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Supporting Information

Mechanistic Insights into Nitric Oxide Generation from Nitrite via O-atom Transfer in the Unsymmetrical β-Diketiminato Copper(II) Nitrite Complex

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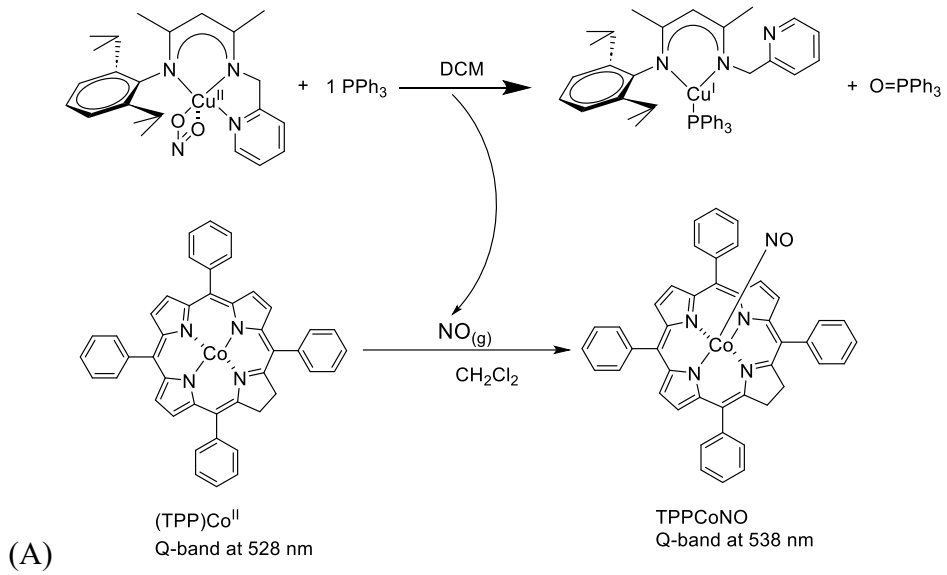


(A)

(B)

Figure S1. (A) A representative scheme showing NO generation (in Chamber 1) and NO trapping (in Chamber 2). (B) A pictorial demonstration of the "H-tube" setup utilized for the NO trapping experiments. The reaction is monitored for more than 3 times for better accuracy.

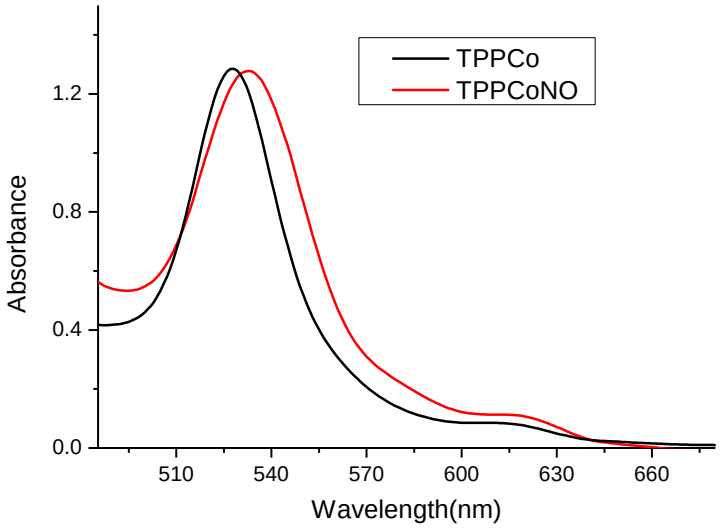


Figure S2. UV-Vis spectra (2 mM in CH_2Cl_2) of [(TPP)Co] (black trace) and [(TPP)CoNO] (red trace) generated by reacting [(TPP)Co] with NO released from the mixture of $LCu^{II}ONO$ and 1 equivalent of PPh_3. The wavelength shift from 528 nm for [(TPP)Co] to 532.4 nm for [(TPP)CoNO] is observed. The amount of NO generated was calculated using the calibration curve in Figure S3B and aligns with the reported literature.[1] The cuvette used for these measurements had a 1 cm path length.

