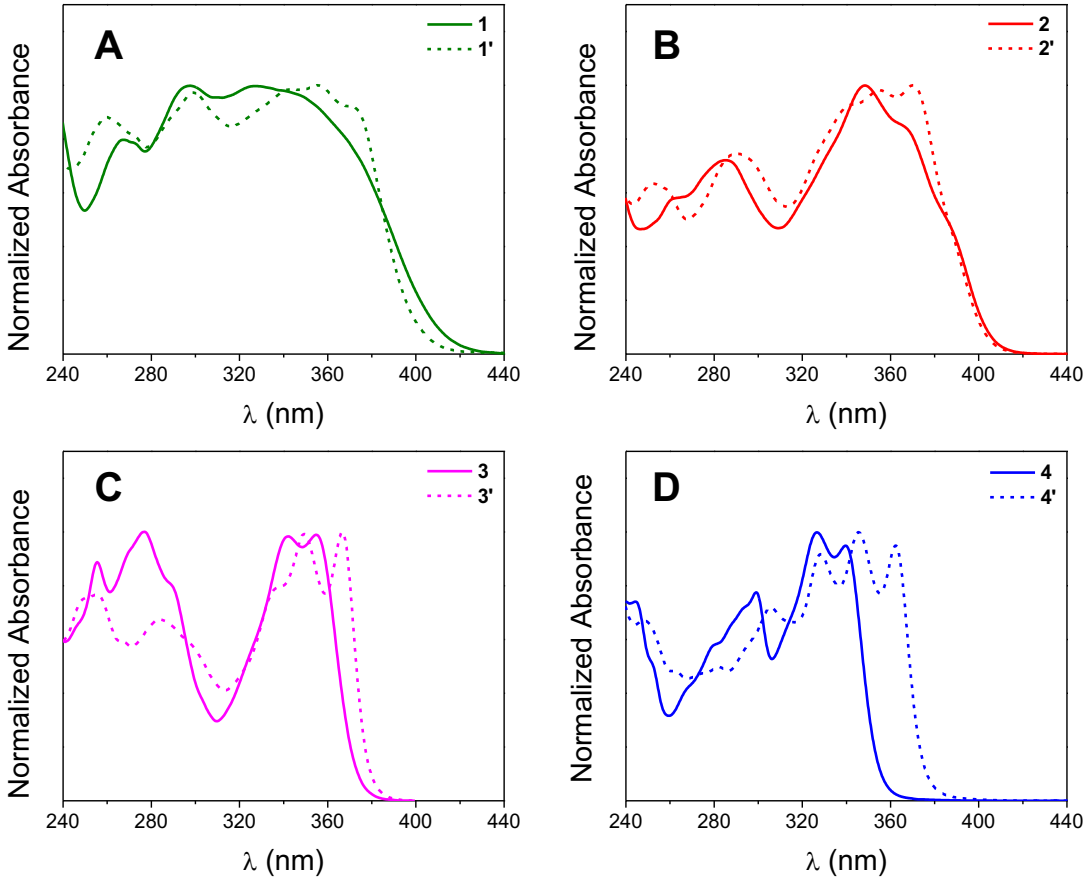


Figure S11. (**A-D**) Normalized UV-visible spectra of BIPs **1**–**4** (solid lines) and BI_2Ps **1'**–**4'** (dashed lines) in DCM. The red shift in the spectra observed in the BI_2Ps series relative to BIPs series with the same terminal proton-accepting group is due to the extended π system provided by the partially conjugated dibenzimidazole.

1.6. IR Data

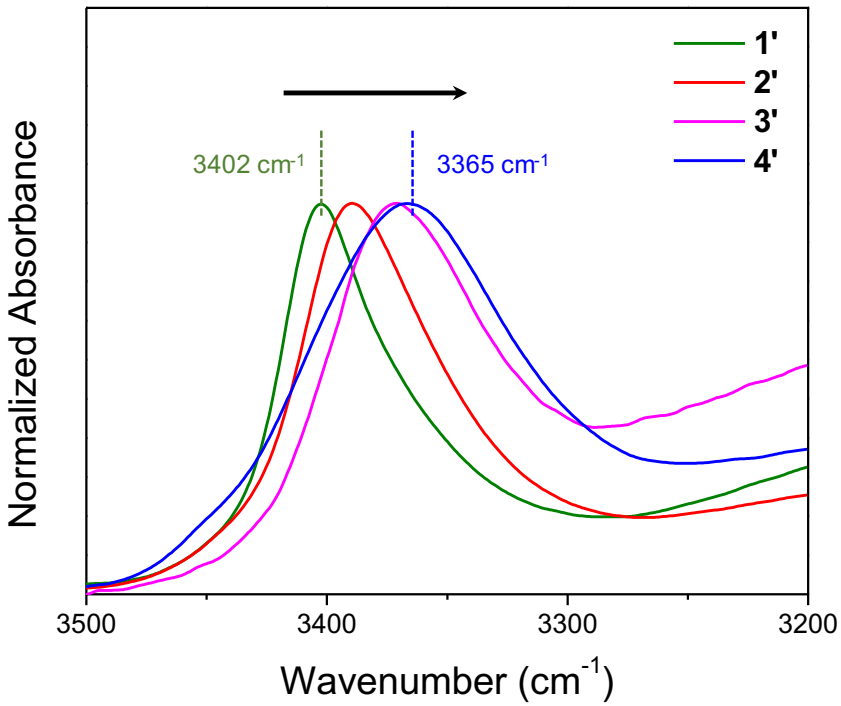


Figure S12. Normalized infrared spectra of BI_2Ps **1'**–**4'** in the 3200-3500 cm^{-1} region showing the benzimidazole NH stretching vibrational mode (ν_{NH}). The ν_{NH} of **1'** appears at 3402 cm^{-1} and shifts to 3365 cm^{-1} (ν_{NH} of **4'**) across the BI_2Ps series. The progressive shift to lower frequencies supports the increasing hydrogen bond network strength due to the increase in the basicity of the terminal proton-accepting group, consistent with the trend observed in the ^1H NMR.

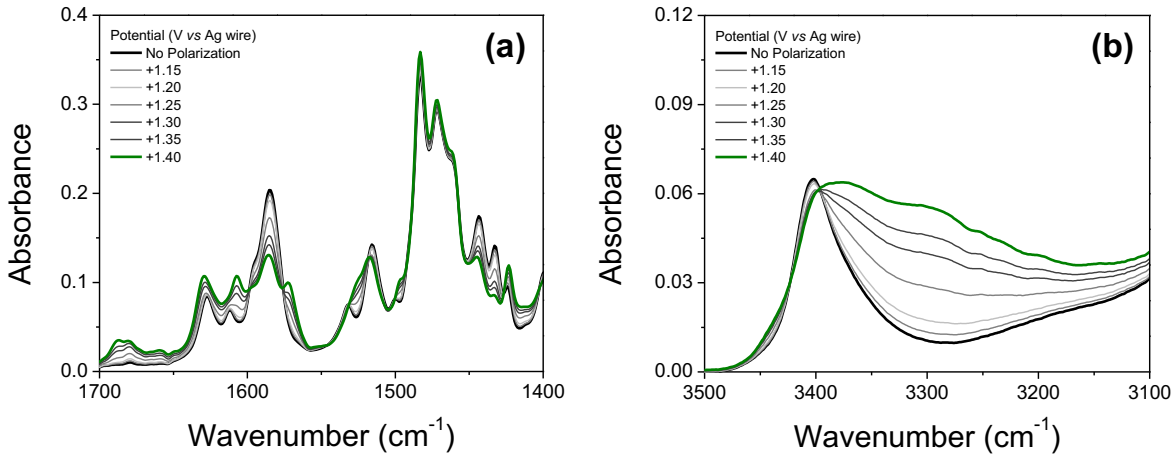


Figure S13. IRSEC spectra of **1'** (19 mM solutions) polarized in 50 mV steps in the **(a)** 1700–1400 cm^{-1} region and **(b)** 3500–3100 cm^{-1} region. Solvent: DCM, 0.1 M $TBAPF_6$.

1.7. Kinetic Isotope Effect (KIE)

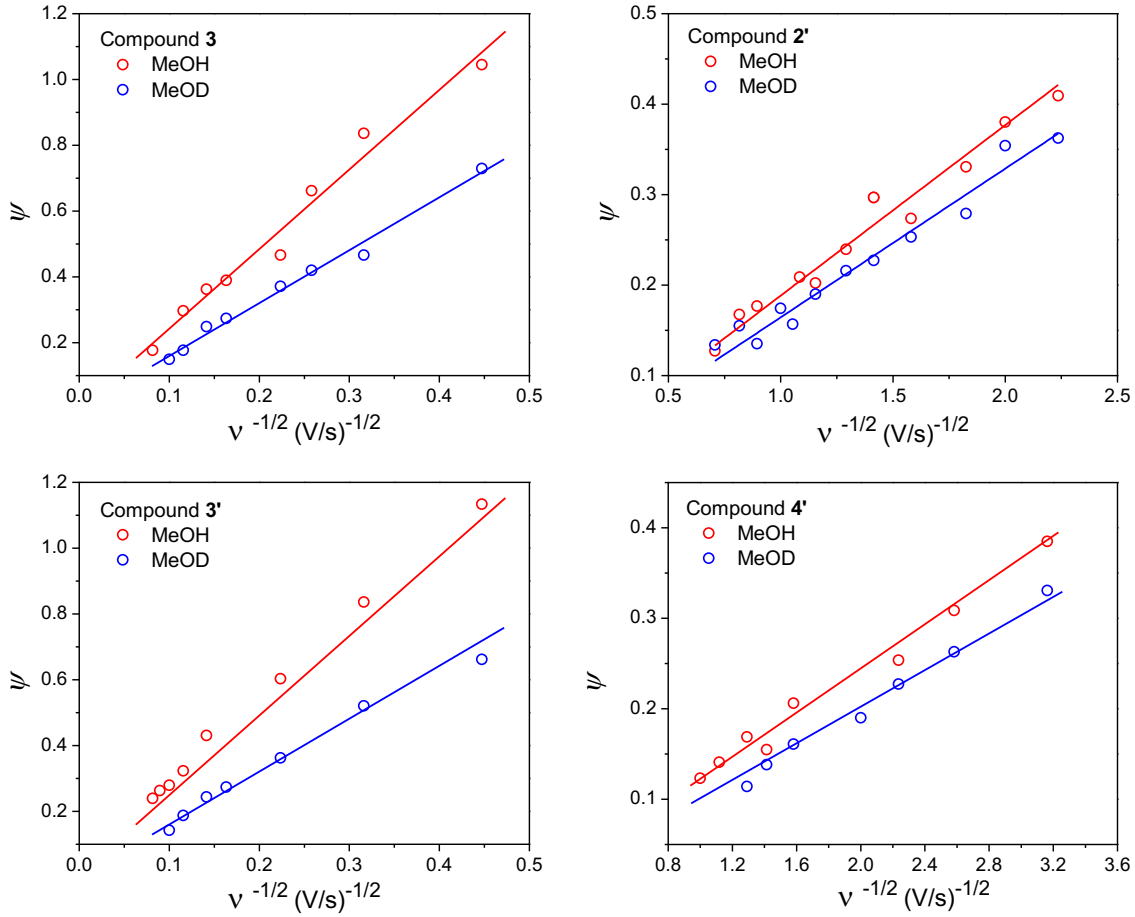


Figure S14. Plots of ψ *vs* $v^{-1/2}$ for the investigated compounds in DCM or ACN + 2% MeOH (red circles) and DCM or ACN + 2% MeOD (blue circles). The solid red and solid blue lines are the linear fits for the data collected in MeOH and MeOD, respectively. The relation between ψ, scan rate v, and rate constant are given in the Experimental Results, KIE Measurements, page S4.

Table S21. Apparent standard rate constants of electron transfer (k_{app}) for the investigated compounds determined in DCM or ACN (+ 2% MeOH or MeOD) and kinetic isotope effects (KIEs).

	3[a]	**2'**[a]	**3'**[a]	**4'**[b]
k_{app}[c] (cm s^{-1})	8.47 x 10^{-2}	6.45 x 10^{-3}	9.22 x 10^{-2}	4.20 x 10^{-3}
k_{app}[d] (cm s^{-1})	5.60 x 10^{-2}	4.97 x 10^{-3}	5.47 x 10^{-2}	3.50 x 10^{-3}
KIE	1.5 ± 0.3	1.3 ± 0.3	1.7 ± 0.3	1.2 ± 0.3

[a] Determined in DCM
[b] Determined in ACN
[c] Determined in the solvent + 2% MeOH
[d] Determined in the solvent + 2% MeOD

Table S22. Experimental Kinetic Isotope Effect (KIE)

Compound	*KIE*
1	1.2 ± 0.3[a]
2	1.1 ± 0.3[a]
3	1.5 ± 0.3
4	0.9 ± 0.5[b]
1'	n/a
2'	1.3 ± 0.3
3'	1.7 ± 0.3
4'	1.2 ± 0.3

[a] Values from ref. 3
[b] Values from ref. 9

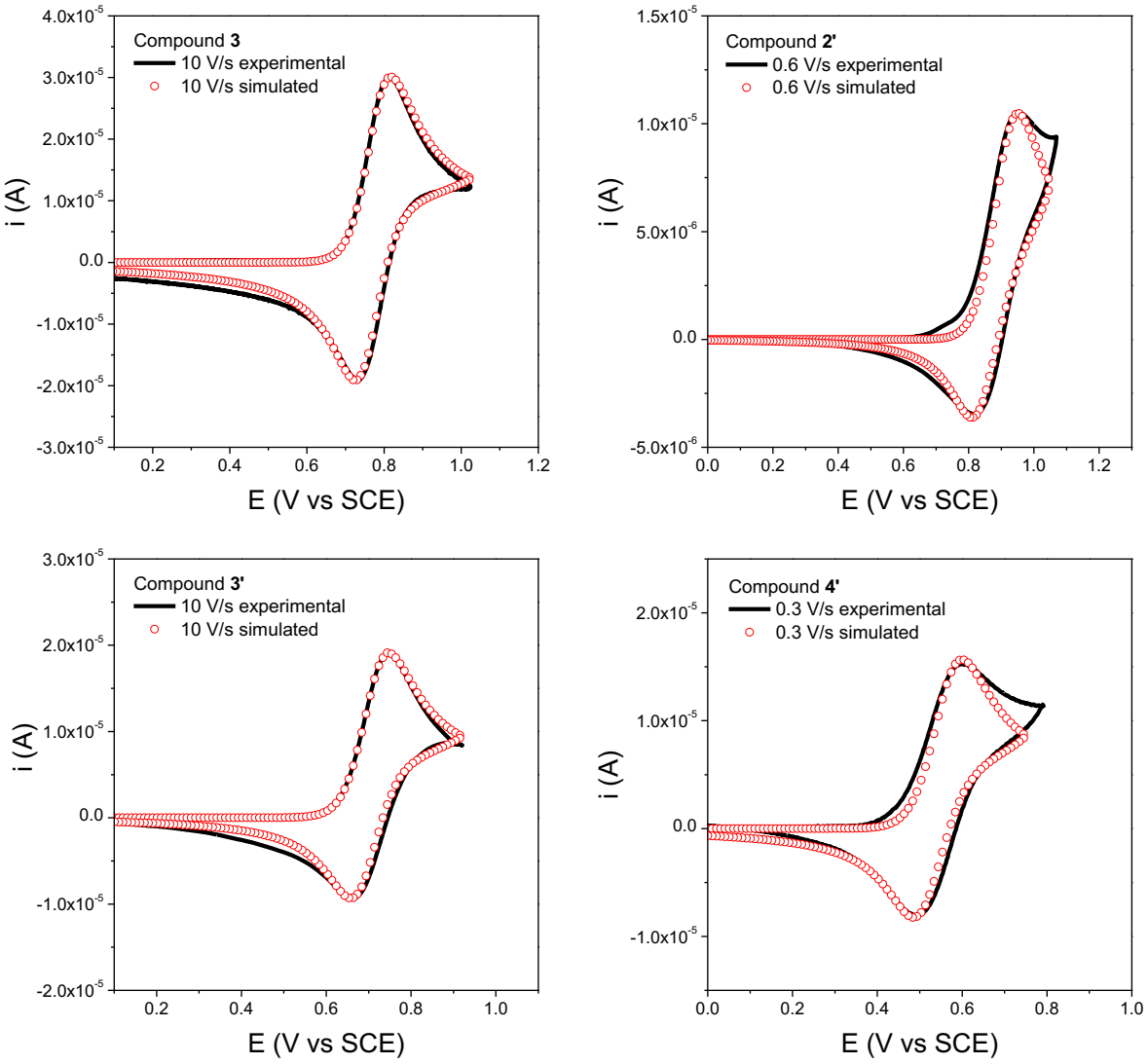


Figure S15. Experimental (black line) and simulated (red circles) cyclic voltammograms of compounds **3, 2', 3'** in DCM + 2% MeOH and **4'** in ACN in + 2% MeOH. Scan rates are indicated in the plots.

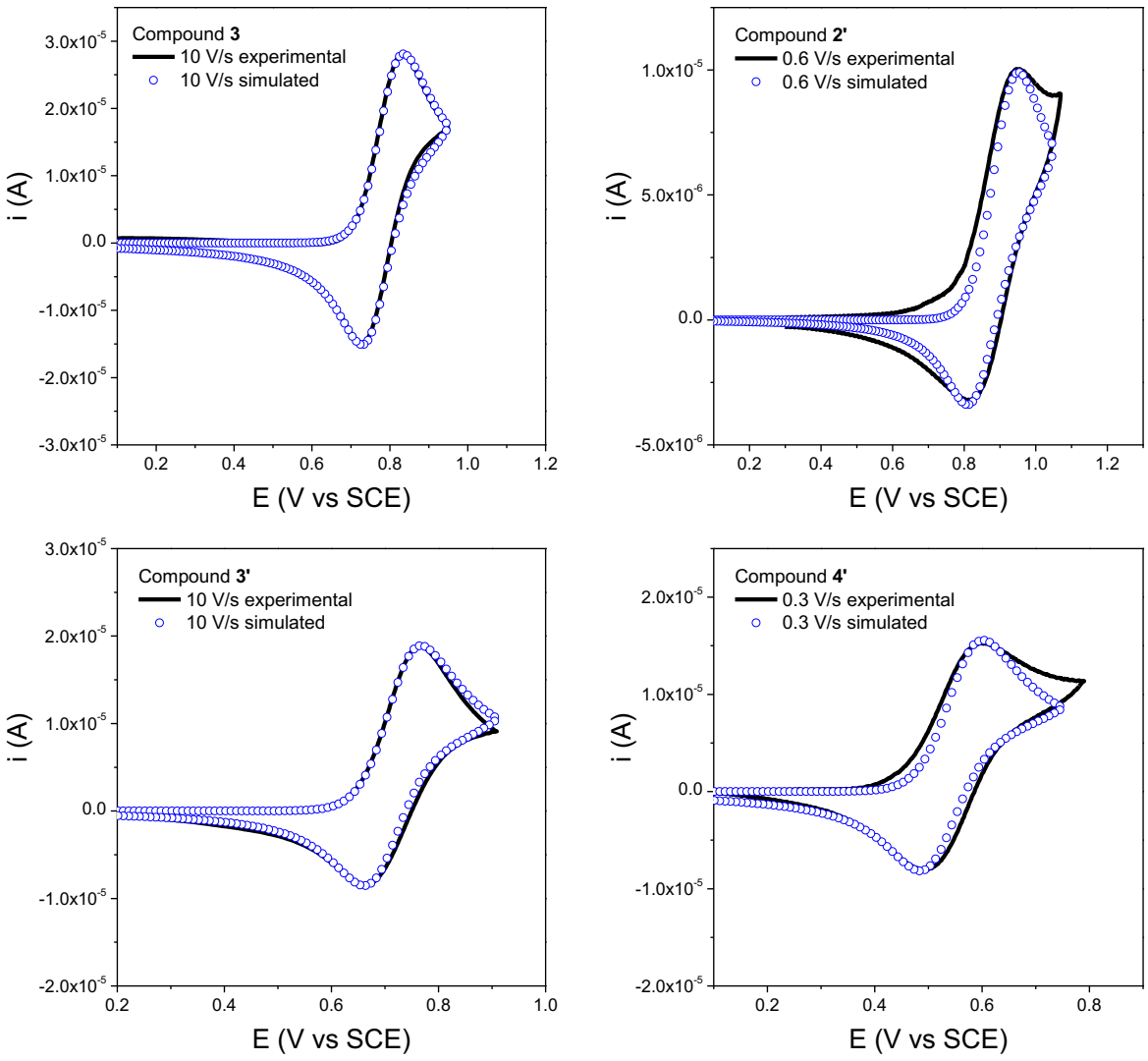


Figure S16. Experimental (black line) and simulated (blue circles) cyclic voltammograms of compounds **3, 2', 3'** in DCM + 2% MeOH and **4'** in ACN in + 2% MeOH. Scan rates are indicated in the plots.

2. Thermodynamic Analysis of E3PT

As shown in our previous report involving reversible PCET reactions that yield E*n*PT (*n* = 1–4) products, proton translocation is accompanied by a loss in redox potential.[5] For example, the potential of a redox couple involving *no* proton coupled electron transfer is ~1.5 V *vs* SCE. Conversely, the potential of the redox couple involving formation of an E4PT product is ~0.7 V *vs* SCE.[5] The calculated redox potentials for the compounds studied herein are given in Table S25. A thermodynamic (not mechanistic) description to address this change in the redox potential is presented below:

$E_{1/2}$ (E0PT) = $E_{1/2}$ (no proton transfer from the oxidized phenol to the benzimidazole)
$E_{1/2}$ (E1PT) = $E_{1/2}$ + 2.3RT/F × ΔpK_a (1)
$E_{1/2}$ (E2PT) = $E_{1/2}$ + 2.3RT/F × ΔpK_a (1) + 2.3RT/F × ΔpK_a (2)
$E_{1/2}$ (E3PT) = $E_{1/2}$ + 2.3RT/F × ΔpK_a (1) + 2.3RT/F × ΔpK_a (2) + 2.3RT/F × ΔpK_a (3)

Herein, the ΔpK_a terms are converted to an effective $\Delta E_{1/2}$ in units of volts by multiplying by the factor 2.3RT/F, and $\Delta pK_a = pK_{a\ initial} - pK_{a\ final}$ (note that because $\Delta pK_a = -\log(K_{final} - K_{initial})$, ΔpK_a is $pK_{a\ initial} - pK_{a\ final}$). $E_{1/2}$ is the redox potential for the redox reaction $BIP^{\bullet+} + e^- \rightarrow BIP$ with no proton transfer. The ΔpK_a values are determined from the change in Gibbs free energy calculated at intermediate proton locations following oxidation of the phenol for each of the E*n*PT systems. Thus, each ΔpK_a describes the shift in redox potential as each intermediate proton transfer occurs. Because the sum of $E_{1/2}$ and the individual ΔpK_a values yields the redox potential for a given E*n*PT process, the impact of each proton transfer can be elucidated. Importantly, the π-conjugated framework supporting the Grotthuss-type hydrogen-bonded network as well as the electron donating/withdrawing nature of substituents modulate the ΔpK_a values. Because the ΔpK_a terms are negative (i.e., all proton transfer reactions following oxidation are exoergic), there is a monotonic decrease of the phenoxyl radical/phenol couple redox potential with increasing proton translocation distance (e.g., the number (*n*) of proton transfer reactions for each system). For the molecules studied, the sum of $E_{1/2}$ and all of the individual ΔpK_a values for each molecule yields the experimentally observed redox potential, indicating that all protons transfer.

3. Computational Methods

The computational methods follow closely those used in Ref. 5. All electronic structure calculations were performed with density functional theory (DFT) using the B3LYP-D3(BJ) functional with empirical dispersion[10–12] and the 6-31G** basis set for all atoms.[13,14] All geometries were optimized in ACN solution using the conductor-like polarizable continuum model (C-PCM).[15] with the Bondi atomic radii,[16] including the nonelectrostatic contributions of dispersion,[17] repulsion,[17] and cavitation energies.[18] This electronic structure method has previously been shown to perform well for similar calculations on substituted benzimidazole-phenol constructs.[3,9] Specifically, previous benchmarking studies[3,9] on 14 substituted BIP systems obtained similar redox potentials for six different density functionals, and the computed redox potentials were in good agreement with available experimental data. All DFT calculations reported in this paper were performed using the Gaussian 16 electronic structure program.[19]

Thermochemical data were calculated at T=298.15 K, and all calculated free energies include zero-point energy, entropic contributions, and solvation effects. The solution free energies were calculated using the standard Gibbs relation $\Delta G^0=\Delta H^0-T\Delta S^0$, after empirically scaling the vibrational frequencies by 0.9576 (*vide infra*). The relative redox potentials were computed from the corresponding reaction free energies using an experimentally known reference potential within a thermodynamic cycle, as outlined elsewhere.[3,9,20] In the current work, the reference potential used for computing the redox potentials of all compounds was the experimental value of $E_{1/2}$ for the E2PT compound **2**. This computational protocol has been shown previously to yield good agreement between the calculations and experimental data, even when the calculations were performed prior to the experimental measurement of the redox potentials in a predictive manner.[3,9] The structures and energies for all of the systems studies are provided in Table S27-Table S69.

To aid with the assignment of band changes in the IRSEC spectra, we computed infrared spectra for the compounds **2'** and **4'**, which clearly show the formation of the final E3PT product. For the optimized DFT structures discussed above, frequency calculations were performed for both the reduced (neutral) and oxidized (+1) species. All frequency calculations were computed at the same level of theory as described above. To make direct comparison with experimental IRSEC spectra, all computed frequencies were empirically scaled by a factor of 0.9576, corresponding to

an alignment of the computed and experimental C=NH^+ protonated azomethine stretch for compound **2'**. Simulated spectra are depicted in Figure S19.

To simulate line broadening, the peaks were dressed with an artificial Lorentzian function for a full-width-half-maximum (FWHM) of 12 cm^{-1}. Selected vibrations are given in Table S26. Band assignments were performed by visually inspecting displacements along the computed normal mode of each vibration. Consistent with experiment, computational oxidation of compound **2'** results in a strong peak that grows in around 1653 cm^{-1} from the azomethine C=NH^+ stretch, shifted from the weaker reduced azomethine C=N stretch of 1606 cm^{-1}.

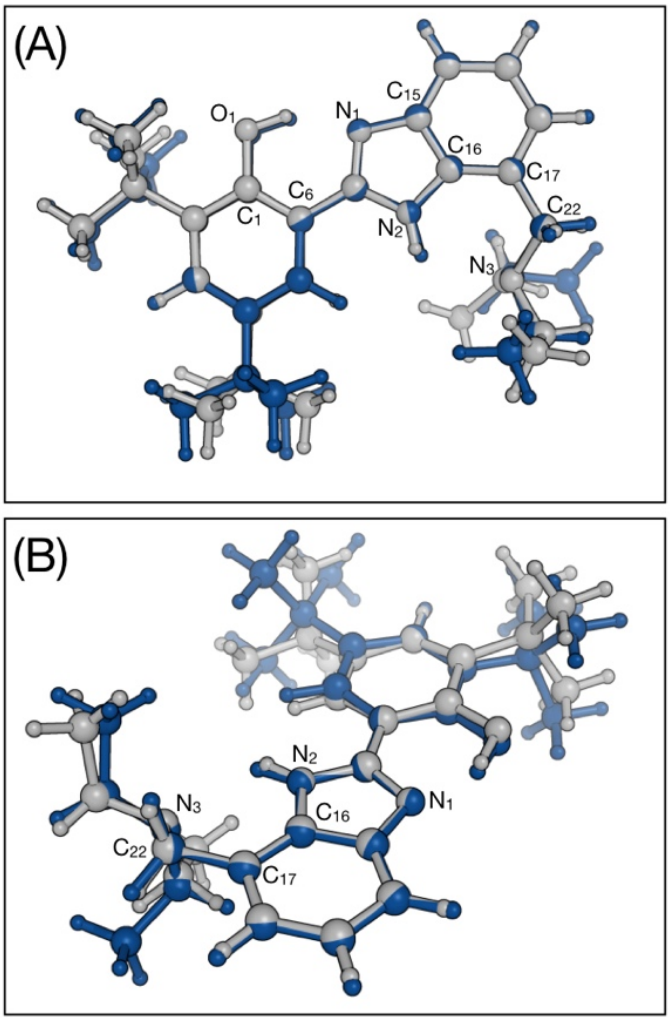


Figure S17. Two views of the superimposed structures of compound **4** showing the generally good agreement between the crystal structure (gray) and optimized structure (blue) from DFT. Select atoms are labelled according to the crystal structure shown in Figure S17 and the bond lengths and angles reported in Table S23.

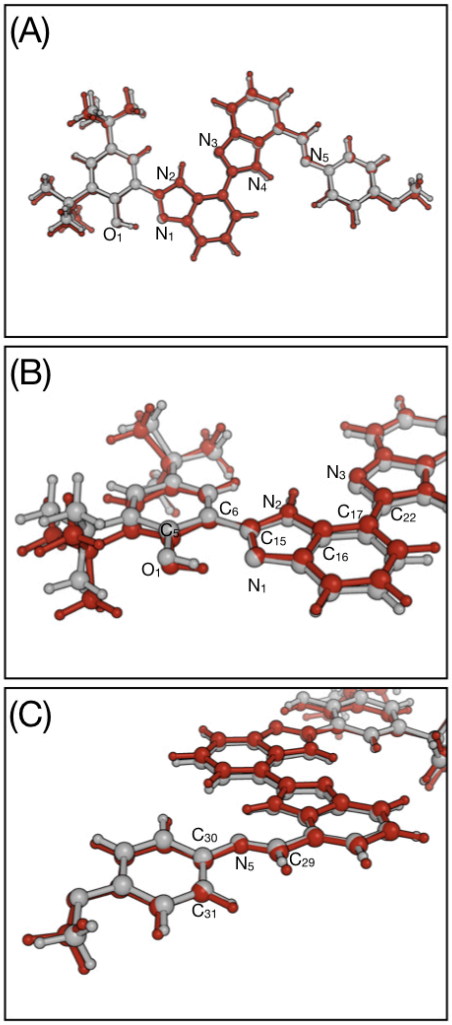


Figure S18. Three views of the superimposed structures of **2'** showing the generally good agreement between the crystal structure (gray) and optimized structure (red) from DFT. Select atoms are labelled according to the crystal structure shown in Figure S10 and the bond lengths and angles reported in Table S24.

Table S23. Selected bond lengths and dihedral angles of **4**.

	Bond Distances (Å)			Dihedral Angles (°)	
	$O_1\cdots N_1$	$N_2\cdots N_3$	$O_1\cdots N_3$	$C_1–C_6–C_{15}–N_1$	$C_{16}–C_{17}–C_{22}–N_3$
Expt.	2.5934	2.8485	7.0057	-7.9957	31.0019
Calc.	2.5779	2.8417	6.9672	1.8933	37.0396

Table S24. Selected bond lengths and dihedral angles of **2'**.

	Bond Distances (Å)				Dihedral Angles (°)			
	$O_1\cdots N_1$	$N_2\cdots N_3$	$N_4\cdots N_5$	$O_1\cdots N_5$	$C_5–C_6–C_{15}–N_2$	$C_{16}–C_{17}–C_{22}–N_3$	$C_{28}–C_{27}–C_{29}–N_5$	$C_{29}–N_5–C_{30}–C_{31}$
Expt.	2.5928	2.7983	2.8403	11.1962	3.6001	-5.2878	2.1088	-20.4486
Calc.	2.5650	2.8317	2.8330	11.2077	1.7783	0.8632	1.7073	-12.7172

Table S25. Redox potentials calculated for formation of E*n*PT products of the BIP and BI_2P analogs in ACN.

Compound	Experimental $E_{1/2}$ (V *vs* SCE)	Calculated $E_{1/2}$ (V *vs* SCE)			
		E0PT	E1PT	E2PT	E3PT
BIP	0.97	1.38	1.03	-	-
1	0.99	1.42	1.06	1.00	-
2	0.93	1.44	1.04	0.93[a]	-
3	0.77	1.38	1.02	0.77	-
4	0.61	1.34	0.94	0.61	-
BI_2P	0.85	1.39	0.99	0.85	-
1'	0.93	1.38	0.98	0.86	0.91
2'	0.87	1.40	1.00	0.88	0.77
3'	0.71	1.39	1.05	0.87	0.72
4'	0.55	1.39	1.00	0.78	0.55

[a]This couple was used as the reference reaction for all other calculated potentials, so the experimental and calculated values agree by construction.

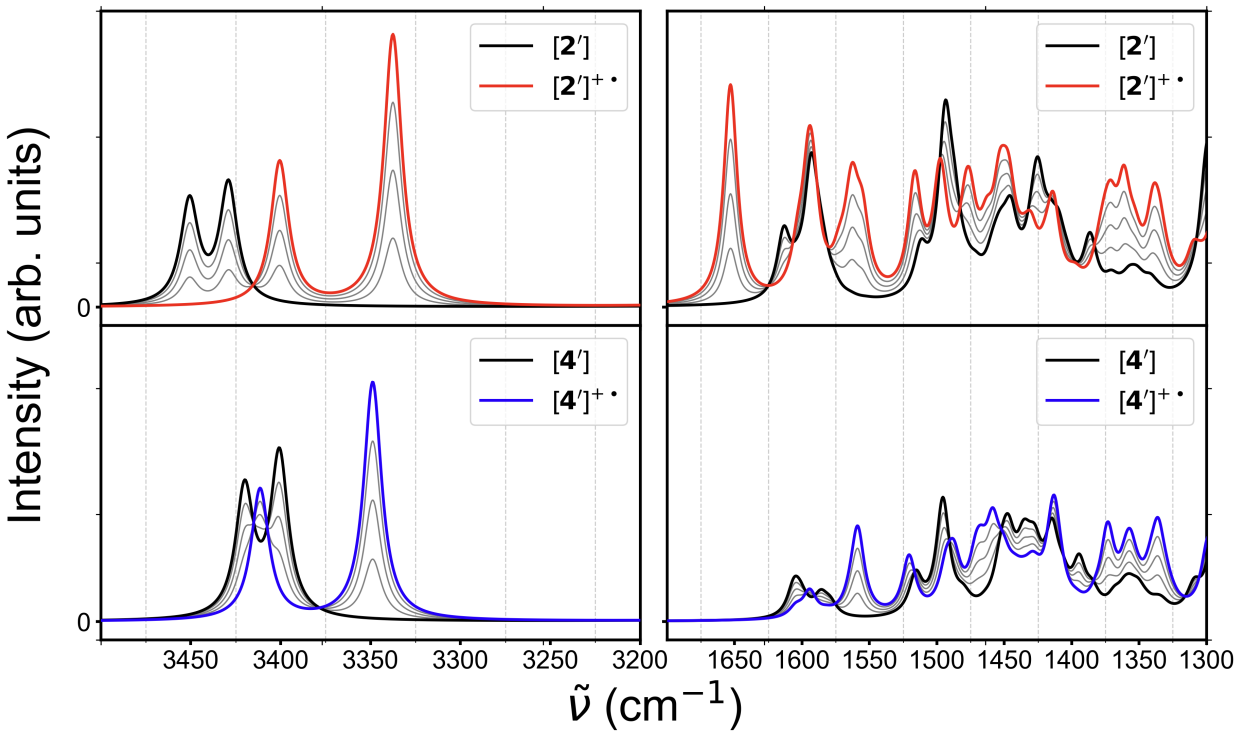


Figure S19. Computed IRSEC spectra for compounds **2'** (red) and **4'** (blue). Each peak was scaled empirically by a factor of 0.9576 and dressed with a Lorentzian function for a FWHM of 12 cm^{-1}. To simulate the increasing applied potential, spectra corresponding to the reduced, neutral (black) and oxidized, positively charged (colored) were computed. The thin gray lines correspond to an interpolation between the reduced and oxidized computed spectra.

Table S26. Selected peaks and assignments in simulated IRSEC spectrum of **2'** and **4'**.

2'		**2'$^{+\bullet}$**	
$\tilde{\nu}$ (cm^{-1})	assignment[a]	$\tilde{\nu}$ (cm^{-1})	assignment[a]
1494	phenol-Bz C–C str	1454	phenol C-H bend
1604-1577	ring C=C str	1595-1555	ring C=C str
1614	imine C=N str	1653	imine C=NH^{+} str
3451, 3429	Bz N–H str	3401, 3338	Bz N–H str

4'		**4'$^{+\bullet}$**	
$\tilde{\nu}$ (cm^{-1})	assignment[a]	$\tilde{\nu}$ (cm^{-1})	assignment[a]
1496	phenol-Bz C–C str	1493	phenol-Bz C–C str
1516	Bz-Bz C–C str	1520	Bz-Bz C=C str
1605-1579	ring C=C str	1559	Phenol ring C=C str
-	-	1604-1581	Bz ring C=C str
3420, 3401	Bz N–H str	3412, 3348	Bz N–H str

[a]Approximate mode description.

3.1. Optimized Cartesian Coordinates of Species Studied

The following tables provide the optimized Cartesian coordinates and free energies (reported in units of Hartrees) of all species studied. The geometries were optimized in the solution phase (ACN) using the B3LYP-D3(BJ) functional with the 6-31G** basis set for all atoms.

Table S27. Cartesian coordinates for unsubstituted BIP: (-1000.80519705 E_h)

atom	x	y	z
C	-0.471458	2.719484	0.449446
C	-1.870896	2.899434	0.320592
C	-2.404404	4.188273	0.207597
C	-1.515514	5.259854	0.225606
C	-0.126578	5.064352	0.355299
C	0.422475	3.788870	0.471314
C	-1.519831	0.753900	0.441671
H	-3.472467	4.338437	0.105016
H	-1.899202	6.269915	0.139362
H	0.530497	5.926235	0.365965
N	-2.491547	1.659258	0.321221
C	-3.065621	-1.188072	0.361099
C	-1.741809	-0.684252	0.459140
C	-0.662359	-1.574525	0.544186
C	-0.852013	-2.950864	0.541338
C	-2.170926	-3.418278	0.452513
C	-3.288959	-2.584110	0.363647
H	0.346171	-1.182500	0.607184
H	-2.335262	-4.484412	0.449782
C	0.361435	-3.884124	0.601115
C	-4.707273	-3.168116	0.261933
O	-4.118027	-0.343065	0.261195
H	-3.764828	0.594321	0.261303
N	-0.289627	1.351498	0.527396
H	0.593815	0.873521	0.617013
C	1.238427	-3.636853	-0.643377
H	1.558584	-2.593461	-0.695228
H	2.132373	-4.266551	-0.611170
H	0.688908	-3.870071	-1.559477
C	1.188818	-3.576662	1.864650
H	0.601837	-3.754672	2.769604
H	2.074142	-4.218000	1.899514
H	1.525273	-2.537047	1.875973
C	-0.044366	-5.363375	0.629422
H	-0.647339	-5.600201	1.510162
H	-0.613723	-5.641478	-0.261463
H	0.852742	-5.986472	0.660207
C	-5.348896	-2.751146	-1.077972
H	-6.364469	-3.152491	-1.144862
H	-5.397317	-1.667275	-1.175800
H	-4.771308	-3.148338	-1.917249
C	-5.570618	-2.668111	1.439509
H	-5.672952	-1.584240	1.425258

H	-6.568417	-3.113162	1.383976
H	-5.120135	-2.959813	2.392421
C	-4.695632	-4.704951	0.315402
H	-4.127150	-5.136724	-0.512518
H	-4.268712	-5.072971	1.252049
H	-5.722476	-5.071537	0.245765
H	1.489708	3.635650	0.573005

Table S28. Cartesian coordinates for unsubstituted BIP$^{\bullet+}$: E0PT. (-1000.61237749 E_h)

atom	x	y	z
C	-0.420761	2.705251	0.278930
C	-1.838098	2.846846	0.159783
C	-2.418240	4.122660	0.039894
C	-1.562171	5.207694	0.047430
C	-0.155806	5.051064	0.172263
C	0.440103	3.804413	0.291527
C	-1.406241	0.720633	0.300373
H	-3.490206	4.236763	-0.056141
H	-1.967156	6.208312	-0.042171
H	0.468317	5.936310	0.173996
N	-2.409169	1.606112	0.180140
C	-3.003558	-1.174915	0.362788
C	-1.627201	-0.694771	0.350453
C	-0.578096	-1.613272	0.383299
C	-0.831591	-2.977669	0.453932
C	-2.191897	-3.418167	0.506621
C	-3.280028	-2.580997	0.471296
H	0.440481	-1.254879	0.344866
H	-2.364765	-4.481326	0.578282
C	0.271959	-4.022058	0.473069
C	-4.717822	-3.101213	0.537476
O	-3.995305	-0.330935	0.271772
H	-3.616358	0.633132	0.207392
N	-0.194763	1.354885	0.364662
H	0.704811	0.909392	0.477146
C	-5.439314	-2.491586	1.759964
H	-5.499773	-1.405967	1.694396
H	-6.455496	-2.890714	1.811077
H	-4.921209	-2.758449	2.684583
C	-4.744100	-4.629736	0.690420
H	-5.782608	-4.960946	0.748783
H	-4.277493	-5.134155	-0.159787
H	-4.235432	-4.950076	1.603403
C	-5.467699	-2.733967	-0.761960
H	-5.544430	-1.655341	-0.892466
H	-4.955363	-3.155608	-1.630060
H	-6.477606	-3.150193	-0.723926
C	0.131690	-4.873241	1.755180
H	-0.833638	-5.380857	1.802500
H	0.915135	-5.635343	1.766437
H	0.238856	-4.252393	2.647274
C	1.671611	-3.395652	0.445206
H	1.834330	-2.813429	-0.465290
H	1.837810	-2.746116	1.308067
H	2.420558	-4.189997	0.472105
C	0.103679	-4.931882	-0.765584
H	0.878140	-5.703199	-0.751903
H	-0.869201	-5.427487	-0.774489
H	0.205309	-4.354777	-1.687318
H	1.511225	3.685590	0.387660

Table S29. Cartesian coordinates for unsubstituted $BIP^{\bullet+}$: E1PT. (-1000.62760437 E_h)

atom	x	y	z
C	-0.481460	2.798619	0.402486
C	-1.872035	2.988894	0.269299
C	-2.427965	4.262474	0.146150
C	-1.537118	5.329379	0.160857
C	-0.145848	5.137431	0.294966
C	0.410645	3.869764	0.419724
C	-1.474773	0.791547	0.411596
H	-3.495229	4.403818	0.040391
H	-1.920937	6.337841	0.067851
H	0.505711	6.002522	0.301456
N	-2.433935	1.725085	0.281265
C	-3.053551	-1.163975	0.326475
C	-1.685513	-0.638078	0.446022
C	-0.614068	-1.496644	0.569681
C	-0.790316	-2.896495	0.585733
C	-2.098795	-3.412224	0.479185
C	-3.225227	-2.621697	0.352200
H	0.392149	-1.106942	0.653944
H	-2.220848	-4.483589	0.496563
C	0.439351	-3.787275	0.689241
C	-4.622235	-3.224154	0.237603
O	-4.028082	-0.379597	0.204790
N	-0.287106	1.429849	0.490081
H	0.607905	0.969745	0.581397
H	-3.408364	1.439051	0.205075
C	-5.507223	-2.706211	1.394068
H	-5.624162	-1.625218	1.345914
H	-6.494337	-3.171184	1.328223
H	-5.068504	-2.969290	2.360135
C	-4.585072	-4.758574	0.317183
H	-3.998342	-5.192908	-0.496315
H	-4.167537	-5.102147	1.267000
H	-5.604894	-5.140512	0.238441
C	0.085091	-5.279205	0.716093
H	-0.524337	-5.534592	1.586668
H	-0.453221	-5.580549	-0.185678
H	1.005580	-5.864192	0.767624
C	1.338260	-3.507667	-0.536970
H	0.818024	-3.757584	-1.464670
H	1.637220	-2.458209	-0.581338
H	2.242745	-4.117698	-0.473057
C	1.215558	-3.435173	1.976803
H	0.603499	-3.613459	2.863694
H	2.106549	-4.064317	2.040687
H	1.538619	-2.391955	1.983161
C	-5.247676	-2.831054	-1.119733
H	-6.246755	-3.268581	-1.194294
H	-5.332022	-1.750328	-1.221679
H	-4.645652	-3.215480	-1.946953
H	1.476466	3.716867	0.524609

Table S30. Cartesian coordinates for unsubstituted BI_2P. (-1379.53872842 E_h)

atom	x	y	z
C	1.602618	1.144917	0.128626
C	0.385313	1.849031	-0.057173
C	0.396748	3.245373	-0.166291
C	1.623471	3.895664	-0.077190
C	2.823154	3.179740	0.115227
C	2.835308	1.791115	0.220849
C	-0.128404	-0.248034	0.057269
H	-0.526897	3.792600	-0.314835
H	1.662511	4.975748	-0.159959
H	3.758652	3.723164	0.180893
C	-2.285657	-1.450144	0.020173
C	-3.087877	-2.612399	0.060747
C	-2.489434	-3.870998	0.174964
C	-1.097350	-3.921679	0.248894
C	-0.310240	-2.760726	0.209880
C	-0.885638	-1.487825	0.091946
C	-4.433965	-0.904610	-0.084634
H	-3.089742	-4.771733	0.207176
H	-0.605371	-4.882608	0.340331
H	0.767715	-2.855356	0.274637
N	-0.674974	0.955844	-0.094834
C	-6.909588	-0.761726	-0.180642
C	-5.648875	-0.108643	-0.152941
C	-5.587486	1.292288	-0.170729
C	-6.739025	2.069202	-0.215708
C	-7.968669	1.394891	-0.242198
C	-8.096567	0.003430	-0.224548
H	-4.618166	1.776740	-0.142417
H	-8.873143	1.982124	-0.272846
C	-6.632124	3.598474	-0.229863
C	-9.479794	-0.666960	-0.243392
O	-6.986669	-2.112790	-0.163422
H	-6.053680	-2.472808	-0.103034
N	-3.160868	-0.393883	-0.073313
N	-4.420188	-2.237918	-0.009653
H	-2.843054	0.567472	-0.127756
N	1.236006	-0.184270	0.191200
H	1.855680	-0.968396	0.328855
C	-5.840322	4.040700	-1.476576
H	-5.727094	5.128792	-1.487527
H	-4.842108	3.596118	-1.489279
H	-6.358450	3.741082	-2.391539
C	-5.885712	4.069476	1.034268
H	-4.882358	3.639668	1.084131
H	-5.786592	5.158884	1.031313
H	-6.426108	3.776067	1.938273
C	-8.010839	4.271352	-0.261618
H	-8.574040	3.987272	-1.154753
H	-8.604440	4.005706	0.617394
H	-7.886992	5.356823	-0.271485
C	-9.618449	-1.552658	-1.499440
H	-8.844880	-2.318887	-1.533314
H	-10.596211	-2.043609	-1.501087

H	-9.544283	-0.944693	-2.405067
C	-9.669753	-1.521662	1.028189
H	-10.653490	-2.000309	1.008122
H	-8.908076	-2.295749	1.107737
H	-9.619667	-0.892668	1.921086
C	-10.616406	0.366139	-0.274526
H	-10.598643	1.017203	0.603172
H	-10.573734	0.995667	-1.166959
H	-11.573240	-0.161600	-0.281721
H	3.756307	1.240795	0.369148

Table S31. Cartesian coordinates for unsubstituted $BI_2P^{\bullet+}$: E0PT. (-1379.34492803 E_h)

atom	x	y	z
C	1.646939	1.115110	0.108527
C	0.435383	1.830938	-0.072492
C	0.456660	3.228418	-0.171446
C	1.687975	3.867163	-0.077905
C	2.882512	3.139714	0.109621
C	2.885007	1.751082	0.205468
C	-0.092347	-0.261510	0.029944
H	-0.462833	3.783738	-0.314244
H	1.736584	4.947348	-0.152453
H	3.821808	3.675886	0.179339
C	-2.270395	-1.422790	-0.008161
C	-3.102304	-2.575442	0.032785
C	-2.531547	-3.853292	0.142508
C	-1.148285	-3.924017	0.210901
C	-0.330476	-2.771642	0.172899
C	-0.867444	-1.489743	0.060354
C	-4.391451	-0.826490	-0.108176
H	-3.151230	-4.739585	0.174627
H	-0.669730	-4.891554	0.297863
H	0.744260	-2.894913	0.236185
N	-0.630783	0.946660	-0.114699
C	-6.868966	-0.742718	-0.196474
C	-5.591184	-0.041137	-0.177039
C	-5.567285	1.348376	-0.211504
C	-6.754648	2.075464	-0.277547
C	-7.993982	1.363471	-0.319600
C	-8.102843	-0.004859	-0.278408
H	-4.614663	1.858617	-0.183341
H	-8.896832	1.953414	-0.374154
C	-6.791319	3.592842	-0.288850
C	-9.453483	-0.723409	-0.295150
O	-6.898061	-2.044153	-0.136356
H	-5.917312	-2.404150	-0.078937
N	-3.109846	-0.349029	-0.097582
N	-4.409070	-2.166454	-0.033424
H	-2.758820	0.604432	-0.151236
N	1.270467	-0.211660	0.163315
H	1.884046	-1.002300	0.293711
C	-7.521761	4.065384	-1.566536
H	-8.536270	3.666505	-1.625324
H	-7.586994	5.156013	-1.558136
H	-6.977469	3.756510	-2.461819
C	-7.576995	4.068356	0.956053
H	-7.652983	5.158275	0.936392
H	-8.588388	3.657457	0.977542
H	-7.063615	3.772035	1.873545
C	-5.388920	4.211274	-0.259146
H	-4.846349	3.929508	0.646718
H	-4.800757	3.905632	-1.127868
H	-5.477346	5.299313	-0.275035
C	-9.530272	-1.681604	-1.503746
H	-8.763897	-2.454382	-1.458254
H	-10.509881	-2.165963	-1.513912

H	-9.414113	-1.129224	-2.439508
C	-10.612388	0.277467	-0.408649
H	-10.636191	0.968732	0.437449
H	-10.556370	0.861632	-1.330611
H	-11.552588	-0.277258	-0.416563
C	-9.636172	-1.510772	1.021460
H	-10.611635	-2.003830	1.011209
H	-8.867115	-2.271131	1.149368
H	-9.605998	-0.833971	1.878911
H	3.801584	1.192672	0.349564

Table S32. Cartesian coordinates for unsubstituted $BI_2P^{\bullet+}$: E1PT. (-1379.36048500 E_h)

atom	x	y	z
C	1.571475	1.090663	-0.051939
C	0.330271	1.764651	-0.181248
C	0.304538	3.146925	-0.408707
C	1.522379	3.810144	-0.505930
C	2.748394	3.124113	-0.371332
C	2.796747	1.752184	-0.143624
C	-0.128012	-0.325123	0.129754
H	-0.638165	3.671073	-0.512124
H	1.535215	4.879256	-0.683966
H	3.675674	3.679610	-0.450062
C	-2.276052	-1.523925	0.231200
C	-3.069848	-2.679731	0.314595
C	-2.499980	-3.943637	0.469632
C	-1.110065	-3.990267	0.535371
C	-0.312959	-2.835168	0.436917
C	-0.873913	-1.564708	0.277209
C	-4.409903	-0.899014	0.087645
H	-3.108620	-4.835163	0.534487
H	-0.620867	-4.947997	0.661357
H	0.763429	-2.942413	0.488429
N	-0.709029	0.857503	-0.058698
C	-6.905230	-0.767801	-0.166467
C	-5.605043	-0.095902	-0.027136
C	-5.524207	1.279932	0.007566
C	-6.679701	2.084989	-0.091364
C	-7.931178	1.451122	-0.243057
C	-8.096825	0.079970	-0.282518
H	-4.561705	1.760599	0.129446
H	-8.805092	2.077881	-0.323109
C	-6.538743	3.597587	0.010580
C	-9.471251	-0.562033	-0.437287
O	-6.974554	-2.022938	-0.184175
N	-3.135477	-0.454971	0.097585
N	-4.377944	-2.240093	0.215794
H	-2.771802	0.493002	-0.001847
N	1.238938	-0.234120	0.145465
H	1.886840	-0.998705	0.262523
H	-5.249060	-2.767888	0.186620
C	-7.873113	4.324828	-0.198216
H	-7.711078	5.401807	-0.118499
H	-8.294766	4.117480	-1.184936
H	-8.609153	4.041663	0.558092
C	-5.529752	4.093783	-1.046795
H	-4.543425	3.645635	-0.909793
H	-5.878109	3.863873	-2.056269
H	-5.420195	5.177369	-0.957279
C	-6.004355	3.932608	1.421813
H	-6.703867	3.596779	2.190769
H	-5.038008	3.459034	1.607640
H	-5.878648	5.014047	1.517078
C	-9.505536	-1.377612	-1.749046
H	-8.749479	-2.161806	-1.744471
H	-10.490537	-1.837856	-1.863643

H	-9.331191	-0.726873	-2.609581
C	-10.587969	0.490780	-0.496065
H	-10.617980	1.098579	0.411732
H	-10.478287	1.159069	-1.353882
H	-11.547950	-0.021011	-0.592387
C	-9.760024	-1.486945	0.768265
H	-10.757242	-1.919892	0.653838
H	-9.030574	-2.291529	0.835588
H	-9.742721	-0.916477	1.700369
H	3.736452	1.223674	-0.041667

Table S33. Cartesian coordinates for unsubstituted $BI_2P^{\bullet+}$: E2PT. (-1379.36613557 E_h)

atom	x	y	z
C	1.543637	1.143265	-0.200865
C	0.313513	1.818421	-0.326095
C	0.252443	3.188355	-0.574351
C	1.468817	3.853083	-0.697793
C	2.698940	3.177336	-0.569176
C	2.761390	1.809555	-0.320176
C	-0.107816	-0.347334	0.048012
H	-0.696150	3.699963	-0.671462
H	1.470927	4.918480	-0.893343
H	3.621021	3.736663	-0.670045
C	-2.276001	-1.505284	0.202179
C	-3.035205	-2.697140	0.321961
C	-2.439081	-3.945696	0.487074
C	-1.044709	-3.980443	0.528480
C	-0.269042	-2.819327	0.395623
C	-0.863326	-1.562996	0.227317
C	-4.347658	-0.922355	0.087698
H	-3.029581	-4.848142	0.579059
H	-0.542767	-4.930569	0.661383
H	0.809790	-2.907608	0.427143
N	-0.670885	0.857672	-0.158825
C	-6.869052	-0.781867	-0.133552
C	-5.558935	-0.129091	-0.016095
C	-5.463475	1.248263	0.004104
C	-6.604873	2.066020	-0.090235
C	-7.869993	1.447113	-0.216938
C	-8.052097	0.079288	-0.238067
H	-4.482748	1.694705	0.108205
H	-8.737140	2.084234	-0.291400
C	-6.444655	3.579886	-0.015224
C	-9.439101	-0.546939	-0.360735
O	-6.958166	-2.038735	-0.142848
N	-3.105924	-0.421031	0.063143
N	-4.342378	-2.280647	0.239248
N	1.231256	-0.190954	0.028955
H	1.900501	-0.936786	0.157550
H	-5.205946	-2.814767	0.230105
H	-1.689220	0.958321	-0.174845
C	-9.513584	-1.377109	-1.660886
H	-8.765991	-2.169389	-1.662696
H	-10.506025	-1.827557	-1.749023
H	-9.350356	-0.739655	-2.533656
C	-5.434694	4.044969	-1.084907
H	-5.308250	5.128344	-1.015359
H	-4.455298	3.582790	-0.944376
H	-5.790897	3.803165	-2.089093
C	-10.543206	0.519393	-0.409897
H	-10.545803	1.140143	0.489587
H	-10.442700	1.175088	-1.278565
H	-11.512642	0.020652	-0.478314
C	-9.717606	-1.455024	0.859445
H	-8.999933	-2.271097	0.917279
H	-9.668895	-0.877084	1.786045

H	-10.724498	-1.872674	0.774033
C	-7.769970	4.321676	-0.232463
H	-8.202429	4.095801	-1.210583
H	-8.505141	4.067411	0.534951
H	-7.593960	5.398391	-0.180527
C	-5.899743	3.935067	1.386224
H	-6.598696	3.620262	2.164892
H	-4.938398	3.452184	1.574216
H	-5.761458	5.016561	1.464871
H	3.703071	1.285787	-0.222005

Table S34. Cartesian coordinates for **1**. (-1417.60070286 E_h)

atom	x	y	z
C	-0.475377	2.735531	0.550582
C	-1.874687	2.918177	0.478109
C	-2.407406	4.210624	0.428782
C	-1.516685	5.286483	0.456794
C	-0.131117	5.092530	0.533208
C	-1.506795	0.772300	0.515659
H	-3.477413	4.367340	0.367313
H	-1.905189	6.297042	0.420381
H	0.531295	5.950465	0.555928
N	-2.488326	1.674595	0.460859
C	-3.031414	-1.181445	0.389968
C	-1.713145	-0.665512	0.490621
C	-0.620815	-1.543071	0.535623
C	-0.793213	-2.920355	0.482847
C	-2.106811	-3.400443	0.372618
C	-3.235581	-2.578191	0.321665
H	0.380383	-1.134424	0.608815
H	-2.257550	-4.467454	0.320600
C	0.430275	-3.841765	0.515682
C	-4.645709	-3.174012	0.187181
O	-4.097120	-0.348112	0.352182
H	-3.758238	0.592288	0.385542
N	-0.276473	1.379041	0.574102
H	0.646914	0.965789	0.621973
C	1.292743	-3.569419	-0.733500
H	1.606690	-2.523414	-0.772898
H	2.190505	-4.194297	-0.718971
H	0.736109	-3.792753	-1.647716
C	1.267773	-3.545381	1.775411
H	0.691241	-3.740272	2.683647
H	2.156957	-4.182026	1.792389
H	1.599372	-2.504222	1.799067
C	0.039312	-5.325433	0.528385
H	-0.559800	-5.577434	1.407600
H	-0.527960	-5.600879	-0.364527
H	0.942769	-5.939578	0.551379
C	-5.300519	-2.673816	-1.117983
H	-6.311871	-3.081721	-1.205527
H	-5.362025	-1.586636	-1.141570
H	-4.725333	-3.008066	-1.986029
C	-5.509129	-2.768813	1.399818
H	-5.619518	-1.687456	1.466607
H	-6.503497	-3.216643	1.313236
H	-5.054001	-3.126297	2.327739
C	-4.614953	-4.709729	0.132617
H	-4.048359	-5.074900	-0.728076
H	-4.178388	-5.141870	1.036806
H	-5.638353	-5.081496	0.043220
C	0.433145	3.806901	0.579244
C	1.864463	3.605243	0.651377
N	2.368413	2.415606	0.682479

H	2.470578	4.513941	0.681536
C	3.755582	2.210553	0.761858
C	4.167441	0.871229	0.876194
C	4.736419	3.222585	0.733358
C	5.510546	0.538614	0.966259
H	3.407866	0.098134	0.893252
C	6.080754	2.900852	0.821959
H	4.456564	4.263626	0.638719
C	6.477574	1.556676	0.940148
H	5.818184	-0.495149	1.053375
H	6.831051	3.681479	0.798752
C	7.864333	1.229513	1.022532
N	8.996276	0.964919	1.084075

Table S35. Cartesian coordinates for **1**$^{\bullet+}$: E0PT. (-1417.40700695 E_h)

atom	x	y	z
C	-0.377947	2.682076	0.062980
C	-1.788434	2.826492	-0.025369
C	-2.362083	4.099901	-0.178004
C	-1.499580	5.185298	-0.226844
C	-0.099791	5.030931	-0.125825
C	-1.351593	0.705291	0.194624
H	-3.434823	4.220890	-0.254150
H	-1.905249	6.182515	-0.342332
H	0.532741	5.909890	-0.162086
N	-2.357095	1.582625	0.061375
C	-2.958458	-1.176442	0.384363
C	-1.577462	-0.709206	0.320009
C	-0.540633	-1.632338	0.371476
C	-0.807218	-2.997199	0.489680
C	-2.167732	-3.425674	0.579648
C	-3.247617	-2.579055	0.539879
H	0.481186	-1.287031	0.310571
H	-2.347101	-4.485017	0.682814
C	0.288953	-4.047175	0.527242
C	-4.689022	-3.079969	0.640141
O	-3.940648	-0.326728	0.294797
H	-3.549693	0.636943	0.179019
N	-0.140128	1.343776	0.196448
H	0.797059	0.969150	0.303292
C	-5.385841	-2.434352	1.858458
H	-5.426616	-1.349200	1.774572
H	-6.408500	-2.813865	1.924883
H	-4.864931	-2.695971	2.782862
C	-4.731300	-4.603845	0.827311
H	-5.773059	-4.921034	0.902971
H	-4.279795	-5.132045	-0.016541
H	-4.217995	-4.910409	1.742369
C	-5.454474	-2.731995	-0.656252
H	-5.511038	-1.656119	-0.815142
H	-4.968836	-3.189901	-1.521081
H	-6.471552	-3.125766	-0.586987
C	0.191337	-4.809950	1.868144
H	-0.777920	-5.297158	1.990866
H	0.965354	-5.581036	1.898349
H	0.344358	-4.130017	2.708944
C	1.690487	-3.437203	0.406806
H	1.819068	-2.904975	-0.539049
H	1.900037	-2.744776	1.225959
H	2.432905	-4.236971	0.445443
C	0.068935	-5.031643	-0.644357
H	0.843236	-5.802352	-0.612647
H	-0.903364	-5.524995	-0.587776
H	0.136574	-4.512382	-1.602905
C	0.501784	3.779239	0.021699
C	1.938754	3.620054	0.143207
N	2.466912	2.456207	0.308826
H	2.536971	4.534701	0.111216
C	3.862253	2.339168	0.390035

C	4.742325	3.142554	-0.357529
C	4.381523	1.340518	1.230035
C	6.113577	2.973952	-0.240741
H	4.345814	3.878130	-1.045999
C	5.751267	1.174337	1.362093
H	3.694180	0.712343	1.782793
C	6.624881	1.994099	0.626733
H	6.792161	3.587699	-0.819240
H	6.152934	0.414489	2.019916
C	8.036287	1.819351	0.745863
N	9.187707	1.677072	0.840328

Table S36. Cartesian coordinates for **1**$^{\bullet+}$: E1PT. (-1417.42192640 E_h)

atom	x	y	z
C	-0.460401	2.801689	0.252324
C	-1.845919	2.993558	0.130906
C	-2.394863	4.270483	-0.004050
C	-1.498425	5.336159	-0.006314
C	-0.111177	5.144895	0.119947
C	-1.438755	0.799756	0.316641
H	-3.461592	4.418909	-0.103541
H	-1.880086	6.344160	-0.106989
H	0.546634	6.005870	0.113275
N	-2.403718	1.728240	0.173511
C	-3.007924	-1.161690	0.291908
C	-1.642977	-0.627071	0.402399
C	-0.568862	-1.472253	0.582326
C	-0.741341	-2.871511	0.655156
C	-2.046848	-3.396238	0.551627
C	-3.175310	-2.617039	0.377239
H	0.432228	-1.070573	0.672056
H	-2.166614	-4.466116	0.617155
C	0.488084	-3.752521	0.826669
C	-4.570358	-3.227468	0.284981
O	-3.983608	-0.385345	0.134719
N	-0.252814	1.445593	0.363710
H	0.683917	1.061496	0.457790
H	-3.377901	1.437311	0.111113
C	-5.447742	-2.682320	1.435484
H	-5.560269	-1.601589	1.367287
H	-6.437503	-3.143333	1.382759
H	-5.006404	-2.930217	2.404205
C	-4.527255	-4.759114	0.402994
H	-3.937268	-5.209809	-0.399138
H	-4.109512	-5.077998	1.361302
H	-5.545575	-5.146493	0.332467
C	0.137382	-5.243782	0.902205
H	-0.492342	-5.468332	1.766646
H	-0.379937	-5.579328	0.000291
H	1.058016	-5.822896	0.997115
C	1.422403	-3.521374	-0.382832
H	0.926418	-3.803554	-1.314426
H	1.728061	-2.475740	-0.459278
H	2.321529	-4.131836	-0.270021
C	1.221525	-3.343359	2.122613
H	0.571277	-3.461542	2.992227
H	2.098493	-3.981242	2.255791
H	1.561731	-2.305916	2.083860
C	-5.209276	-2.870843	-1.075934
H	-6.204001	-3.320828	-1.133319
H	-5.305935	-1.793557	-1.198511
H	-4.609147	-3.266161	-1.899261
C	0.450521	3.870432	0.250751
C	1.881035	3.652104	0.374977
N	2.356628	2.458487	0.473766
H	2.514223	4.542801	0.391145
C	3.743247	2.257018	0.538957

C	4.672996	3.077463	-0.125131
C	4.197283	1.145074	1.266910
C	6.030703	2.810897	-0.033506
H	4.327901	3.905716	-0.731100
C	5.553607	0.878579	1.372821
H	3.470126	0.504204	1.750459
C	6.477123	1.713690	0.721641
H	6.747146	3.440139	-0.545596
H	5.904586	0.028389	1.943356
C	7.874048	1.432919	0.808917
N	9.012792	1.201892	0.876154

Table S37. Cartesian coordinates for **1**$^{\bullet+}$: E2PT. (-1417.42528819 E_h)

atom	x	y	z
C	-0.553785	2.830205	0.383354
C	-1.947475	3.052363	0.269591
C	-2.481193	4.333383	0.158612
C	-1.582094	5.408564	0.167266
C	-0.203794	5.216853	0.281851
C	-1.480427	0.887725	0.410254
H	-3.547396	4.495663	0.065695
H	-1.968567	6.416107	0.084040
H	0.460749	6.072438	0.285367
N	-2.496027	1.790581	0.291214
C	-3.006042	-1.135315	0.341821
C	-1.664858	-0.549314	0.453447
C	-0.555105	-1.358989	0.581505
C	-0.666914	-2.762168	0.603080
C	-1.953031	-3.339007	0.496404
C	-3.112513	-2.599711	0.365734
H	0.420313	-0.895973	0.655645
H	-2.025826	-4.415337	0.514378
C	0.603861	-3.595248	0.706879
C	-4.482510	-3.261552	0.241278
O	-4.017415	-0.393885	0.229798
N	-0.283137	1.496550	0.469191
H	-3.464637	1.491695	0.229746
C	-5.115704	-2.885713	-1.117091
H	-6.103841	-3.347349	-1.195610
H	-5.224974	-1.807111	-1.218783
H	-4.502144	-3.255142	-1.942913
C	-5.396309	-2.790368	1.394636
H	-5.552132	-1.713938	1.355907
H	-6.364965	-3.291427	1.316526
H	-4.955316	-3.046927	2.361629
C	-4.383981	-4.792944	0.311542
H	-3.775197	-5.198575	-0.500520
H	-3.957860	-5.125494	1.261614
H	-5.387145	-5.215510	0.223838
C	0.321043	-5.102170	0.735042
H	-0.278442	-5.384025	1.604543
H	-0.202902	-5.428392	-0.166621
H	1.266845	-5.645620	0.788649
C	1.365705	-3.202419	1.990266
H	2.297097	-3.771463	2.045913
H	1.617685	-2.139442	1.997678
H	0.774701	-3.424211	2.881988
C	1.489093	-3.274116	-0.518263
H	0.976253	-3.532414	-1.447874
H	1.749566	-2.213807	-0.551675
H	2.414920	-3.852141	-0.462105
C	0.347834	3.923836	0.390964
C	1.749187	3.730340	0.503293
N	2.276771	2.531671	0.588769
H	2.409631	4.588343	0.523029
C	3.637755	2.194243	0.717761
C	3.938702	0.834011	0.854899

C	4.653055	3.158590	0.712161
C	5.258071	0.430462	0.994540
H	3.140299	0.100729	0.850947
C	5.971304	2.756111	0.853014
H	4.430909	4.210285	0.593926
C	6.279790	1.392705	0.996104
H	5.499180	-0.618391	1.103668
H	6.764481	3.492364	0.849876
C	7.642200	0.986282	1.137551
N	8.753203	0.660354	1.249035
H	1.601958	1.749398	0.571954

Table S38. Cartesian coordinates for **1'**. (-1796.33573006 E_h)

atom	x	y	z
C	1.623611	1.097373	-0.176312
C	0.410966	1.808106	-0.336715
C	0.439412	3.190977	-0.551669
C	1.681779	3.825087	-0.594476
C	2.875948	3.109607	-0.422930
C	-0.115157	-0.267769	-0.036810
H	-0.481032	3.747384	-0.681869
H	1.729091	4.895057	-0.757039
H	3.824690	3.633181	-0.454585
C	-2.279736	-1.448501	0.132953
C	-3.081294	-2.606374	0.252340
C	-2.481116	-3.862142	0.386619
C	-1.087009	-3.917939	0.389530
C	-0.300366	-2.764146	0.254383
C	-0.877764	-1.493593	0.121343
C	-4.430008	-0.902961	0.096223
H	-3.082044	-4.757948	0.482805
H	-0.593783	-4.876985	0.492524
H	0.779039	-2.860441	0.249772
N	-0.657631	0.929802	-0.243936
C	-6.892957	-0.757472	-0.161231
C	-5.644255	-0.106732	0.016813
C	-5.590688	1.290572	0.112474
C	-6.739980	2.067918	0.024481
C	-7.955219	1.398466	-0.183764
C	-8.073425	0.009348	-0.286683
H	-4.632522	1.768128	0.283153
H	-8.854115	1.990719	-0.263050
C	-6.647433	3.589404	0.187534
C	-9.434312	-0.659435	-0.534041
O	-6.962570	-2.108102	-0.223945
H	-6.046780	-2.471024	-0.054718
N	-3.157021	-0.393662	0.042800
N	-4.415555	-2.231869	0.220548
H	-2.846253	0.560747	-0.097147
N	1.258835	-0.210211	0.009410
H	1.927161	-0.956074	0.159237
C	-5.649280	4.158630	-0.839104
H	-5.552840	5.241111	-0.714498
H	-4.657890	3.715737	-0.715366
H	-5.986328	3.958728	-1.859741
C	-6.146350	3.905800	1.611051
H	-5.172537	3.446849	1.797209
H	-6.045376	4.986249	1.748430
H	-6.846916	3.526002	2.359565
C	-8.004122	4.277587	-0.013613
H	-8.408041	4.089560	-1.011832
H	-8.739276	3.937878	0.720627
H	-7.885793	5.357416	0.105232
C	-9.388132	-1.438106	-1.865675
H	-8.609145	-2.200011	-1.853720

H	-10.350537	-1.926227	-2.046517
H	-9.194206	-0.755473	-2.697431
C	-9.781865	-1.615416	0.626930
H	-10.748441	-2.090899	0.434526
H	-9.028326	-2.392283	0.742923
H	-9.857984	-1.061039	1.566313
C	-10.569155	0.371493	-0.636560
H	-10.702162	0.924244	0.297307
H	-10.396849	1.092586	-1.439677
H	-11.504458	-0.151291	-0.852386
C	2.882036	1.721834	-0.213010
C	4.117233	0.987731	-0.037816
N	4.126186	-0.295265	0.110428
H	5.034473	1.583571	-0.023741
C	5.349764	-0.970122	0.227161
C	5.345245	-2.186153	0.931531
C	6.550716	-0.517575	-0.352358
C	6.512456	-2.915107	1.097341
H	4.413427	-2.532875	1.360710
C	7.721975	-1.242460	-0.195947
H	6.559294	0.389391	-0.943245
C	7.711549	-2.441906	0.536538
H	6.506923	-3.842688	1.654999
H	8.642319	-0.898964	-0.651082
C	8.918368	-3.185678	0.704147
N	9.902216	-3.791109	0.847586

Table S39. Cartesian coordinates for **1'**$^{\bullet+}$: E0PT. (-1796.14151559 E_h)

atom	x	y	z
C	1.667684	1.113832	-0.087570
C	0.462715	1.838897	-0.238828
C	0.489598	3.239094	-0.257282
C	1.724024	3.872622	-0.118115
C	2.911573	3.140772	0.041194
C	-0.056360	-0.259052	-0.274469
H	-0.425537	3.806649	-0.375133
H	1.772375	4.954642	-0.130598
H	3.853041	3.666701	0.153031
C	-2.230534	-1.422365	-0.376150
C	-3.057820	-2.577996	-0.421078
C	-2.480569	-3.857394	-0.456753
C	-1.095656	-3.927497	-0.437834
C	-0.282285	-2.773104	-0.380761
C	-0.826026	-1.489069	-0.347382
C	-4.355390	-0.830839	-0.370031
H	-3.096246	-4.746237	-0.493921
H	-0.612824	-4.896368	-0.463935
H	0.794036	-2.896314	-0.369368
N	-0.598354	0.954388	-0.346273
C	-6.833611	-0.752975	-0.283991
C	-5.558123	-0.047986	-0.319721
C	-5.537797	1.341118	-0.287753
C	-6.726391	2.065380	-0.205957
C	-7.963318	1.350437	-0.150546
C	-8.068961	-0.018216	-0.190931
H	-4.586993	1.854301	-0.321345
H	-8.866876	1.937939	-0.083541
C	-6.764793	3.582494	-0.183217
C	-9.417245	-0.740425	-0.158512
O	-6.859148	-2.054760	-0.334848
H	-5.877828	-2.413039	-0.383941
N	-3.075564	-0.349205	-0.351297
N	-4.367505	-2.171750	-0.415692
H	-2.732669	0.607871	-0.324620
N	1.307205	-0.208169	-0.118356
H	1.973384	-0.964285	-0.017159
C	-7.566068	4.067601	-1.414194
H	-8.576946	3.655116	-1.427902
H	-7.643883	5.157133	-1.383075
H	-7.062518	3.780796	-2.340097
C	-7.479315	4.042875	1.107864
H	-7.542150	5.133649	1.112521
H	-8.493791	3.645165	1.174273
H	-6.925213	3.723005	1.993245
C	-5.363392	4.202641	-0.224741
H	-4.764012	3.889133	0.633428
H	-4.831749	3.930230	-1.139923
H	-5.452564	5.290338	-0.196937
C	-9.611230	-1.528022	-1.473340
H	-8.840547	-2.285390	-1.609313
H	-10.584430	-2.025137	-1.452593
H	-9.592933	-0.851067	-2.331019

C	-10.577802	0.256985	-0.031626
H	-10.515138	0.838332	0.891734
H	-10.611095	0.950821	-0.875255
H	-11.516242	-0.300492	-0.016930
C	-9.479001	-1.699684	1.050093
H	-10.458740	-2.183385	1.071702
H	-8.713653	-2.472717	0.994458
H	-9.350973	-1.148563	1.985055
C	2.918293	1.738212	0.062612
C	4.141331	0.980559	0.238269
N	4.133836	-0.309572	0.251648
H	5.065359	1.556807	0.342485
C	5.328509	-1.003767	0.480510
C	5.492211	-2.242578	-0.162783
C	6.331159	-0.541851	1.353139
C	6.646656	-2.986459	0.022561
H	4.704081	-2.602012	-0.812603
C	7.484708	-1.285598	1.552532
H	6.189953	0.387684	1.890471
C	7.650971	-2.510227	0.883520
H	6.776510	-3.934663	-0.483676
H	8.254587	-0.930028	2.225467
C	8.836116	-3.278137	1.089411
N	9.803251	-3.903611	1.258135

Table S40. Cartesian coordinates for **1'**$^{\bullet+}$: E1PT. (-1796.15667338 E_h)

atom	x	y	z
C	1.586283	1.042730	-0.158194
C	0.362240	1.735273	-0.305895
C	0.357489	3.132864	-0.397874
C	1.580651	3.797576	-0.329605
C	2.788297	3.098474	-0.173149
C	-0.112145	-0.371427	-0.215472
H	-0.572997	3.674234	-0.519191
H	1.604401	4.878081	-0.401308
H	3.721588	3.647664	-0.122982
C	-2.262826	-1.569344	-0.159103
C	-3.056030	-2.727726	-0.121647
C	-2.483835	-4.000203	-0.112114
C	-1.092833	-4.053344	-0.146432
C	-0.296533	-2.894512	-0.186624
C	-0.860676	-1.615903	-0.188156
C	-4.398746	-0.934749	-0.119595
H	-3.091188	-4.894367	-0.082142
H	-0.603779	-5.019256	-0.145410
H	0.780359	-3.002180	-0.226726
N	-0.682282	0.825776	-0.332046
C	-6.903619	-0.783657	-0.200336
C	-5.593279	-0.123617	-0.105763
C	-5.501072	1.248926	-0.012328
C	-6.652903	2.064688	-0.042959
C	-7.914890	1.442223	-0.150537
C	-8.093301	0.073874	-0.216850
H	-4.529733	1.715837	0.089747
H	-8.787313	2.075609	-0.171721
C	-6.500345	3.575890	0.066227
C	-9.481283	-0.555006	-0.289735
O	-6.982630	-2.036832	-0.260147
N	-3.123289	-0.492780	-0.155843
N	-4.365420	-2.281309	-0.098984
H	-2.766636	0.460206	-0.213818
N	1.253849	-0.286307	-0.108787
H	1.938223	-1.024068	0.007283
H	-5.240220	-2.804090	-0.095833
C	-7.833238	4.311184	-0.125883
H	-7.662096	5.387441	-0.057456
H	-8.271777	4.098216	-1.104121
H	-8.559604	4.039858	0.643867
C	-5.504726	4.072756	-1.003370
H	-4.516546	3.624289	-0.882585
H	-5.867660	3.845458	-2.008351
H	-5.393391	5.156098	-0.913396
C	-5.946545	3.902992	1.471338
H	-6.637426	3.567346	2.248185
H	-4.979775	3.424856	1.642500
H	-5.815489	4.983671	1.568921
C	-9.615882	-1.376296	-1.591857
H	-8.870136	-2.168203	-1.639046
H	-10.612003	-1.825099	-1.631426
H	-9.499642	-0.730493	-2.465787

C	-10.588389	0.509131	-0.284684
H	-10.565656	1.115910	0.623946
H	-10.516628	1.177358	-1.146504
H	-11.557364	0.007386	-0.329734
C	-9.697015	-1.471659	0.937688
H	-10.707078	-1.888299	0.900335
H	-8.978958	-2.289723	0.953437
H	-9.599703	-0.901517	1.865003
C	2.826593	1.699717	-0.083996
C	4.074655	0.980716	0.072083
N	4.110738	-0.307907	0.126340
H	4.984698	1.585473	0.121475
C	5.346240	-0.940454	0.323210
C	5.571103	-2.159276	-0.339494
C	6.337372	-0.425658	1.178549
C	6.777156	-2.827141	-0.196252
H	4.792226	-2.559267	-0.976659
C	7.541900	-1.094530	1.337017
H	6.149796	0.487475	1.729640
C	7.771583	-2.294124	0.642650
H	6.957169	-3.757310	-0.720319
H	8.305600	-0.698130	1.994109
C	9.016211	-2.974693	0.797461
N	10.033065	-3.526994	0.923890

Table S41. Cartesian coordinates for **1'**$^{\bullet+}$: E2PT. (-1796.16070572 E_h)

atom	x	y	z
C	2.955553	1.619313	-0.182038
C	1.648995	2.125210	-0.265412
C	1.401696	3.495472	-0.343881
C	2.513799	4.335156	-0.328253
C	3.821241	3.831240	-0.230851
C	1.548508	-0.109384	-0.169095
H	0.393632	3.882435	-0.411685
H	2.367176	5.405973	-0.390786
H	4.657063	4.520654	-0.215204
C	-0.431814	-1.567395	-0.125067
C	-1.018520	-2.857355	-0.106975
C	-0.252628	-4.020771	-0.094623
C	1.134600	-3.866389	-0.099271
C	1.742223	-2.602320	-0.119939
C	0.975790	-1.431042	-0.135133
C	-2.565815	-1.265236	-0.104212
H	-0.709836	-5.001937	-0.080685
H	1.764050	-4.747009	-0.089668
H	2.823259	-2.539592	-0.130637
N	0.815405	1.018951	-0.250263
C	-5.095811	-1.447632	-0.095657
C	-3.873202	-0.635345	-0.059375
C	-3.952300	0.740419	0.024908
C	-5.191007	1.404761	0.092951
C	-6.373304	0.630513	0.086427
C	-6.382127	-0.747132	-0.000627
H	-3.033215	1.311614	0.048305
H	-7.315604	1.151570	0.150614
C	-5.208225	2.926735	0.170105
C	-7.684502	-1.544236	-0.014969
O	-5.028241	-2.701130	-0.203406
N	-1.403290	-0.598945	-0.123431
N	-2.372484	-2.618275	-0.098896
N	2.850263	0.243922	-0.129490
H	3.671427	-0.349388	-0.049213
H	-3.155369	-3.263664	-0.106715
H	-0.207908	0.972120	-0.267935
C	-7.811826	-2.297068	-1.358106
H	-6.989674	-2.997447	-1.495610
H	-8.753722	-2.852121	-1.372919
H	-7.818605	-1.591777	-2.193385
C	-4.491399	3.494568	-1.075100
H	-4.473840	4.585948	-1.017353
H	-3.460135	3.141845	-1.141501
H	-5.013722	3.205749	-1.990414
C	-8.912848	-0.634121	0.135612
H	-8.893901	-0.078708	1.076765
H	-8.989971	0.084204	-0.684673
H	-9.812772	-1.252320	0.126399
C	-7.696745	-2.552031	1.155442
H	-6.871688	-3.257765	1.074360
H	-7.619108	-2.029317	2.112610
H	-8.639165	-3.106089	1.146278

C	-6.630439	3.498830	0.220079
H	-7.197814	3.236129	-0.676288
H	-7.179982	3.140554	1.094221
H	-6.576632	4.588007	0.280470
C	-4.446332	3.366417	1.439496
H	-4.955364	3.010450	2.338309
H	-3.424120	2.982100	1.445471
H	-4.400698	4.457701	1.480884
C	4.081072	2.457172	-0.155594
C	5.427079	1.921608	-0.045721
N	5.627519	0.650331	0.018778
H	6.242615	2.648767	-0.000911
C	6.937943	0.155439	0.080722
C	8.020530	0.762646	-0.581166
C	7.147934	-1.024422	0.813306
C	9.292957	0.220207	-0.481296
H	7.856842	1.643701	-1.188785
C	8.418807	-1.566146	0.927243
H	6.303495	-1.494032	1.301833
C	9.499704	-0.942110	0.280450
H	10.126215	0.682270	-0.994731
H	8.583121	-2.469088	1.501058
C	10.808276	-1.503685	0.381972
N	11.873107	-1.966838	0.462304

Table S42. Cartesian coordinates for **1'**$^{\bullet+}$: E3PT. (-1796.16206454 E_h)

atom	x	y	z
C	1.510943	1.181275	0.620999
C	0.288757	1.890610	0.714737
C	0.243232	3.258213	0.958606
C	1.465184	3.931063	1.113083
C	2.683460	3.261334	1.017565
C	-0.052087	-0.267274	0.328733
H	-0.698974	3.786894	1.029054
H	1.458610	4.996498	1.304010
H	3.611956	3.806889	1.135869
C	-2.208178	-1.469641	0.026634
C	-2.927386	-2.679915	-0.151539
C	-2.291626	-3.916633	-0.255652
C	-0.899284	-3.917500	-0.174079
C	-0.165447	-2.734429	0.010634
C	-0.797710	-1.491824	0.119045
C	-4.295168	-0.932668	-0.072159
H	-2.850166	-4.833215	-0.396123
H	-0.366637	-4.857331	-0.251149
H	0.914364	-2.776948	0.079230
N	-0.678792	0.931204	0.516461
C	-6.828075	-0.835154	-0.166840
C	-5.523344	-0.161997	-0.140047
C	-5.446836	1.215654	-0.208660
C	-6.600821	2.011933	-0.315617
C	-7.863802	1.374675	-0.308398
C	-8.027681	0.006855	-0.230022
H	-4.467641	1.677308	-0.202946
H	-8.743332	1.996182	-0.369599
C	-6.447558	3.522798	-0.451868
C	-9.412768	-0.637901	-0.218195
O	-6.897783	-2.093307	-0.136170
N	-3.074630	-0.403022	0.071147
N	-4.246003	-2.293773	-0.199723
N	1.284144	-0.146990	0.384374
H	-5.091503	-2.846675	-0.294704
H	-1.694186	1.023394	0.490107
C	-5.629572	3.817258	-1.728947
H	-5.484497	4.895975	-1.829826
H	-4.646684	3.342569	-1.696112
H	-6.157017	3.458658	-2.616268
C	-7.795834	4.246567	-0.557497
H	-8.367156	3.907426	-1.425186
H	-8.404910	4.097118	0.337506
H	-7.621400	5.318928	-0.669984
C	-5.685323	4.062451	0.777061
H	-6.230603	3.847519	1.699330
H	-4.689754	3.620174	0.856916
H	-5.567901	5.145501	0.686764
C	-9.570976	-1.563683	-1.445410
H	-8.837257	-2.367942	-1.429499
H	-10.573892	-1.999530	-1.443621
H	-9.448699	-0.997529	-2.372530
C	-10.530596	0.413835	-0.270687

H	-10.488215	1.094933	0.582999
H	-10.489117	1.009046	-1.186395
H	-11.496029	-0.096497	-0.245569
C	-9.595406	-1.452204	1.082437
H	-10.589123	-1.908761	1.087341
H	-8.846643	-2.238126	1.166388
H	-9.519517	-0.799529	1.956048
C	2.739868	1.870966	0.772314
C	3.989985	1.212736	0.666540
N	4.088921	-0.076671	0.438351
H	4.900472	1.788587	0.770850
C	5.269887	-0.833226	0.298154
C	5.123574	-2.183346	-0.042011
C	6.541773	-0.273293	0.473582
C	6.247718	-2.974528	-0.228317
H	4.133623	-2.603964	-0.169782
C	7.665178	-1.062926	0.287935
H	6.668839	0.764134	0.750160
C	7.524071	-2.414962	-0.067814
H	6.141062	-4.016844	-0.497096
H	8.651892	-0.638903	0.418338
C	8.688147	-3.219115	-0.268921
N	9.636291	-3.872223	-0.434657
H	3.193511	-0.578401	0.338574

Table S43. Cartesian coordinates for **2**. (-1439.88109971 E_h)

atom	x	y	z
C	-0.538732	2.762726	0.647831
C	-1.940434	2.924870	0.587435
C	-2.495034	4.210034	0.599917
C	-1.619265	5.294909	0.667440
C	-0.228402	5.118441	0.727116
C	-1.535216	0.784683	0.529041
H	-3.567606	4.353331	0.551754
H	-2.021273	6.301078	0.675836
H	0.420219	5.985676	0.780063
N	-2.532686	1.672525	0.517235
C	-3.032887	-1.184643	0.338277
C	-1.721182	-0.654214	0.448680
C	-0.618250	-1.518974	0.465507
C	-0.773788	-2.896999	0.381345
C	-2.081409	-3.391157	0.262963
C	-3.220172	-2.581578	0.235433
H	0.378485	-1.100677	0.543607
H	-2.218898	-4.458585	0.185949
C	0.460954	-3.804087	0.398923
C	-4.623753	-3.190407	0.090523
O	-4.109159	-0.363941	0.327378
H	-3.779595	0.579219	0.391299
N	-0.316501	1.408451	0.610687
H	0.616692	1.015683	0.647899
C	1.322633	-3.502287	-0.843783
H	1.624858	-2.452293	-0.867577
H	2.227641	-4.116788	-0.836193
H	0.770670	-3.719224	-1.762380
C	1.292841	-3.519437	1.665328
H	0.716785	-3.736060	2.568934
H	2.188695	-4.146832	1.673668
H	1.613272	-2.475452	1.707764
C	0.087567	-5.292410	0.388113
H	-0.512056	-5.563816	1.261250
H	-0.473102	-5.561784	-0.510760
H	0.998034	-5.896326	0.405928
C	-5.285346	-2.670150	-1.203151
H	-6.293238	-3.085190	-1.297479
H	-5.357019	-1.583293	-1.203968
H	-4.709488	-2.981646	-2.079131
C	-5.491989	-2.821349	1.311262
H	-5.609970	-1.742885	1.405441
H	-6.482815	-3.274031	1.210285
H	-5.036839	-3.200180	2.230670
C	-4.577204	-4.724120	0.005436
H	-4.010615	-5.067516	-0.864236
H	-4.133439	-5.169262	0.899758
H	-5.597309	-5.104074	-0.087612
C	0.356010	3.842780	0.716828
C	1.793751	3.653017	0.781250
N	2.309713	2.470425	0.782169

H	2.391795	4.566774	0.834460
C	3.700218	2.266000	0.851960
C	4.126927	0.930746	0.968654
C	4.680276	3.272017	0.812988
C	5.472781	0.608555	1.051685
H	3.375021	0.149043	0.994246
C	6.034279	2.960816	0.890451
H	4.397134	4.313154	0.715931
C	6.438976	1.624029	1.012660
H	5.799493	-0.420339	1.141959
H	6.765771	3.756815	0.855023
O	7.736110	1.222605	1.096633
C	8.750744	2.217548	0.956410
H	8.676016	2.974138	1.742879
H	9.699495	1.691931	1.045292
H	8.689316	2.705430	-0.020671

Table S44. Cartesian coordinates for **2**$^{\bullet+}$: E0PT. (-1439.68821524 E_h)

atom	x	y	z
C	-0.330266	2.621962	0.068479
C	-1.736568	2.819245	-0.030984
C	-2.254516	4.115929	-0.188017
C	-1.343257	5.161157	-0.227985
C	0.051281	4.951908	-0.118378
C	-1.377414	0.685549	0.202687
H	-3.320163	4.283815	-0.273141
H	-1.705602	6.174822	-0.345455
H	0.716690	5.806829	-0.153223
N	-2.351863	1.597982	0.055773
C	-3.024042	-1.162313	0.358900
C	-1.636851	-0.717638	0.341392
C	-0.612137	-1.652951	0.458313
C	-0.899677	-3.006593	0.596832
C	-2.270438	-3.415832	0.620521
C	-3.337589	-2.556693	0.517213
H	0.413832	-1.315153	0.443555
H	-2.468000	-4.471445	0.733016
C	0.182618	-4.063869	0.733276
C	-4.789207	-3.037697	0.568118
O	-3.990110	-0.294437	0.228980
H	-3.584375	0.656329	0.129468
N	-0.143331	1.280109	0.209173
H	0.786606	0.880402	0.306136
C	-5.513385	-2.377613	1.762945
H	-5.540804	-1.292677	1.669911
H	-6.540859	-2.747495	1.806631
H	-5.016636	-2.635997	2.701594
C	-4.859469	-4.560010	0.758056
H	-5.907255	-4.863359	0.801267
H	-4.387900	-5.096548	-0.069442
H	-4.379985	-4.870260	1.689848
C	-5.506937	-2.682557	-0.752688
H	-5.548376	-1.606078	-0.911961
H	-4.995859	-3.142761	-1.601655
H	-6.529665	-3.066538	-0.719632
C	-0.007144	-4.791530	2.083878
H	-0.986881	-5.267909	2.154634
H	0.756621	-5.566764	2.183842
H	0.096186	-4.091203	2.915685
C	1.592940	-3.461902	0.690195
H	1.786664	-2.955500	-0.258920
H	1.748622	-2.745139	1.500409
H	2.328343	-4.261180	0.800703
C	0.036027	-5.078120	-0.422848
H	0.791548	-5.859548	-0.310183
H	-0.946699	-5.554094	-0.427590
H	0.187802	-4.588257	-1.387248
C	0.601193	3.678751	0.032432
C	2.028712	3.439113	0.154595
N	2.480874	2.239591	0.295750
H	2.675051	4.319974	0.131312
C	3.859416	1.985695	0.380487

C	4.864181	2.865044	-0.055479
C	4.244387	0.740706	0.909396
C	6.209200	2.526567	0.053127
H	4.599044	3.810841	-0.512904
C	5.581010	0.399938	1.036326
H	3.471458	0.051908	1.231860
C	6.576413	1.292472	0.609145
H	6.961304	3.212933	-0.311140
H	5.876049	-0.553528	1.457260
O	7.860661	0.874048	0.758652
C	8.898578	1.724155	0.266174
H	8.892810	2.691157	0.776941
H	9.832731	1.206948	0.476220
H	8.795402	1.882591	-0.810740

Table S45. Cartesian coordinates for **2**$^{\bullet+}$: E1PT. (-1439.70330508 E_h)

atom	x	y	z
C	-0.510576	2.841719	0.215897
C	-1.897653	3.014936	0.086749
C	-2.459814	4.284430	-0.065963
C	-1.570792	5.356256	-0.083590
C	-0.180019	5.180085	0.037161
C	-1.461581	0.828548	0.310840
H	-3.527624	4.423234	-0.166786
H	-1.961095	6.359830	-0.197269
H	0.468432	6.047756	0.009944
N	-2.438607	1.742516	0.146374
C	-2.998062	-1.158716	0.281697
C	-1.648625	-0.597837	0.435382
C	-0.574251	-1.415920	0.714933
C	-0.732988	-2.810782	0.861311
C	-2.020047	-3.363846	0.688649
C	-3.144302	-2.613190	0.401548
H	0.411242	-0.986991	0.842665
H	-2.128104	-4.432066	0.792023
C	0.480119	-3.656975	1.222854
C	-4.513262	-3.254259	0.199008
O	-3.978362	-0.404987	0.056149
N	-0.285671	1.490681	0.352525
H	0.663788	1.133162	0.444651
H	-3.407696	1.438630	0.075066
C	-5.516845	-2.694689	1.232657
H	-5.631826	-1.617638	1.128597
H	-6.489422	-3.170794	1.080968
H	-5.183776	-2.916851	2.249764
C	-4.457826	-4.779792	0.369205
H	-3.787167	-5.243348	-0.358452
H	-4.128979	-5.063187	1.372218
H	-5.457972	-5.189056	0.212940
C	0.144358	-5.150137	1.329809
H	-0.615960	-5.337647	2.091461
H	-0.208271	-5.553997	0.377853
H	1.046200	-5.696781	1.613291
C	1.573146	-3.466318	0.148315
H	1.217151	-3.788644	-0.832699
H	1.890888	-2.423664	0.074612
H	2.448736	-4.063531	0.414779
C	1.017704	-3.168728	2.587434
H	0.263211	-3.291501	3.367808
H	1.899814	-3.752930	2.861509
H	1.306793	-2.116312	2.551377
C	-5.001969	-2.949278	-1.235893
H	-5.975510	-3.420213	-1.395564
H	-5.099669	-1.877118	-1.399391
H	-4.303245	-3.356540	-1.971447
C	0.395537	3.914277	0.187724
C	1.830096	3.696628	0.283022
N	2.300768	2.502947	0.405338
H	2.465238	4.583427	0.222079
C	3.682763	2.271910	0.503158

C	4.627207	3.227922	0.909791
C	4.132509	0.978126	0.184451
C	5.982364	2.915815	0.967721
H	4.307009	4.219517	1.207591
C	5.480802	0.661659	0.224505
H	3.403701	0.233122	-0.114715
C	6.418093	1.631672	0.611127
H	6.687187	3.665619	1.300136
H	5.831911	-0.329580	-0.034993
O	7.717916	1.234877	0.625535
C	8.710122	2.217499	0.929262
H	8.591673	2.597121	1.947834
H	9.669333	1.712211	0.836084
H	8.661931	3.052304	0.224145

Table S46. Cartesian coordinates for **2**$^{\bullet+}$: E2PT. (-1439.71014512 E_h)

atom	x	y	z
C	-0.437185	2.696377	0.019815
C	-1.819888	2.963796	-0.124344
C	-2.305785	4.256641	-0.309605
C	-1.367225	5.293769	-0.343874
C	0.003951	5.055397	-0.198124
C	-1.438264	0.795678	0.160606
H	-3.364547	4.451941	-0.423009
H	-1.712637	6.309712	-0.486489
H	0.700455	5.885089	-0.226143
N	-2.417113	1.728292	-0.029113
C	-3.060679	-1.141865	0.346191
C	-1.686878	-0.624692	0.308700
C	-0.611908	-1.484493	0.413215
C	-0.793204	-2.870851	0.571131
C	-2.112318	-3.376578	0.635715
C	-3.238967	-2.585843	0.532758
H	0.387171	-1.070301	0.367358
H	-2.238204	-4.439785	0.767497
C	0.431459	-3.774417	0.639185
C	-4.646414	-3.171624	0.605179
O	-4.040418	-0.360187	0.220808
N	-0.219438	1.358232	0.191909
H	-3.396951	1.462516	-0.056185
C	-5.401188	-2.871374	-0.709714
H	-6.395366	-3.324778	-0.668772
H	-5.508838	-1.799047	-0.862866
H	-4.866632	-3.296040	-1.563306
C	-5.403224	-2.549227	1.800861
H	-5.474032	-1.466973	1.700758
H	-6.413512	-2.965046	1.846063
H	-4.895697	-2.784812	2.740143
C	-4.620274	-4.695076	0.801239
H	-4.122045	-5.203794	-0.028317
H	-4.115146	-4.975071	1.729285
H	-5.647285	-5.062792	0.852930
C	0.067083	-5.242637	0.894683
H	-0.456651	-5.367991	1.845840
H	-0.563857	-5.646160	0.098959
H	0.981256	-5.838609	0.931776
C	1.366433	-3.291664	1.768366
H	2.252946	-3.929672	1.801340
H	1.696302	-2.262704	1.607788
H	0.866515	-3.345341	2.738401
C	1.175630	-3.669153	-0.710344
H	0.545644	-4.019764	-1.531332
H	1.472346	-2.638962	-0.918898
H	2.077334	-4.286332	-0.681086
C	0.504006	3.753842	-0.011670
C	1.899137	3.518146	0.161901
N	2.377724	2.315793	0.357688
H	2.587689	4.353451	0.144169
C	3.714456	1.926946	0.574559
C	4.773566	2.838596	0.604208

C	3.956832	0.560616	0.777377
C	6.067239	2.393239	0.845194
H	4.607020	3.896245	0.446153
C	5.244380	0.114829	1.019824
H	3.132519	-0.144279	0.749291
C	6.309676	1.028287	1.064294
H	6.876232	3.109821	0.866681
H	5.445371	-0.935791	1.186914
O	7.530152	0.506603	1.331105
C	8.637756	1.406833	1.429567
H	8.463427	2.158193	2.204368
H	9.496268	0.795460	1.698913
H	8.824449	1.905698	0.474827
H	1.674260	1.559738	0.367319

Table S47. Cartesian coordinates for **2'**. (-1818.61629462 E_h)

atom	x	y	z
O	9.605950	4.398598	22.547417
H	10.468935	4.474389	22.040894
O	20.452035	5.552057	11.427704
N	11.294166	4.641470	20.631179
N	10.626298	4.934497	18.519823
H	10.067373	5.060355	17.683254
N	11.114189	5.344028	15.760624
N	13.212655	5.383357	14.968403
H	14.222468	5.361811	14.890006
N	15.057200	5.607024	12.828781
C	8.593674	4.468284	21.653905
C	7.256089	4.340676	22.105408
C	6.249314	4.400068	21.144650
H	5.222623	4.299087	21.469591
C	6.481316	4.580385	19.767711
C	7.797108	4.703461	19.352697
H	8.022123	4.833154	18.302577
C	8.858860	4.652606	20.274394
C	6.938149	4.116215	23.591585
C	7.589477	2.800510	24.069923
H	8.670990	2.825795	23.945396
H	7.363382	2.638708	25.128037
H	7.194987	1.952306	23.503477
C	7.464343	5.299865	24.429406
H	6.958723	6.226048	24.141871
H	7.262759	5.121389	25.489948
H	8.536934	5.435161	24.298052
C	5.426432	4.005010	23.842629
H	4.986481	3.163942	23.300655
H	5.255166	3.845624	24.910043
H	4.898821	4.916379	23.548881
C	5.292859	4.616210	18.802477
C	4.558181	3.262199	18.861468
H	3.683278	3.276372	18.204930
H	5.214627	2.449802	18.538303
H	4.217617	3.041575	19.875975
C	4.321447	5.734506	19.228734
H	3.961330	5.578476	20.248280
H	4.810572	6.711351	19.186940
H	3.454322	5.756121	18.562545
C	5.732598	4.876019	17.355748
H	4.854791	4.899767	16.705772
H	6.249743	5.834698	17.260303
H	6.399569	4.090843	16.989231
C	10.236542	4.750124	19.822369
C	12.001080	4.930024	18.487819
C	12.904605	5.053956	17.422176
C	14.264558	4.980281	17.755514
H	15.010422	5.067040	16.974009
C	14.687067	4.799011	19.081152
H	15.749415	4.746569	19.286619

C	13.778994	4.683875	20.133853
H	14.113254	4.542423	21.154215
C	12.416724	4.746519	19.825645
C	12.406051	5.251580	16.072589
C	11.078912	5.552024	14.389678
C	9.996432	5.736329	13.519838
H	8.978605	5.720142	13.890737
C	10.274126	5.941730	12.168423
H	9.456221	6.084861	11.472421
C	11.591293	5.969222	11.681468
H	11.765403	6.131953	10.623480
C	12.696829	5.784105	12.524726
C	12.398444	5.579189	13.882790
C	14.062815	5.807714	12.031483
H	14.186185	6.007204	10.962915
C	16.385944	5.596023	12.369260
C	16.783451	5.540976	11.023563
H	16.041515	5.492960	10.235370
C	18.130373	5.527182	10.672129
H	18.409427	5.478586	9.628437
C	19.113430	5.561594	11.671137
C	18.731338	5.601649	13.019856
H	19.501132	5.619254	13.782509
C	17.387071	5.612232	13.357482
H	17.081873	5.639692	14.397374
C	20.881649	5.528146	10.066267
H	20.517720	6.403696	9.520973
H	21.969390	5.543875	10.097846
H	20.542913	4.620609	9.558160

Table S48. Cartesian coordinates for **2'**$^{\bullet+}$: E0PT. (-1818.42481793 E_h)

atom	x	y	z
O	9.614095	4.389502	22.547252
H	10.477305	4.471783	22.043969
O	20.365752	5.556099	11.463145
N	11.304476	4.654119	20.631097
N	10.633005	4.927185	18.517869
H	10.065302	5.036798	17.685773
N	11.125927	5.275460	15.744334
N	13.226752	5.375495	14.961418
H	14.238097	5.380597	14.903949
N	15.060365	5.664637	12.822546
C	8.602634	4.467823	21.653774
C	7.264392	4.339322	22.103212
C	6.258648	4.409653	21.142144
H	5.231641	4.308162	21.465836
C	6.491474	4.603740	19.766913
C	7.807750	4.725304	19.353951
H	8.034931	4.865975	18.305594
C	8.868647	4.661513	20.275866
C	6.944762	4.103665	23.587291
C	7.594072	2.783803	24.056950
H	8.675669	2.808040	23.932829
H	7.367606	2.615922	25.114010
H	7.198111	1.939615	23.485593
C	7.471890	5.280668	24.433823
H	6.969559	6.209926	24.150504
H	7.267043	5.096218	25.492685
H	8.545193	5.413768	24.306117
C	5.432672	3.992809	23.836153
H	4.992048	3.156160	23.287888
H	5.260221	3.826314	24.902259
H	4.906650	4.906997	23.548397
C	5.304077	4.653779	18.800993
C	4.569678	3.299026	18.839879
H	3.695142	3.322657	18.183173
H	5.226137	2.491218	18.505529
H	4.228476	3.064406	19.851038
C	4.331204	5.765362	19.241419
H	3.967501	5.593436	20.257109
H	4.819895	6.742990	19.216081
H	3.466371	5.796675	18.572680
C	5.746101	4.934814	17.358744
H	4.869385	4.966644	16.707743
H	6.262064	5.895598	17.278758
H	6.415043	4.156050	16.982165
C	10.245781	4.754703	19.823890
C	12.006711	4.924189	18.483084
C	12.912075	5.041187	17.417630
C	14.273545	4.975147	17.750501
H	15.020422	5.056134	16.969640
C	14.695970	4.805564	19.076410
H	15.758139	4.757401	19.282904
C	13.786836	4.696461	20.129540
H	14.121498	4.564396	21.150972

C	12.424801	4.753220	19.822406
C	12.412795	5.222462	16.068549
C	11.098378	5.477996	14.374198
C	10.022735	5.623006	13.499145
H	9.004637	5.574370	13.865651
C	10.289640	5.840184	12.134547
H	9.461635	5.954907	11.446778
C	11.590109	5.915020	11.651966
H	11.766778	6.086435	10.596861
C	12.711966	5.763041	12.507987
C	12.422809	5.543859	13.877753
C	14.039099	5.833485	12.008108
H	14.161869	6.045848	10.945345
C	16.344710	5.634782	12.377472
C	16.750327	5.576562	11.005637
H	16.005734	5.541683	10.221790
C	18.077531	5.550486	10.665686
H	18.372011	5.506400	9.626808
C	19.063750	5.573146	11.690198
C	18.680710	5.610380	13.059958
H	19.458720	5.617017	13.812463
C	17.354641	5.635787	13.389055
H	17.031073	5.662952	14.421750
C	20.863096	5.528271	10.107486
H	20.526656	6.413099	9.566797
H	21.944871	5.532678	10.203573
H	20.531334	4.620561	9.602914

Table S49. Cartesian coordinates for **2'**$^{\bullet+}$: E1PT. (-1818.43769015 E_h)

atom	x	y	z
C	1.561875	0.882961	-0.255370
C	0.356301	1.599751	-0.435873
C	0.400335	2.951856	-0.801646
C	1.652308	3.539224	-0.974028
C	2.841845	2.811848	-0.791588
C	-0.184101	-0.426514	0.093529
H	-0.513218	3.514960	-0.949505
H	1.714814	4.582084	-1.260628
H	3.796269	3.303934	-0.942723
C	-2.369251	-1.532641	0.384729
C	-3.186862	-2.648886	0.628199
C	-2.645269	-3.909758	0.878544
C	-1.255750	-3.996814	0.877867
C	-0.434614	-2.881584	0.632029
C	-0.968788	-1.615487	0.376472
C	-4.492378	-0.861324	0.282208
H	-3.274362	-4.769515	1.064057
H	-0.787065	-4.953253	1.072825
H	0.640606	-3.012514	0.641874
N	-0.718867	0.755006	-0.209790
C	-6.995787	-0.687538	0.197979
C	-5.675284	-0.045426	0.127357
C	-5.567419	1.315053	-0.067451
C	-6.711987	2.126380	-0.232520
C	-7.983436	1.515384	-0.196600
C	-8.176322	0.161571	0.003206
H	-4.590267	1.780886	-0.089022
H	-8.849714	2.144515	-0.328390
C	-6.528929	3.627163	-0.412299
C	-9.568225	-0.461200	0.038830
O	-7.093817	-1.921400	0.416981
N	-3.207534	-0.457921	0.177627
N	-4.486043	-2.180979	0.552694
H	-2.833626	0.463086	-0.045836
N	1.186413	-0.392247	0.079901
H	1.861268	-1.120666	0.283672
H	-5.371899	-2.675187	0.653964
C	-7.857439	4.361277	-0.634234
H	-7.660417	5.428156	-0.759115
H	-8.370819	4.008463	-1.532160
H	-8.532720	4.243816	0.216571
C	-5.609675	3.887744	-1.625595
H	-4.626220	3.431181	-1.497779
H	-6.057659	3.497374	-2.542222
H	-5.468202	4.964862	-1.743749
C	-5.858831	4.184388	0.864044
H	-6.495844	4.025479	1.737142
H	-4.893881	3.709134	1.052044
H	-5.693583	5.258321	0.745975
C	-9.677847	-1.545088	-1.058328
H	-8.951048	-2.340126	-0.900716
H	-10.683386	-1.973768	-1.041420
H	-9.511092	-1.108730	-2.046657

C	-10.666655	0.582571	-0.212160
H	-10.669351	1.361913	0.554421
H	-10.557017	1.059383	-1.189497
H	-11.637932	0.084046	-0.186146
C	-9.815572	-1.091311	1.428764
H	-10.821238	-1.519146	1.455163
H	-9.092011	-1.876623	1.639287
H	-9.748612	-0.330708	2.211234
C	2.832314	1.459712	-0.424715
C	4.054250	0.697593	-0.230698
N	4.017243	-0.534370	0.147975
H	4.993856	1.229500	-0.408089
C	5.207269	-1.268596	0.295531
C	6.382321	-1.027733	-0.442655
C	5.204054	-2.321350	1.219348
C	7.514997	-1.800222	-0.235703
H	6.399114	-0.251658	-1.198978
C	6.341483	-3.093041	1.446181
H	4.293446	-2.524341	1.771346
C	7.506635	-2.833004	0.715063
H	8.419337	-1.626538	-0.806843
H	6.310489	-3.889773	2.176799
O	8.664800	-3.537248	0.843227
C	8.662147	-4.654642	1.732702
H	7.923489	-5.399745	1.423748
H	9.661370	-5.082523	1.679427
H	8.451291	-4.341574	2.759248

Table S50. Cartesian coordinates for **2'**$^{\bullet+}$: E2PT. (-1818.44299022 E_h)

atom	x	y	z
O	9.586180	4.418389	22.529234
O	20.348578	5.578206	11.483271
N	11.395169	4.654909	20.622440
N	10.674812	4.917834	18.515927
N	11.160773	5.286563	15.799903
N	13.182591	5.346379	14.985411
H	14.191174	5.341265	14.851396
N	14.952069	5.601309	12.849998
C	8.649827	4.479935	21.689170
C	7.242962	4.352268	22.090950
C	6.282103	4.418406	21.110835
H	5.242663	4.319487	21.390130
C	6.571454	4.609420	19.730979
C	7.908299	4.731444	19.336608
H	8.161764	4.866575	18.295063
C	8.939504	4.671655	20.262427
C	6.895268	4.125727	23.561201
C	7.551998	2.814972	24.050795
H	8.635599	2.860202	23.957152
H	7.294733	2.650942	25.100753
H	7.185023	1.962697	23.472610
C	7.402353	5.313980	24.406868
H	6.900936	6.238961	24.109472
H	7.177405	5.131788	25.461478
H	8.477315	5.446472	24.296181
C	5.379659	4.003348	23.776806
H	4.958406	3.161722	23.220935
H	5.186911	3.836951	24.839104
H	4.852826	4.913076	23.476909
C	5.419717	4.650348	18.735004
C	4.691281	3.288976	18.775479
H	3.844080	3.307632	18.084584
H	5.362043	2.480342	18.475275
H	4.310594	3.067923	19.774793
C	4.434251	5.765089	19.147001
H	4.034149	5.597784	20.148975
H	4.922654	6.742369	19.129823
H	3.595953	5.786576	18.445796
C	5.894442	4.918236	17.300998
H	5.029248	4.943228	16.635402
H	6.409294	5.879316	17.222557
H	6.568918	4.135464	16.944425
C	10.309764	4.760913	19.797381
C	12.046101	4.898512	18.528124
C	12.962564	5.006354	17.456786
C	14.327535	4.931090	17.756540
H	15.056298	5.005613	16.958166
C	14.775365	4.762849	19.075434
H	15.840497	4.707513	19.261317
C	13.888444	4.664601	20.147811
H	14.241387	4.535889	21.162870
C	12.528426	4.731518	19.851517
C	12.468439	5.199468	16.118248

C	11.019941	5.501108	14.436785
C	9.906779	5.675461	13.613725
H	8.900420	5.646030	14.009449
C	10.162206	5.886195	12.259698
H	9.329196	6.022424	11.581501
C	11.469465	5.928515	11.744906
H	11.617727	6.095441	10.684345
C	12.594443	5.753118	12.560590
C	12.324561	5.540833	13.921632
C	13.957076	5.790798	12.052280
H	14.071631	5.988128	10.983638
C	16.282310	5.598480	12.400385
C	16.685427	5.558048	11.055744
H	15.947016	5.513916	10.264058
C	18.033389	5.552080	10.712178
H	18.319006	5.513861	9.669912
C	19.010600	5.581508	11.718337
C	18.621412	5.608633	13.065935
H	19.387575	5.622699	13.832105
C	17.275891	5.610129	13.396159
H	16.963625	5.626708	14.434208
C	20.789700	5.559286	10.124554
H	20.429668	6.436625	9.579978
H	21.876991	5.575707	10.166281
H	20.455533	4.652848	9.611934
H	11.284438	4.533675	21.624572
H	10.442365	5.200798	16.522280

Table S51. Cartesian coordinates for **2'**$^{\bullet+}$: E3PT. (-1818.44750807 E_h)

atom	x	y	z
C	1.519626	1.083941	0.090097
C	0.332664	1.840557	-0.059568
C	0.354498	3.211041	-0.299813
C	1.608651	3.827003	-0.397829
C	2.794878	3.102291	-0.258235
C	-0.112544	-0.303737	0.301217
H	-0.560474	3.778686	-0.412508
H	1.660648	4.892320	-0.583484
H	3.748434	3.609526	-0.344237
C	-2.321523	-1.446206	0.451083
C	-3.079372	-2.633515	0.628239
C	-2.483969	-3.875602	0.846151
C	-1.090371	-3.906838	0.883501
C	-0.317977	-2.747521	0.705705
C	-0.909511	-1.499346	0.490251
C	-4.396629	-0.877419	0.295181
H	-3.074738	-4.772873	0.979254
H	-0.587533	-4.850954	1.054278
H	0.762567	-2.811160	0.736443
N	-0.681838	0.919432	0.083720
C	-6.926117	-0.758171	0.155450
C	-5.612017	-0.104014	0.114092
C	-5.519351	1.258504	-0.094513
C	-6.663390	2.054694	-0.282543
C	-7.933475	1.430860	-0.257823
C	-8.113184	0.077939	-0.055292
H	-4.534731	1.708412	-0.108401
H	-8.804205	2.050730	-0.405329
C	-6.494258	3.556153	-0.488454
C	-9.501167	-0.559726	-0.037991
O	-7.017883	-1.997933	0.363312
N	-3.157440	-0.373095	0.249307
N	-4.387206	-2.226654	0.521425
N	1.225425	-0.236964	0.311942
H	-5.251825	-2.755014	0.585165
H	-1.692034	1.050484	0.049066
C	-5.602620	3.799906	-1.725388
H	-5.457767	4.874815	-1.862020
H	-4.620226	3.337386	-1.612083
H	-6.072670	3.399226	-2.626594
C	-7.830960	4.280024	-0.696080
H	-8.356703	3.915173	-1.582039
H	-8.491758	4.165411	0.166584
H	-7.644069	5.347358	-0.834340
C	-5.800526	4.144815	0.759385
H	-6.410805	3.991256	1.652559
H	-4.824143	3.686208	0.929623
H	-5.653188	5.219344	0.622948
C	-9.589312	-1.638501	-1.141039
H	-8.852903	-2.424120	-0.980447
H	-10.589006	-2.081713	-1.137673
H	-9.418120	-1.194787	-2.125582
C	-10.608332	0.473137	-0.296506

H	-10.624808	1.251708	0.470819
H	-10.495457	0.953402	-1.271898
H	-11.575350	-0.034490	-0.279649
C	-9.760587	-1.199286	1.344502
H	-10.760617	-1.641528	1.358057
H	-9.028695	-1.975151	1.561476
H	-9.713914	-0.441423	2.131404
C	2.782950	1.713906	-0.017062
C	4.001257	0.980522	0.085103
N	4.016103	-0.314898	0.273434
H	4.946313	1.498938	-0.019307
C	5.124622	-1.183880	0.327264
C	6.448418	-0.739772	0.187360
C	4.858244	-2.544158	0.502718
C	7.480342	-1.660143	0.217130
H	6.676525	0.308994	0.046890
C	5.894095	-3.471966	0.530733
H	3.833138	-2.880597	0.609834
C	7.215148	-3.031000	0.384756
H	8.508450	-1.338773	0.108004
H	5.668859	-4.520328	0.664916
O	8.297774	-3.843568	0.392049
C	8.075105	-5.251792	0.512572
H	7.478579	-5.625403	-0.324217
H	9.061514	-5.710074	0.496351
H	7.572066	-5.490470	1.453269
H	3.085916	-0.752432	0.362913

Table S52. Cartesian coordinates for **3**. (-1328.98358689 E_h)

atom	x	y	z
C	-0.446806	2.665094	0.444510
C	-1.842084	2.872315	0.368082
C	-2.349517	4.173770	0.278134
C	-1.435641	5.228006	0.268782
C	-0.051043	5.005308	0.342181
C	-1.514468	0.720678	0.464828
H	-3.416313	4.350498	0.213382
H	-1.801391	6.245608	0.200609
H	0.629643	5.849435	0.327292
N	-2.479183	1.640159	0.384982
C	-3.080132	-1.203522	0.389943
C	-1.750811	-0.713497	0.473579
C	-0.676987	-1.613102	0.528914
C	-0.879529	-2.987383	0.503825
C	-2.203531	-3.441691	0.413882
C	-3.314907	-2.596567	0.354935
H	0.333478	-1.224807	0.587283
H	-2.377629	-4.505920	0.386705
C	0.324102	-3.933837	0.543544
C	-4.739298	-3.163797	0.252023
O	-4.128028	-0.348823	0.336557
H	-3.768093	0.585103	0.346265
N	-0.273737	1.303647	0.507619
H	0.642560	0.875513	0.565821
C	1.191978	-3.688334	-0.707440
H	1.527865	-2.649443	-0.754140
H	2.076460	-4.331780	-0.688579
H	0.630717	-3.906265	-1.620129
C	1.166742	-3.644413	1.801416
H	0.585027	-3.819257	2.710414
H	2.042992	-4.298613	1.825281
H	1.518150	-2.609658	1.815589
C	-0.097602	-5.408795	0.566702
H	-0.697693	-5.643518	1.449978
H	-0.674742	-5.677261	-0.322080
H	0.793122	-6.041346	0.589341
C	-5.407952	-2.667094	-1.047502
H	-6.426135	-3.061597	-1.115307
H	-5.453079	-1.579380	-1.079211
H	-4.850297	-3.016666	-1.920976
C	-5.569325	-2.722012	1.475889
H	-5.662027	-1.637704	1.522836
H	-6.572357	-3.155456	1.422067
H	-5.097625	-3.067264	2.400216
C	-4.740498	-4.700527	0.216731
H	-4.188108	-5.086107	-0.644281
H	-4.303577	-5.130371	1.121810
H	-5.771526	-5.053794	0.141175
C	0.484223	3.713863	0.432064
C	1.921992	3.469687	0.486904
N	2.407297	2.288640	0.586840
H	2.567649	4.355065	0.434249
C	3.857489	2.157034	0.636115

C	4.284600	1.679777	2.031910
C	4.318292	1.163624	-0.439290
H	4.336865	3.130802	0.442693
C	5.797624	1.447127	2.101834
H	3.968465	2.416035	2.777033
H	3.754879	0.745656	2.256375
C	5.830899	0.927088	-0.371701
H	4.029706	1.536730	-1.426320
H	3.787064	0.216400	-0.281963
C	6.260893	0.461620	1.023474
H	6.315849	2.404044	1.961383
H	6.070180	1.081871	3.096604
H	6.352556	1.861000	-0.616900
H	6.126783	0.193994	-1.128268
H	7.347386	0.336861	1.065829
H	5.818728	-0.522143	1.224895

Table S53. Cartesian coordinates for **3**$^{\bullet+}$: E0PT. (-1328.79032557 E_h)

atom	x	y	z
C	-0.404012	2.702618	0.291236
C	-1.816977	2.858572	0.257157
C	-2.381096	4.144452	0.175396
C	-1.505540	5.217940	0.135990
C	-0.100217	5.045206	0.168027
C	-1.382140	0.727229	0.365651
H	-3.454168	4.281131	0.144506
H	-1.901098	6.224225	0.075330
H	0.539106	5.919439	0.129096
N	-2.389189	1.615357	0.304690
C	-2.983102	-1.166808	0.409419
C	-1.604842	-0.689539	0.416113
C	-0.559764	-1.608249	0.454223
C	-0.818040	-2.975913	0.495377
C	-2.178991	-3.416159	0.509413
C	-3.264998	-2.576658	0.473580
H	0.459853	-1.251174	0.448680
H	-2.354186	-4.480411	0.551221
C	0.284707	-4.020097	0.514558
C	-4.704340	-3.096190	0.487938
O	-3.969219	-0.317788	0.336899
H	-3.584374	0.651720	0.307101
N	-0.168675	1.360195	0.361154
H	0.779819	0.993609	0.397056
C	-5.463573	-2.517800	1.702781
H	-5.542756	-1.432873	1.651366
H	-6.472910	-2.936470	1.725454
H	-4.960539	-2.788752	2.634385
C	-4.734521	-4.628326	0.600914
H	-5.774148	-4.960213	0.623441
H	-4.245184	-5.110486	-0.249252
H	-4.249111	-4.971263	1.518236
C	-5.413648	-2.695578	-0.824409
H	-5.488839	-1.613890	-0.929830
H	-4.873979	-3.093179	-1.687426
H	-6.423622	-3.113295	-0.828998
C	0.120891	-4.898665	1.775611
H	-0.846584	-5.404004	1.796313
H	0.901792	-5.663382	1.781329
H	0.216665	-4.298454	2.682904
C	1.685083	-3.394253	0.523828
H	1.864738	-2.794631	-0.372054
H	1.837304	-2.761834	1.401954
H	2.432017	-4.190461	0.548746
C	0.138407	-4.905362	-0.744868
H	0.915694	-5.673801	-0.733533
H	-0.832115	-5.404298	-0.778296
H	0.252214	-4.310274	-1.653539
C	0.489976	3.785991	0.246299
C	1.936425	3.577421	0.256640
N	2.433727	2.400983	0.334561
H	2.564301	4.472904	0.188809
C	3.884097	2.269571	0.332841

C	4.354065	1.743007	1.696559
C	4.303557	1.311856	-0.790591
H	4.356526	3.249080	0.155661
C	5.867612	1.501892	1.709143
H	4.068095	2.454486	2.476686
H	3.827331	0.804044	1.906585
C	5.816375	1.066375	-0.778723
H	3.986807	1.721817	-1.754141
H	3.771822	0.362690	-0.649014
C	6.291089	0.551922	0.584292
H	6.386108	2.460872	1.585578
H	6.167595	1.101684	2.682217
H	6.334428	2.005532	-1.010318
H	6.082050	0.358336	-1.569291
H	7.377938	0.424108	0.584868
H	5.853162	-0.437307	0.768217

Table S54. Cartesian coordinates for **3**$^{\bullet+}$: E1PT. (-1328.80569033 E_h)

atom	x	y	z
C	-0.463413	2.781407	0.365296
C	-1.848965	2.991914	0.283837
C	-2.381630	4.279878	0.190346
C	-1.466893	5.329447	0.184887
C	-0.077374	5.114046	0.265219
C	-1.457954	0.788725	0.392042
H	-3.448025	4.447413	0.121996
H	-1.834307	6.345545	0.115039
H	0.593870	5.964876	0.252803
N	-2.418410	1.730438	0.304799
C	-3.043659	-1.160331	0.328012
C	-1.672627	-0.638749	0.422926
C	-0.598928	-1.498090	0.516645
C	-0.777937	-2.897535	0.516683
C	-2.089660	-3.410655	0.435185
C	-3.218092	-2.617737	0.347688
H	0.408132	-1.107270	0.588109
H	-2.212041	-4.482121	0.442447
C	0.451817	-3.790630	0.579500
C	-4.619689	-3.216599	0.271694
O	-4.018025	-0.372326	0.231649
N	-0.265613	1.420634	0.430818
H	0.678076	1.039027	0.485363
H	-3.396164	1.450081	0.257044
C	-5.467117	-2.705099	1.459436
H	-5.580800	-1.623087	1.424934
H	-6.458042	-3.165017	1.420223
H	-5.000514	-2.979164	2.409163
C	-4.582984	-4.751618	0.339886
H	-4.023773	-5.181138	-0.495206
H	-4.133726	-5.102116	1.272510
H	-5.605456	-5.131521	0.292123
C	0.095889	-5.282246	0.581679
H	-0.500993	-5.553915	1.456012
H	-0.456208	-5.565190	-0.317879
H	1.015982	-5.869540	0.608177
C	1.332368	-3.486106	-0.653921
H	0.797679	-3.711114	-1.579788
H	1.639090	-2.437793	-0.676592
H	2.233324	-4.103531	-0.617398
C	1.250898	-3.464456	1.860008
H	0.655966	-3.661623	2.754611
H	2.143147	-4.094218	1.894277
H	1.573882	-2.421110	1.881024
C	-5.285693	-2.814012	-1.063477
H	-6.283544	-3.257803	-1.114674
H	-5.380237	-1.733033	-1.152237
H	-4.704098	-3.186247	-1.910719
C	0.465789	3.831147	0.358472
C	1.901869	3.566750	0.425429
N	2.350676	2.372274	0.526176
H	2.565372	4.437315	0.380832
C	3.795217	2.192162	0.584544

C	4.199356	1.705782	1.983660
C	4.230095	1.182741	-0.486858
H	4.303848	3.149921	0.391311
C	5.706794	1.439780	2.059276
H	3.897257	2.450142	2.726226
H	3.647850	0.783924	2.206205
C	5.737143	0.912575	-0.414422
H	3.953003	1.559746	-1.475533
H	3.676798	0.248562	-0.327174
C	6.154738	0.444167	0.983462
H	6.245419	2.385690	1.921924
H	5.966604	1.068517	3.055121
H	6.278634	1.833861	-0.663879
H	6.016812	0.169465	-1.167076
H	7.238776	0.301689	1.029212
H	5.695678	-0.531559	1.186515

Table S55. Cartesian coordinates for **3**$^{\bullet+}$: E2PT. (-1328.81640591 E_h)

atom	x	y	z
C	-0.513901	2.748533	0.452659
C	-1.904544	2.999607	0.350615
C	-2.417954	4.291626	0.253002
C	-1.501115	5.347311	0.259660
C	-0.122142	5.124659	0.354094
C	-1.479313	0.824926	0.463075
H	-3.482299	4.471331	0.169822
H	-1.867263	6.363362	0.186641
H	0.560715	5.966067	0.349926
N	-2.478690	1.750168	0.361307
C	-3.056947	-1.158687	0.358573
C	-1.700807	-0.608756	0.479801
C	-0.612889	-1.451382	0.585539
C	-0.761578	-2.850668	0.579623
C	-2.062109	-3.391595	0.460093
C	-3.200890	-2.619650	0.345094
H	0.374853	-1.016253	0.665393
H	-2.163064	-4.465615	0.451165
C	0.485163	-3.720992	0.668470
C	-4.585727	-3.244692	0.193805
O	-4.051457	-0.391438	0.264656
N	-0.269980	1.405073	0.524018
H	-3.452917	1.470973	0.299060
C	-5.197017	-2.819333	-1.160082
H	-6.193028	-3.258787	-1.262025
H	-5.283952	-1.736311	-1.233355
H	-4.581844	-3.178258	-1.989498
C	-5.499588	-2.782796	1.350079
H	-5.627952	-1.702100	1.340491
H	-6.479647	-3.256802	1.248035
H	-5.076197	-3.076091	2.314399
C	-4.523012	-4.779295	0.224872
H	-3.918000	-5.178094	-0.593381
H	-4.112416	-5.146927	1.168750
H	-5.534783	-5.176544	0.119281
C	0.160444	-5.220059	0.677665
H	-0.447027	-5.496469	1.543379
H	-0.370427	-5.521858	-0.228472
H	1.091165	-5.789457	0.725131
C	1.259404	-3.369920	1.956657
H	2.167672	-3.975465	2.007793
H	1.552575	-2.317819	1.975687
H	0.657930	-3.577754	2.844674
C	1.376831	-3.408805	-0.554198
H	0.857595	-3.647803	-1.485534
H	1.661443	-2.354329	-0.578219
H	2.289352	-4.008404	-0.504959
C	0.403426	3.825579	0.450141
C	1.816598	3.610234	0.511019
N	2.350473	2.429848	0.585363
H	2.489265	4.462003	0.483213
C	3.789867	2.161395	0.644023
C	4.180589	1.671749	2.043054

C	4.173067	1.146245	-0.438929
H	4.288239	3.113475	0.442880
C	5.682849	1.370574	2.098001
H	3.905655	2.428599	2.781911
H	3.610702	0.763543	2.272195
C	5.674553	0.839449	-0.375940
H	3.897680	1.538505	-1.420956
H	3.600351	0.224874	-0.276122
C	6.094690	0.363743	1.018494
H	6.239134	2.304799	1.954362
H	5.941988	0.994639	3.091555
H	6.233699	1.746813	-0.634957
H	5.922618	0.087484	-1.129756
H	7.175535	0.199289	1.051999
H	5.616863	-0.601095	1.228519
H	1.700978	1.631684	0.611722

Table S56. Cartesian coordinates for **3'**. (-1707.71783793 E_h)

atom	x	y	z
C	1.549318	1.005753	-0.114039
C	0.335484	1.717826	-0.252160
C	0.361539	3.098279	-0.488219
C	1.604893	3.721126	-0.583365
C	2.802129	2.998518	-0.441510
C	-0.187380	-0.356562	0.077641
H	-0.559989	3.657308	-0.598616
H	1.654848	4.788189	-0.765085
H	3.751790	3.516309	-0.519066
C	-2.361477	-1.515219	0.227233
C	-3.182756	-2.660115	0.335857
C	-2.601333	-3.922416	0.491835
C	-1.208288	-3.994385	0.529642
C	-0.402251	-2.852190	0.403848
C	-0.959932	-1.575890	0.245971
C	-4.500886	-0.938436	0.123950
H	-3.214852	-4.810642	0.578379
H	-0.730019	-4.958663	0.653361
H	0.675292	-2.963538	0.430316
N	-0.731353	0.842584	-0.125549
C	-6.962605	-0.746439	-0.134448
C	-5.696641	-0.120026	0.002440
C	-5.607322	1.278701	0.020735
C	-6.737090	2.079710	-0.095473
C	-7.972475	1.432298	-0.243810
C	-8.127429	0.043031	-0.265873
H	-4.635762	1.742659	0.145060
H	-8.858454	2.041092	-0.338532
C	-6.600475	3.604859	-0.024680
C	-9.513183	-0.599618	-0.429211
O	-7.063756	-2.096631	-0.146630
H	-6.152486	-2.475084	0.012095
N	-3.220043	-0.449629	0.101968
N	-4.510659	-2.266326	0.263400
H	-2.886569	0.499523	-0.024948
N	1.186092	-0.301443	0.094448
H	1.863664	-1.044338	0.217904
C	-5.607833	4.087449	-1.099560
H	-5.484720	5.172426	-1.036871
H	-4.624606	3.629590	-0.966453
H	-5.967504	3.840021	-2.101772
C	-6.060130	3.989582	1.367271
H	-5.091363	3.521006	1.556742
H	-5.935405	5.073555	1.444157
H	-6.749449	3.667436	2.152407
C	-7.942111	4.317028	-0.242187
H	-8.369488	4.081556	-1.220636
H	-8.672689	4.041128	0.522788
H	-7.795415	5.398696	-0.188356
C	-9.548638	-1.418679	-1.735724
H	-8.785035	-2.196265	-1.734713

H	-10.527915	-1.891882	-1.854997
H	-9.379546	-0.767714	-2.597771
C	-9.826148	-1.513008	0.775983
H	-10.816458	-1.960234	0.648802
H	-9.092339	-2.310884	0.874145
H	-9.834645	-0.930926	1.701583
C	-10.628330	0.455024	-0.503073
H	-10.662588	1.070937	0.399286
H	-10.511698	1.118307	-1.364059
H	-11.590702	-0.053223	-0.602180
C	2.808347	1.617999	-0.206645
C	4.049414	0.864612	-0.068522
N	4.066334	-0.402148	0.121986
H	4.976746	1.445899	-0.144657
C	5.374594	-1.037058	0.221878
C	5.510061	-1.750770	1.573546
C	5.558341	-2.034113	-0.931485
H	6.170400	-0.277496	0.148640
C	6.858748	-2.470406	1.686243
H	5.391624	-1.022238	2.381321
H	4.692883	-2.476268	1.666944
C	6.908353	-2.751912	-0.827009
H	5.472689	-1.504809	-1.885237
H	4.742526	-2.766178	-0.892150
C	7.066609	-3.451859	0.526991
H	7.664244	-1.725334	1.677074
H	6.922213	-2.992608	2.645642
H	7.714363	-2.017861	-0.949870
H	7.010192	-3.474096	-1.642998
H	8.053076	-3.920786	0.597686
H	6.324476	-4.256710	0.602658

Table S57. Cartesian coordinates for **3'**$^{\bullet+}$: E0PT. (-1707.52387182 E_h)

atom	x	y	z
C	1.589454	0.997184	0.008760
C	0.380186	1.719628	-0.112394
C	0.410474	3.112551	-0.261830
C	1.654736	3.737032	-0.286197
C	2.848432	3.004099	-0.161536
C	-0.148620	-0.368937	0.077409
H	-0.508436	3.678348	-0.356892
H	1.710374	4.812917	-0.401285
H	3.799049	3.525403	-0.183315
C	-2.339671	-1.498053	0.091564
C	-3.191689	-2.635994	0.129551
C	-2.641098	-3.921888	0.251640
C	-1.259707	-4.013197	0.332641
C	-0.421198	-2.875147	0.286414
C	-0.937207	-1.586455	0.158149
C	-4.448218	-0.865778	-0.035959
H	-3.274048	-4.798835	0.283324
H	-0.797746	-4.987594	0.431936
H	0.650719	-3.014984	0.353316
N	-0.688666	0.840889	-0.063179
C	-6.919589	-0.732846	-0.202113
C	-5.630465	-0.056784	-0.125277
C	-5.578513	1.332815	-0.136731
C	-6.749029	2.083965	-0.220430
C	-8.000457	1.397057	-0.304147
C	-8.136468	0.030548	-0.297446
H	-4.617458	1.823713	-0.074470
H	-8.890813	2.005119	-0.363297
C	-6.756838	3.601884	-0.212397
C	-9.499491	-0.659383	-0.374783
O	-6.973597	-2.035193	-0.181073
H	-6.005444	-2.414557	-0.082684
N	-3.159133	-0.410942	-0.009872
N	-4.490696	-2.205446	0.043071
H	-2.784828	0.533887	-0.071183
N	1.221870	-0.320455	0.127074
H	1.897377	-1.070515	0.218984
C	-7.452306	4.103146	-1.498751
H	-8.473811	3.727318	-1.581821
H	-7.493792	5.194724	-1.479907
H	-6.897661	3.791631	-2.386773
C	-7.558234	4.077048	1.022309
H	-7.624045	5.167760	1.008784
H	-8.573478	3.675018	1.025314
H	-7.061330	3.771027	1.945686
C	-5.344225	4.194047	-0.148856
H	-4.824289	3.896529	0.765187
H	-4.743902	3.883749	-1.007477
H	-5.412519	5.283657	-0.157833
C	-9.573909	-1.521836	-1.653249
H	-8.799250	-2.288076	-1.669956
H	-10.548404	-2.014855	-1.696182
H	-9.467629	-0.898105	-2.543887

C	-10.638188	0.369546	-0.424148
H	-10.648240	1.004214	0.465427
H	-10.572040	1.012009	-1.305709
H	-11.589407	-0.164496	-0.468911
C	-9.717630	-1.542979	0.874221
H	-10.714477	-1.988434	0.824167
H	-8.983659	-2.344568	0.938544
H	-9.660505	-0.941835	1.784821
C	2.850404	1.612458	-0.014894
C	4.089654	0.852269	0.100555
N	4.104727	-0.422870	0.221495
H	5.016835	1.437715	0.069965
C	5.413791	-1.059482	0.308565
C	5.556509	-1.788863	1.651290
C	5.594640	-2.041418	-0.857575
H	6.208402	-0.298291	0.242730
C	6.908569	-2.504753	1.748411
H	5.440631	-1.069570	2.467687
H	4.741870	-2.517754	1.740726
C	6.948348	-2.754397	-0.769112
H	5.501624	-1.501515	-1.804564
H	4.782213	-2.777478	-0.822303
C	7.116715	-3.469798	0.575532
H	7.710699	-1.756015	1.746232
H	6.978212	-3.039714	2.700264
H	7.750509	-2.015409	-0.887790
H	7.048845	-3.466453	-1.594041
H	8.106300	-3.933518	0.635903
H	6.379821	-4.280067	0.644188

Table S58. Cartesian coordinates for **3'**$^{\bullet+}$: E1PT. (-1707.53964549 E_h)

atom	x	y	z
C	1.533853	0.991660	-0.027606
C	0.306962	1.686921	-0.127561
C	0.305085	3.073053	-0.333098
C	1.535997	3.715786	-0.438275
C	2.747920	3.009121	-0.334256
C	-0.171026	-0.402880	0.161412
H	-0.626952	3.619468	-0.412196
H	1.566488	4.787010	-0.598120
H	3.686949	3.544794	-0.418799
C	-2.331272	-1.576306	0.253960
C	-3.138748	-2.722689	0.330082
C	-2.582255	-3.993060	0.482317
C	-1.192809	-4.055549	0.552166
C	-0.381793	-2.909359	0.460785
C	-0.930122	-1.633526	0.303862
C	-4.456153	-0.925043	0.100576
H	-3.200517	-4.878309	0.541802
H	-0.715733	-5.019633	0.676002
H	0.693919	-3.023314	0.515483
N	-0.740907	0.790424	-0.001870
C	-6.948922	-0.758953	-0.159742
C	-5.639365	-0.105415	-0.022146
C	-5.538109	1.269424	-0.000512
C	-6.681224	2.090753	-0.108597
C	-7.942208	1.474336	-0.251934
C	-8.128236	0.105436	-0.279036
H	-4.568731	1.737319	0.115671
H	-8.807007	2.113012	-0.336353
C	-6.516947	3.602431	-0.029702
C	-9.512400	-0.516949	-0.426861
O	-7.036059	-2.013019	-0.173339
N	-3.176598	-0.496756	0.119113
N	-4.441296	-2.266850	0.226202
H	-2.799995	0.447152	0.027718
N	1.198035	-0.326512	0.156301
H	1.892512	-1.060068	0.239961
H	-5.318841	-2.783647	0.193544
C	-7.840849	4.346266	-0.246598
H	-7.662737	5.422048	-0.187336
H	-8.269879	4.127428	-1.227707
H	-8.578154	4.088397	0.517473
C	-5.503996	4.066447	-1.097856
H	-4.524242	3.605559	-0.956397
H	-5.858948	3.826430	-2.102670
H	-5.378185	5.149483	-1.025034
C	-5.972607	3.952127	1.374045
H	-6.672689	3.636335	2.150978
H	-5.010793	3.470533	1.562868
H	-5.834531	5.033380	1.453019
C	-9.563446	-1.335488	-1.736113
H	-8.819864	-2.131521	-1.730814
H	-10.556027	-1.780100	-1.846540
H	-9.380466	-0.690673	-2.599314

C	-10.613615	0.551847	-0.484401
H	-10.627925	1.165673	0.419644
H	-10.500037	1.213159	-1.347084
H	-11.582087	0.054440	-0.570399
C	-9.810588	-1.434817	0.781670
H	-10.815620	-1.850749	0.672852
H	-9.094619	-2.251661	0.846321
H	-9.779247	-0.863413	1.712864
C	2.781784	1.625523	-0.130517
C	4.035800	0.886644	-0.033381
N	4.070220	-0.383055	0.132889
H	4.954136	1.480456	-0.118246
C	5.386335	-1.007256	0.192796
C	5.562194	-1.731873	1.534113
C	5.546576	-1.992473	-0.974286
H	6.173079	-0.240213	0.106170
C	6.916982	-2.445896	1.603667
H	5.461926	-1.010776	2.351026
H	4.751237	-2.462178	1.643041
C	6.902867	-2.703450	-0.911343
H	5.432881	-1.455306	-1.920654
H	4.736315	-2.729827	-0.920780
C	7.097035	-3.416688	0.430877
H	7.718874	-1.697302	1.578066
H	7.009908	-2.975591	2.556539
H	7.701771	-1.963721	-1.045287
H	6.988551	-3.416046	-1.737513
H	8.086072	-3.883658	0.471846
H	6.358683	-4.223796	0.517346

Table S59. Cartesian coordinates for **3'**$^{\bullet+}$: E2PT. (-1707.54479388 E_h)

atom	x	y	z
C	1.523456	1.060882	-0.159370
C	0.309822	1.754406	-0.286227
C	0.278679	3.128526	-0.525125
C	1.510665	3.770053	-0.635236
C	2.725902	3.074370	-0.502215
C	-0.132818	-0.411414	0.072594
H	-0.656928	3.662624	-0.624815
H	1.535239	4.836465	-0.821864
H	3.661097	3.615045	-0.589345
C	-2.310881	-1.549127	0.213643
C	-3.080784	-2.733987	0.330182
C	-2.494205	-3.987020	0.497159
C	-1.099848	-4.033365	0.544400
C	-0.313760	-2.878747	0.415798
C	-0.899333	-1.618939	0.245439
C	-4.376084	-0.947016	0.089535
H	-3.092084	-4.884909	0.585954
H	-0.607274	-4.988132	0.679016
H	0.765070	-2.969036	0.451122
N	-0.684936	0.802236	-0.129227
C	-6.895854	-0.778130	-0.132121
C	-5.577910	-0.140510	-0.021100
C	-5.465320	1.235764	-0.013932
C	-6.596879	2.066625	-0.111545
C	-7.870137	1.462227	-0.226520
C	-8.069028	0.096551	-0.236045
H	-4.478614	1.670728	0.082042
H	-8.729990	2.109185	-0.300958
C	-6.418023	3.579109	-0.052590
C	-9.464353	-0.513534	-0.346697
O	-6.999521	-2.033877	-0.135857
N	-3.129642	-0.457363	0.070685
N	-4.384092	-2.305382	0.241803
N	1.207563	-0.266280	0.058721
H	1.933295	-0.970886	0.169435
H	-5.252711	-2.831153	0.232254
H	-1.702521	0.911709	-0.146984
C	-9.557569	-1.349880	-1.641728
H	-8.820220	-2.151689	-1.643053
H	-10.556382	-1.787691	-1.720937
H	-9.391300	-0.720072	-2.519430
C	-5.404315	4.021288	-1.128363
H	-5.266183	5.103885	-1.070107
H	-4.429903	3.549916	-0.984040
H	-5.764607	3.773013	-2.129506
C	-10.555440	0.566065	-0.394466
H	-10.543806	1.192367	0.501067
H	-10.453019	1.215063	-1.267926
H	-11.531799	0.079668	-0.452574
C	-9.746249	-1.412502	0.879417
H	-9.039618	-2.238340	0.935179
H	-9.683062	-0.831980	1.803509
H	-10.759343	-1.816708	0.803003

C	-7.734490	4.334704	-0.275967
H	-8.173548	4.100174	-1.249094
H	-8.470296	4.101127	0.497315
H	-7.544800	5.409755	-0.240558
C	-5.866779	3.941816	1.344450
H	-6.568468	3.643269	2.127074
H	-4.910951	3.449330	1.535751
H	-5.715781	5.022358	1.412141
C	2.767127	1.697513	-0.263135
C	4.017192	0.955103	-0.119303
N	4.027473	-0.309244	0.078858
H	4.941320	1.539052	-0.192530
C	5.328048	-0.955189	0.197109
C	5.435322	-1.664205	1.553887
C	5.515350	-1.958471	-0.950210
H	6.130239	-0.202669	0.131180
C	6.776143	-2.394545	1.688080
H	5.311962	-0.931135	2.356645
H	4.609969	-2.381511	1.637446
C	6.858082	-2.686246	-0.823923
H	5.447347	-1.432235	-1.906941
H	4.692901	-2.683218	-0.917760
C	6.993096	-3.381403	0.535072
H	7.587267	-1.655740	1.689147
H	6.820151	-2.914199	2.649889
H	7.671034	-1.958888	-0.939931
H	6.964236	-3.412706	-1.635411
H	7.975323	-3.856387	0.621089
H	6.244882	-4.181228	0.603951

Table S60. Cartesian coordinates for **3'**$^{\bullet+}$: E3PT. (-1707.55376519 E_h)

atom	x	y	z
C	1.567805	1.193257	-0.088834
C	0.366198	1.931621	-0.220117
C	0.362627	3.299389	-0.476495
C	1.603789	3.933830	-0.608047
C	2.804067	3.227862	-0.482625
C	-0.039097	-0.215515	0.167394
H	-0.563114	3.851893	-0.576552
H	1.634666	4.997229	-0.808853
H	3.748474	3.747795	-0.592021
C	-2.226795	-1.399660	0.340695
C	-2.957948	-2.609634	0.468378
C	-2.336212	-3.846358	0.638264
C	-0.942333	-3.849546	0.671195
C	-0.195446	-2.669378	0.525862
C	-0.813497	-1.426711	0.356452
C	-4.314718	-0.869641	0.222978
H	-2.907888	-4.760097	0.738870
H	-0.419175	-4.788501	0.805089
H	0.886363	-2.712186	0.538995
N	-0.631578	0.997693	-0.045085
C	-6.833384	-0.813345	-0.058748
C	-5.550253	-0.116263	0.099512
C	-5.508919	1.264277	0.134995
C	-6.676367	2.039245	0.011922
C	-7.911709	1.377202	-0.183465
C	-8.038727	0.004334	-0.236021
H	-4.550988	1.748369	0.276935
H	-8.795963	1.985428	-0.295692
C	-6.573004	3.556208	0.121422
C	-9.384075	-0.676129	-0.477449
O	-6.884177	-2.072601	-0.041873
N	-3.087557	-0.335899	0.197056
N	-4.274898	-2.227811	0.383749
N	1.297239	-0.130230	0.150663
H	-5.123314	-2.784914	0.367592
H	-1.643615	1.114210	-0.060618
C	-5.572712	4.078005	-0.931262
H	-5.477475	5.162840	-0.836680
H	-4.581583	3.639690	-0.796087
H	-5.916735	3.848767	-1.942672
C	-7.922190	4.255436	-0.087488
H	-8.334153	4.050621	-1.078838
H	-8.655766	3.944854	0.660516
H	-7.786073	5.335178	0.005542
C	-6.049942	3.900650	1.533579
H	-6.745002	3.549838	2.300163
H	-5.076594	3.442352	1.720450
H	-5.942788	4.983861	1.633374
C	-9.296709	-1.530202	-1.762540
H	-8.534251	-2.302297	-1.666232
H	-10.262275	-2.007979	-1.950663
H	-9.053517	-0.905056	-2.625779
C	-10.515615	0.345679	-0.660860

H	-10.670324	0.944483	0.240430
H	-10.320696	1.023686	-1.495524
H	-11.444713	-0.188441	-0.872744
C	-9.747567	-1.575885	0.725200
H	-10.716459	-2.048446	0.540858
H	-8.999452	-2.351847	0.874155
H	-9.826089	-0.981827	1.639413
C	2.816052	1.844674	-0.225437
C	4.052009	1.130166	-0.120349
N	4.109087	-0.148231	0.093569
H	4.992150	1.660822	-0.234821
C	5.333609	-0.947864	0.176006
C	5.423184	-1.606611	1.558043
C	5.332889	-1.987638	-0.951979
H	6.168785	-0.255796	0.042113
C	6.643932	-2.529726	1.646135
H	5.463998	-0.830151	2.326655
H	4.508632	-2.186778	1.727331
C	6.552487	-2.909946	-0.848985
H	5.310183	-1.473637	-1.916380
H	4.414959	-2.582586	-0.875301
C	6.640014	-3.575896	0.528053
H	7.556599	-1.926025	1.574825
H	6.660355	-3.013973	2.626545
H	7.463431	-2.326820	-1.028873
H	6.500596	-3.665759	-1.638169
H	7.538386	-4.197208	0.588020
H	5.780584	-4.244187	0.659885
H	3.207523	-0.634924	0.192027

Table S61. Cartesian coordinates for **4**. (-1252.75009988 E_h)

atom	x	y	z
C	-0.494062	2.775942	0.518039
C	-1.866962	2.936200	0.223179
C	-2.392743	4.222073	0.044678
C	-1.510540	5.294077	0.153819
C	-0.142750	5.108050	0.442438
C	-1.490407	0.795365	0.407789
H	-3.442946	4.372609	-0.174761
H	-1.882299	6.302590	0.013328
H	0.506866	5.973798	0.514396
N	-2.461309	1.683045	0.166874
C	-2.982112	-1.176622	0.186441
C	-1.693909	-0.644164	0.450082
C	-0.635562	-1.502385	0.777507
C	-0.815652	-2.878557	0.855783
C	-2.098562	-3.376563	0.585055
C	-3.192113	-2.572522	0.249213
H	0.338728	-1.078359	0.991442
H	-2.254798	-4.442573	0.644743
C	0.360387	-3.779979	1.246451
C	-4.572902	-3.183511	-0.034588
O	-4.013330	-0.354920	-0.121957
N	-0.293260	1.416115	0.634784
C	-5.006086	-2.845955	-1.477271
H	-5.990347	-3.278462	-1.680403
H	-5.059152	-1.769227	-1.633326
H	-4.297495	-3.268471	-2.195348
C	-5.608166	-2.635417	0.970709
H	-5.693148	-1.552202	0.901102
H	-6.588366	-3.077211	0.767835
H	-5.323387	-2.897916	1.993378
C	-4.561052	-4.714446	0.098899
H	-3.863198	-5.177085	-0.603679
H	-4.292618	-5.033606	1.109373
H	-5.560084	-5.098869	-0.120199
C	-0.038557	-5.260893	1.307747
H	-0.836086	-5.431717	2.035246
H	-0.376177	-5.627787	0.335001
H	0.826259	-5.856274	1.610935
C	0.877984	-3.355450	2.635400
H	1.722973	-3.982497	2.934756
H	1.215679	-2.316058	2.633166
H	0.092539	-3.455068	3.389442
C	1.495030	-3.618117	0.216010
H	1.164031	-3.923157	-0.780165
H	1.830219	-2.579404	0.158837
H	2.353375	-4.234601	0.498334
C	0.402523	3.840506	0.642106
C	1.841779	3.601409	1.025195
H	1.903547	3.487837	2.111807
H	2.439161	4.488801	0.768942
N	2.375046	2.370858	0.426069
C	2.510109	2.477234	-1.035308
C	3.611820	1.924269	1.079686

H	2.765075	1.480585	-1.407603
H	1.522429	2.724794	-1.435136
C	3.540128	3.493948	-1.537213
H	4.087039	1.207070	0.404925
H	4.324454	2.753093	1.211444
C	3.342951	1.251116	2.421567
H	4.541156	3.257608	-1.167976
H	3.572346	3.485933	-2.629458
H	3.292625	4.508983	-1.216596
H	2.710353	0.368875	2.291185
H	4.282434	0.941756	2.886787
H	2.840608	1.928029	3.117528
H	0.644100	1.034579	0.721005
H	-3.675001	0.588757	-0.087661

Table S62. Cartesian coordinates for **4**$^{\bullet+}$: E0PT. (-1252.55883837 E_h)

atom	x	y	z
C	-0.415268	2.745696	0.445127
C	-1.823372	2.917453	0.276154
C	-2.355403	4.213617	0.130899
C	-1.453195	5.260534	0.146467
C	-0.052341	5.061065	0.311225
C	-1.423891	0.784559	0.444991
H	-3.418502	4.371673	0.005550
H	-1.815387	6.274781	0.030483
H	0.599014	5.927659	0.315336
N	-2.414615	1.686028	0.283132
C	-3.004882	-1.122651	0.339904
C	-1.649786	-0.623922	0.509926
C	-0.602201	-1.518906	0.742618
C	-0.842230	-2.880807	0.815281
C	-2.185097	-3.345787	0.643133
C	-3.267096	-2.531837	0.400785
H	0.397435	-1.131654	0.876523
H	-2.347123	-4.411981	0.705574
C	0.260680	-3.895784	1.068829
C	-4.679427	-3.084363	0.190538
O	-3.989351	-0.285384	0.128367
H	-3.623717	0.678134	0.135827
N	-0.207979	1.401372	0.552748
H	0.744192	1.030717	0.552551
C	-5.645523	-2.498077	1.241991
H	-5.729878	-1.416092	1.155666
H	-6.637572	-2.934471	1.099147
H	-5.308056	-2.742590	2.252296
C	-4.699897	-4.614203	0.328892
H	-5.719701	-4.969858	0.169655
H	-4.056399	-5.095355	-0.411771
H	-4.381740	-4.933524	1.324546
C	-5.160521	-2.728043	-1.233572
H	-5.208333	-1.650181	-1.385824
H	-4.489655	-3.157381	-1.982006
H	-6.158712	-3.143758	-1.392710
C	-0.052296	-4.656293	2.376492
H	-1.015358	-5.168632	2.326203
H	0.722352	-5.407552	2.548591
H	-0.068971	-3.972144	3.228009
C	1.637526	-3.231481	1.195998
H	1.906869	-2.692661	0.283723
H	1.669785	-2.529282	2.033233
H	2.393274	-3.999793	1.369636
C	0.294969	-4.897965	-0.106230
H	1.066359	-5.649196	0.079403
H	-0.659530	-5.414634	-0.224466
H	0.528867	-4.387774	-1.043679
C	0.504316	3.802404	0.476899
C	1.965139	3.538124	0.743351
H	2.103388	3.440341	1.824031
H	2.558999	4.405373	0.424545
N	2.413555	2.282458	0.124950

C	2.478571	2.377707	-1.343722
C	3.663354	1.786544	0.721524
H	2.686790	1.371811	-1.718635
H	1.479913	2.650001	-1.698486
C	3.512789	3.358792	-1.902093
H	4.100340	1.080235	0.010879
H	4.397186	2.595737	0.852650
C	3.420288	1.078277	2.049876
H	4.522327	3.097315	-1.575879
H	3.493115	3.335660	-2.994359
H	3.309342	4.384502	-1.585449
H	2.780872	0.202540	1.908121
H	4.368103	0.751069	2.484709
H	2.937044	1.737669	2.775635

Table S63. Cartesian coordinates for **4**$^{\bullet+}$: E1PT. (-1252.57493987 E_h)

atom	x	y	z
C	-0.466721	2.834915	0.505236
C	-1.838780	3.047018	0.283274
C	-2.354029	4.336814	0.141784
C	-1.429340	5.373915	0.213942
C	-0.051965	5.147948	0.431027
C	-1.457756	0.841061	0.422600
H	-3.408207	4.514575	-0.023428
H	-1.776755	6.393782	0.102588
H	0.619211	5.997892	0.478356
N	-2.407029	1.784232	0.244149
C	-3.016786	-1.119541	0.199975
C	-1.672474	-0.586544	0.454931
C	-0.624043	-1.430572	0.754571
C	-0.806223	-2.827324	0.827029
C	-2.091148	-3.353446	0.570984
C	-3.189577	-2.575163	0.258674
H	0.355335	-1.018358	0.961601
H	-2.217612	-4.422976	0.628324
C	0.379319	-3.706543	1.199902
C	-4.560111	-3.185280	-0.016448
O	-3.971355	-0.340998	-0.052942
N	-0.279150	1.470352	0.588979
H	0.680081	1.110569	0.630981
H	-3.373101	1.504150	0.091879
C	-5.588010	-2.641598	1.002386
H	-5.684635	-1.560365	0.924677
H	-6.561369	-3.099407	0.806610
H	-5.289851	-2.897158	2.022436
C	-4.536879	-4.716332	0.103344
H	-3.842145	-5.167834	-0.609243
H	-4.260536	-5.041357	1.109513
H	-5.535110	-5.102823	-0.112358
C	0.011398	-5.195022	1.260375
H	-0.772249	-5.385612	1.997183
H	-0.324146	-5.567380	0.289487
H	0.894527	-5.766918	1.552936
C	1.499895	-3.512739	0.154754
H	1.163488	-3.817271	-0.838849
H	1.829181	-2.472538	0.103051
H	2.361468	-4.124757	0.432952
C	0.895629	-3.266325	2.588389
H	0.118431	-3.385164	3.346959
H	1.752044	-3.884201	2.870091
H	1.219793	-2.223135	2.588885
C	-4.999841	-2.826927	-1.454619
H	-5.978499	-3.271674	-1.653856
H	-5.068925	-1.748481	-1.589076
H	-4.290456	-3.229865	-2.182364
C	0.469259	3.868624	0.595261
C	1.910999	3.564977	0.916692
H	2.009461	3.478259	2.002498
H	2.542781	4.408231	0.607949
N	2.344670	2.287483	0.329226

C	2.468843	2.365261	-1.137681
C	3.558698	1.765155	0.975826
H	2.676976	1.351591	-1.490786
H	1.489081	2.647189	-1.535203
C	3.538474	3.324511	-1.664849
H	3.992824	1.030800	0.292637
H	4.312553	2.554445	1.112449
C	3.253370	1.094446	2.310610
H	4.524892	3.072262	-1.267896
H	3.587174	3.262440	-2.754685
H	3.320801	4.361455	-1.398174
H	2.577560	0.245937	2.171011
H	4.175288	0.733604	2.772980
H	2.784768	1.788370	3.013419

Table S64. Cartesian coordinates for **4**$^{\bullet+}$: E2PT. (-1252.58855869 E_h)

atom	x	y	z
C	-0.505705	2.745929	0.625250
C	-1.856761	3.000288	0.287137
C	-2.329873	4.299867	0.088275
C	-1.399371	5.326898	0.213486
C	-0.044463	5.081645	0.533027
C	-1.467008	0.819265	0.489939
H	-3.363791	4.497823	-0.164809
H	-1.720513	6.349778	0.057548
H	0.642375	5.916718	0.610357
N	-2.433545	1.753021	0.221204
C	-3.022210	-1.160410	0.169989
C	-1.706479	-0.611533	0.519883
C	-0.676072	-1.452518	0.896195
C	-0.853741	-2.843740	0.973270
C	-2.116143	-3.383886	0.630558
C	-3.192406	-2.616054	0.236584
H	0.280326	-1.013314	1.150011
H	-2.237367	-4.454094	0.689575
C	0.311405	-3.717054	1.424469
C	-4.540556	-3.240630	-0.119290
O	-3.963644	-0.396210	-0.175045
N	-0.284908	1.391165	0.742680
H	-3.380472	1.475919	-0.014614
C	-4.901659	-2.902592	-1.582971
H	-5.863087	-3.360431	-1.832274
H	-4.974230	-1.826031	-1.729387
H	-4.148867	-3.303259	-2.267060
C	-5.634732	-2.695628	0.826194
H	-5.737345	-1.616667	0.723042
H	-6.590131	-3.167961	0.581259
H	-5.396807	-2.929560	1.867307
C	-4.513218	-4.770194	0.018806
H	-3.778872	-5.224090	-0.651772
H	-4.285110	-5.082931	1.041031
H	-5.496106	-5.168975	-0.241602
C	-0.069322	-5.199934	1.523985
H	-0.880165	-5.358523	2.239337
H	-0.376295	-5.605659	0.556894
H	0.797103	-5.770310	1.866353
C	0.789908	-3.236094	2.811747
H	1.628268	-3.854421	3.143472
H	1.128072	-2.197943	2.784368
H	-0.011011	-3.316898	3.550679
C	1.467476	-3.561832	0.412607
H	1.167552	-3.903567	-0.580824
H	1.790268	-2.520991	0.335532
H	2.322279	-4.159204	0.740556
C	0.423828	3.792559	0.749041
C	1.839804	3.467312	1.121892
H	1.899505	3.116168	2.152009
H	2.509468	4.315594	1.002356
N	2.359138	2.332427	0.267720
C	2.431671	2.695402	-1.196092

C	3.650793	1.758883	0.790219
H	2.700304	1.773203	-1.710389
H	1.419507	2.972576	-1.487440
C	3.419961	3.807218	-1.493710
H	4.054070	1.146331	-0.015790
H	4.330316	2.591744	0.964717
C	3.428164	0.924821	2.040124
H	4.431670	3.545343	-1.179362
H	3.433308	3.968829	-2.572682
H	3.133966	4.745874	-1.016787
H	2.703898	0.127647	1.853741
H	4.375607	0.464349	2.324593
H	3.078142	1.524039	2.882084
H	1.636832	1.592434	0.348748

Table S65. Cartesian coordinates for **4'**. (-1631.48406116 E_h)

atom	x	y	z
C	1.571349	1.155233	0.354357
C	0.352857	1.850368	0.173857
C	0.374308	3.225428	-0.100151
C	1.618044	3.841586	-0.197405
C	2.820160	3.123308	-0.017620
C	-0.153391	-0.224629	0.540464
H	-0.546861	3.777850	-0.243717
H	1.672107	4.901740	-0.417570
H	3.766824	3.645853	-0.105305
C	-2.315902	-1.411975	0.647675
C	-3.126693	-2.559341	0.800313
C	-2.535114	-3.800941	1.055564
C	-1.143615	-3.848902	1.145900
C	-0.348375	-2.703405	0.981996
C	-0.916333	-1.447562	0.729163
C	-4.454731	-0.876378	0.410253
H	-3.138582	-4.691992	1.177190
H	-0.657311	-4.795881	1.348213
H	0.728568	-2.794960	1.061705
N	-0.707762	0.965456	0.300845
C	-6.904950	-0.737997	0.029466
C	-5.650942	-0.087643	0.161343
C	-5.566888	1.304073	0.019089
C	-6.688289	2.075251	-0.263101
C	-7.910146	1.401797	-0.410480
C	-8.059021	0.017926	-0.276689
H	-4.604331	1.786401	0.144842
H	-8.789929	1.981815	-0.643276
C	-6.546835	3.594568	-0.413738
C	-9.425063	-0.657558	-0.471081
O	-7.003691	-2.079016	0.189877
H	-6.092977	-2.432156	0.404207
N	-3.180646	-0.371153	0.409351
N	-4.455394	-2.191117	0.644425
H	-2.850473	0.571963	0.234774
N	1.214345	-0.154211	0.593334
H	1.911132	-0.891396	0.633944
C	-5.563008	3.896842	-1.561844
H	-5.438641	4.976965	-1.681394
H	-4.579922	3.462674	-1.363372
H	-5.928846	3.486429	-2.506530
C	-5.989456	4.186363	0.896256
H	-5.026509	3.740503	1.155562
H	-5.847537	5.265958	0.791067
H	-6.680937	4.010874	1.724450
C	-7.884944	4.278272	-0.722725
H	-8.319219	3.918620	-1.659428
H	-8.615402	4.115142	0.074001
H	-7.729510	5.355574	-0.819661
C	-9.341017	-1.682835	-1.621548
H	-8.592600	-2.446697	-1.418712
H	-10.311331	-2.169655	-1.757101
H	-9.080729	-1.182048	-2.558423

C	-9.858165	-1.362592	0.831176
H	-10.825986	-1.850575	0.681450
H	-9.131894	-2.115608	1.135350
H	-9.966061	-0.635585	1.640887
C	-10.516620	0.358730	-0.840072
H	-10.660090	1.106229	-0.055438
H	-10.280075	0.880882	-1.771083
H	-11.462776	-0.169550	-0.981613
C	2.829505	1.760607	0.274745
C	4.086123	0.973230	0.545205
H	4.218551	0.889112	1.628206
H	4.957625	1.527126	0.164726
N	4.008054	-0.392483	0.010135
C	3.952992	-0.413776	-1.460924
C	5.074347	-1.250426	0.543730
H	3.790756	-1.453965	-1.757826
H	3.064272	0.147438	-1.763216
C	5.182654	0.141619	-2.184864
H	5.117581	-2.138270	-0.092713
H	6.060539	-0.764670	0.474740
C	4.805573	-1.676349	1.982926
H	6.089792	-0.392257	-1.890453
H	5.059647	0.029613	-3.265015
H	5.329055	1.203689	-1.973471
H	3.861539	-2.223537	2.050095
H	5.609394	-2.323017	2.344087
H	4.748351	-0.816757	2.655635

Table S66. Cartesian coordinates for **4'**$^{\bullet+}$: E0PT. (-1631.29066022 E_h)

atom	x	y	z
C	1.659860	1.151248	0.409435
C	0.460563	1.876389	0.214605
C	0.514400	3.265910	0.031265
C	1.769377	3.864521	0.040544
C	2.951964	3.115892	0.231866
C	-0.086563	-0.206343	0.434081
H	-0.390497	3.842770	-0.117882
H	1.850089	4.935813	-0.104201
H	3.907892	3.628753	0.227708
C	-2.270072	-1.360227	0.375366
C	-3.106659	-2.507827	0.444849
C	-2.548268	-3.777706	0.658466
C	-1.170774	-3.845309	0.801851
C	-0.347282	-2.698100	0.735299
C	-0.872764	-1.424631	0.519732
C	-4.379312	-0.773090	0.101849
H	-3.172779	-4.659769	0.709675
H	-0.700999	-4.805676	0.974908
H	0.722047	-2.817634	0.863597
N	-0.616294	1.002733	0.239180
C	-6.851724	-0.710231	-0.093443
C	-5.575704	-0.003660	-0.104473
C	-5.554241	1.372198	-0.299501
C	-6.741518	2.084221	-0.470898
C	-7.978934	1.368822	-0.452818
C	-8.085522	0.011528	-0.275261
H	-4.605264	1.888211	-0.315335
H	-8.882794	1.943529	-0.588961
C	-6.776052	3.590683	-0.661702
C	-9.432265	-0.714029	-0.270329
O	-6.879869	-2.000190	0.081537
H	-5.895870	-2.350070	0.195455
N	-3.098890	-0.295320	0.159877
N	-4.404770	-2.104579	0.270453
H	-2.741864	0.654927	0.081114
N	1.275385	-0.163474	0.552035
H	1.964072	-0.909994	0.587841
C	-7.458903	3.906039	-2.011630
H	-8.467065	3.489737	-2.062393
H	-7.533428	4.989699	-2.130414
H	-6.876418	3.504169	-2.843633
C	-7.604642	4.210730	0.488303
H	-7.647484	5.294235	0.353991
H	-8.627963	3.830553	0.503462
H	-7.141781	3.997666	1.454408
C	-5.375167	4.213743	-0.654233
H	-4.863062	4.037245	0.294878
H	-4.755941	3.818607	-1.463038
H	-5.463452	5.292811	-0.794117
C	-9.466499	-1.746016	-1.418522
H	-8.697055	-2.507500	-1.297872
H	-10.442584	-2.237624	-1.431711
H	-9.319540	-1.251352	-2.381948

C	-10.594007	0.268423	-0.479653
H	-10.634875	1.022842	0.310413
H	-10.525348	0.780127	-1.442997
H	-11.530943	-0.291210	-0.460234
C	-9.647025	-1.421060	1.086054
H	-10.626821	-1.905423	1.083490
H	-8.888548	-2.179560	1.272295
H	-9.627701	-0.695680	1.903372
C	2.929461	1.737932	0.433086
C	4.160161	0.913655	0.714736
H	4.257110	0.792048	1.797741
H	5.055959	1.458975	0.381677
N	4.067967	-0.431911	0.131952
C	4.080559	-0.406840	-1.340079
C	5.077865	-1.343403	0.685317
H	3.896330	-1.431048	-1.676873
H	3.227160	0.195356	-1.664871
C	5.360259	0.125622	-1.989912
H	5.104943	-2.220253	0.032770
H	6.085809	-0.900257	0.659278
C	4.740113	-1.784874	2.105344
H	6.235558	-0.442798	-1.665840
H	5.285271	0.042586	-3.077010
H	5.527616	1.177451	-1.745668
H	3.758036	-2.265004	2.131199
H	5.484923	-2.496840	2.469763
H	4.722914	-0.941582	2.800590

Table S67. Cartesian coordinates for **4'**$^{\bullet+}$: E1PT. (-1631.30624222 E_h)

atom	x	y	z
C	1.556538	1.123746	0.346291
C	0.327216	1.802686	0.175565
C	0.326412	3.180489	-0.087529
C	1.560512	3.813493	-0.184850
C	2.774628	3.111101	-0.014521
C	-0.141199	-0.282267	0.526152
H	-0.603125	3.720579	-0.222757
H	1.599230	4.875758	-0.397458
H	3.712631	3.648986	-0.101054
C	-2.291295	-1.478363	0.627262
C	-3.087208	-2.627213	0.768205
C	-2.518144	-3.879879	1.000470
C	-1.128527	-3.921652	1.084042
C	-0.330374	-2.772191	0.935245
C	-0.891282	-1.513846	0.702859
C	-4.419529	-0.864136	0.397623
H	-3.126254	-4.767516	1.108215
H	-0.641258	-4.870710	1.269783
H	0.745993	-2.867829	1.010254
N	-0.717487	0.900025	0.299616
C	-6.904863	-0.744867	0.051358
C	-5.605204	-0.070403	0.171320
C	-5.511296	1.299959	0.054834
C	-6.647485	2.093923	-0.214392
C	-7.893307	1.451218	-0.379914
C	-8.070852	0.084880	-0.270681
H	-4.551166	1.784772	0.179324
H	-8.751589	2.063424	-0.607638
C	-6.477443	3.602398	-0.336606
C	-9.429694	-0.573497	-0.484201
O	-6.995627	-1.986514	0.225347
N	-3.145433	-0.420744	0.404820
N	-4.393218	-2.193704	0.617048
H	-2.776444	0.519090	0.255892
N	1.222424	-0.193172	0.574357
H	1.932975	-0.919057	0.607830
H	-5.266342	-2.719013	0.620345
C	-7.801295	4.326193	-0.611880
H	-7.614246	5.399759	-0.681660
H	-8.253459	4.005319	-1.553597
H	-8.525576	4.163717	0.190059
C	-5.499574	3.893965	-1.497082
H	-4.521611	3.438640	-1.326068
H	-5.895979	3.517083	-2.442448
H	-5.359668	4.973892	-1.589174
C	-5.883449	4.148373	0.980856
H	-6.565378	3.969750	1.815161
H	-4.921627	3.688821	1.216635
H	-5.730303	5.226199	0.884510
C	-9.325795	-1.603245	-1.632646
H	-8.595535	-2.377183	-1.404952
H	-10.301565	-2.071612	-1.785826
H	-9.037481	-1.108886	-2.564105

C	-10.503329	0.454122	-0.870434
H	-10.658331	1.196687	-0.083686
H	-10.242603	0.978027	-1.793697
H	-11.449078	-0.066796	-1.035484
C	-9.880878	-1.278159	0.815238
H	-10.854836	-1.745711	0.647298
H	-9.168676	-2.045298	1.115481
H	-9.984419	-0.554545	1.627802
C	2.806250	1.747651	0.267326
C	4.073599	0.975167	0.530547
H	4.211643	0.893874	1.612945
H	4.936585	1.538394	0.145196
N	4.006979	-0.391711	-0.003789
C	3.950700	-0.412799	-1.475344
C	5.083322	-1.239638	0.526844
H	3.795915	-1.454095	-1.772199
H	3.057510	0.142029	-1.776363
C	5.175342	0.151867	-2.200333
H	5.129160	-2.128943	-0.107346
H	6.064839	-0.746070	0.449592
C	4.827773	-1.663072	1.968950
H	6.086492	-0.376261	-1.908070
H	5.051182	0.039942	-3.280321
H	5.315013	1.214681	-1.988408
H	3.887642	-2.215624	2.045248
H	5.638233	-2.304160	2.325028
H	4.771279	-0.802463	2.640353

Table S68. Cartesian coordinates for **4'**$^{\bullet+}$: E2PT. (-1631.31358663 E_h)

atom	x	y	z
C	1.569271	1.211608	0.249827
C	0.358885	1.904956	0.077656
C	0.341335	3.275947	-0.177449
C	1.583129	3.899701	-0.265106
C	2.792335	3.194090	-0.092427
C	-0.093653	-0.261030	0.437420
H	-0.586268	3.816470	-0.311518
H	1.625322	4.962489	-0.470858
H	3.730894	3.731111	-0.170013
C	-2.265505	-1.427294	0.511680
C	-3.020147	-2.619825	0.653416
C	-2.420797	-3.856694	0.885075
C	-1.028550	-3.879008	0.975774
C	-0.257375	-2.715690	0.833362
C	-0.856322	-1.472803	0.601040
C	-4.333548	-0.868752	0.283643
H	-3.007371	-4.760160	0.990492
H	-0.526201	-4.820066	1.161880
H	0.821139	-2.783291	0.912033
N	-0.641571	0.952162	0.211399
C	-6.852267	-0.760505	0.007520
C	-5.544334	-0.096392	0.069446
C	-5.449690	1.272455	-0.082035
C	-6.588030	2.069920	-0.304681
C	-7.850896	1.437549	-0.382278
C	-8.031827	0.076956	-0.237450
H	-4.469578	1.728253	-0.022491
H	-8.717328	2.055764	-0.558494
C	-6.416055	3.577683	-0.450109
C	-9.414414	-0.566741	-0.317632
O	-6.944245	-2.007374	0.165004
N	-3.095537	-0.357374	0.287416
N	-4.325587	-2.218723	0.499808
N	1.241935	-0.116116	0.472087
H	1.982325	-0.819112	0.516581
H	-5.188651	-2.754186	0.509084
H	-1.656118	1.060902	0.153943
C	-9.443450	-1.584252	-1.479879
H	-8.703081	-2.369162	-1.333697
H	-10.435950	-2.039137	-1.540467
H	-9.238779	-1.084583	-2.430717
C	-5.480627	3.859014	-1.646247
H	-5.334312	4.937465	-1.748149
H	-4.501662	3.394627	-1.510561
H	-5.916578	3.483529	-2.575054
C	-10.516344	0.472974	-0.571159
H	-10.565230	1.217398	0.227977
H	-10.369441	0.996020	-1.519765
H	-11.480487	-0.038409	-0.613901
C	-9.731122	-1.281388	1.015322
H	-9.008812	-2.069794	1.217504
H	-9.716013	-0.568448	1.844245
H	-10.731237	-1.720377	0.963000

C	-7.745539	4.307143	-0.683532
H	-8.238363	3.971665	-1.599497
H	-8.438003	4.164607	0.149762
H	-7.555777	5.378406	-0.780794
C	-5.770736	4.127998	0.840755
H	-6.416670	3.949232	1.703664
H	-4.801448	3.664869	1.036623
H	-5.619221	5.205882	0.739932
C	2.820650	1.828388	0.181819
C	4.078494	1.044352	0.459322
H	4.225283	1.009080	1.542528
H	4.945559	1.575592	0.042465
N	3.975255	-0.341469	-0.018111
C	3.984085	-0.424228	-1.489192
C	4.974139	-1.220853	0.606769
H	3.771204	-1.464763	-1.750253
H	3.145614	0.176422	-1.854153
C	5.275474	0.026890	-2.176242
H	5.014202	-2.132432	0.004546
H	5.980931	-0.777602	0.577375
C	4.602689	-1.581056	2.041477
H	6.131981	-0.561763	-1.838901
H	5.181695	-0.100076	-3.257536
H	5.487991	1.080835	-1.981747
H	3.629009	-2.077748	2.070255
H	5.349132	-2.255585	2.468212
H	4.551573	-0.697208	2.682689

Table S69. Cartesian coordinates for **4'**$^{\bullet+}$: E3PT. (-1631.32295325 E_h)

atom	x	y	z
C	1.551373	1.131008	-0.327860
C	0.350526	1.866885	-0.191561
C	0.348369	3.244267	0.031287
C	1.593585	3.859868	0.133880
C	2.796010	3.134152	0.014434
C	-0.058433	-0.299682	-0.491098
H	-0.573561	3.802959	0.131624
H	1.644327	4.927390	0.312656
H	3.741126	3.656029	0.113246
C	-2.259115	-1.473661	-0.572499
C	-3.007778	-2.676050	-0.669489
C	-2.403149	-3.922101	-0.835995
C	-1.010810	-3.938844	-0.900810
C	-0.247976	-2.763771	-0.792625
C	-0.847074	-1.512705	-0.626160
C	-4.338312	-0.915902	-0.418176
H	-2.986480	-4.830915	-0.910616
H	-0.499600	-4.884623	-1.034379
H	0.832513	-2.818188	-0.839663
N	-0.648147	0.925253	-0.314609
C	-6.859276	-0.807852	-0.157276
C	-5.557253	-0.139533	-0.279935
C	-5.478179	1.240304	-0.262763
C	-6.624752	2.041593	-0.126431
C	-7.882896	1.406596	-0.000065
C	-8.050066	0.037262	-0.016626
H	-4.503876	1.701130	-0.364178
H	-8.755697	2.032078	0.103602
C	-6.475749	3.558623	-0.149309
C	-9.429229	-0.607315	0.106226
O	-6.936314	-2.066117	-0.172680
N	-3.104933	-0.398466	-0.422921
N	-4.318699	-2.276674	-0.564071
N	1.271085	-0.214564	-0.508914
H	-5.174693	-2.821352	-0.537627
H	-1.659381	1.040528	-0.282214
C	-5.916265	3.967592	-1.529763
H	-5.784067	5.051955	-1.567358
H	-4.949655	3.497800	-1.723201
H	-6.603575	3.676241	-2.327905
C	-7.807177	4.286053	0.077861
H	-8.533685	4.052410	-0.704354
H	-8.249041	4.027678	1.043651
H	-7.637043	5.364936	0.062813
C	-5.481490	3.990094	0.949008
H	-5.855903	3.722079	1.939898
H	-4.502780	3.525414	0.811808
H	-5.349003	5.074440	0.912164
C	-9.711408	-1.492990	-1.129131
H	-8.980672	-2.294772	-1.215470
H	-10.709278	-1.930639	-1.037261
H	-9.687689	-0.894624	-2.043677
C	-10.544494	0.445423	0.187921

H	-10.445815	1.080584	1.071904
H	-10.558153	1.088054	-0.695889
H	-11.508362	-0.065028	0.249555
C	-9.482516	-1.466785	1.388011
H	-10.469958	-1.928127	1.476746
H	-8.728238	-2.252482	1.363522
H	-9.314826	-0.848573	2.273788
C	2.799599	1.761868	-0.219204
C	4.071901	0.981283	-0.402375
H	4.927531	1.499716	0.025985
H	4.263380	0.818979	-1.464818
N	3.988327	-0.397652	0.216761
C	4.838315	-1.401183	-0.527173
C	4.266099	-0.421285	1.697920
H	4.628577	-2.365535	-0.064382
H	4.449545	-1.415257	-1.545038
C	6.322703	-1.084643	-0.508166
H	4.213549	-1.471327	1.985612
H	5.290306	-0.076055	1.832453
C	3.292352	0.411568	2.513482
H	6.735419	-1.112761	0.500896
H	6.834936	-1.843073	-1.102567
H	6.536970	-0.111308	-0.952487
H	2.258297	0.125717	2.315666
H	3.500559	0.232205	3.570177
H	3.403584	1.477855	2.319522
H	3.005826	-0.705362	0.066451

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