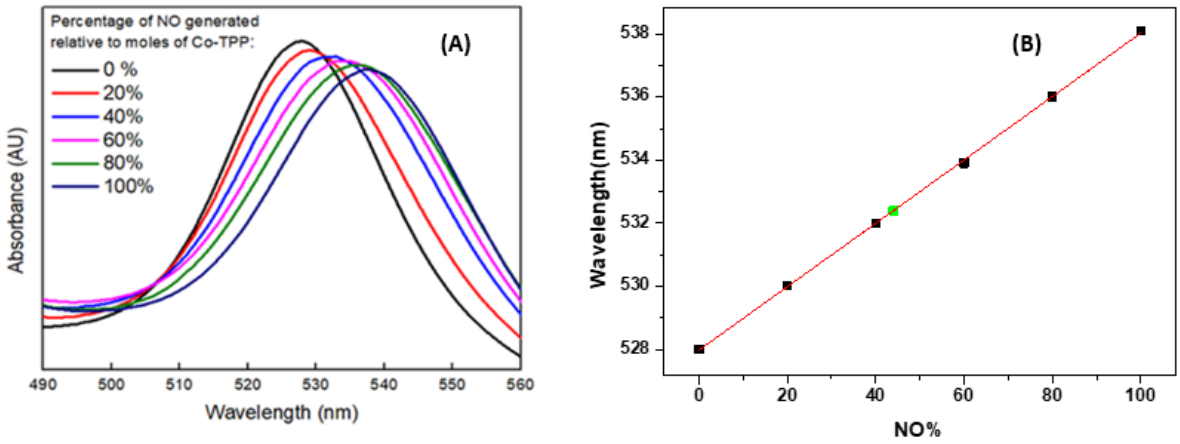


Figure S3. (A) UV-Vis spectra showing the absorbance shift of cobalt(II) porphyrin [(TPP)Co] (2 mM concentration) as NO complexation increases. A calibration curve was constructed by exposing [(TPP)Co] to known concentrations of NO in N_2 (160, 320, 480, 640, and 800 ppm). The peak shift from λ_{max} ~528 nm to ~538 nm was observed, dependent on NO concentration, and the responses were plotted against NO levels. This data was used to generate a graph of λ_{max} shift versus the amount of NO generated. (B) The calibration curve, plotted from the peak maxima, demonstrates a linear relationship between the absorbance shift and the percentage of NO complexation. The green marker indicates the amount of NO released from $LCu^{II}ONO$ upon treatment with 1 equivalent of PPh_3. All measurements were taken in a 1 cm path length cuvette.

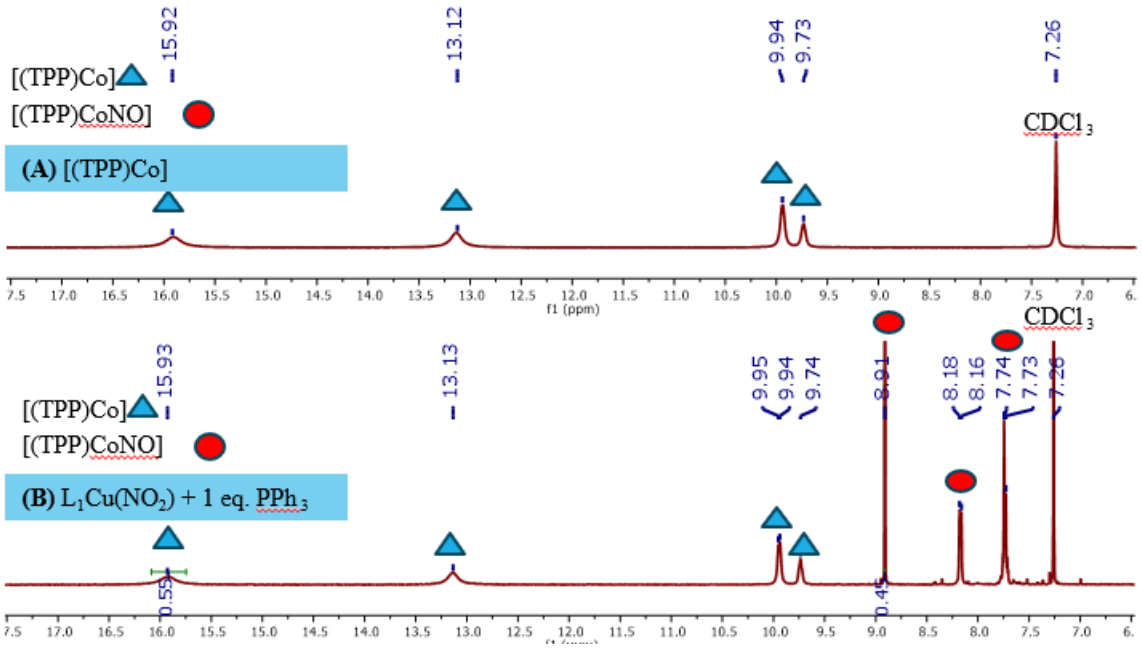


Figure S4. ^{1}H NMR (**400** MHz, $CDCl_3$, 298 K) spectra of [(TPP)Co^{II}] obtained after the NO-trapping experiment: (A) free [(TPP)Co^{II}], indicated by blue triangles, and (B) [(TPP)CoNO], indicated by red circles, after one hour of reaction.[2] The ^{1}H NMR of [(TPP)Co(NO)] (400 MHz, $CDCl_3$): δ 8.91 (s, 2H), 8.17 (d, J = 8 Hz, 2H), 7.73 (d, J = 4 Hz, 3H). The ^{1}H NMR of [(TPP)Co] (400 MHz, $CDCl_3$): δ 15.92 (s, 2H), 13.12 (s, 2H), 9.94 (s, 2H), 9.73 (s, 1H). The yield of NO (100%) was calculated from the relative integrals of the proton NMR resonances of [(TPP)Co(NO)] and unreacted [(TPP)Co] at δ = 15.93 and δ = 8.91 ppm, respectively.

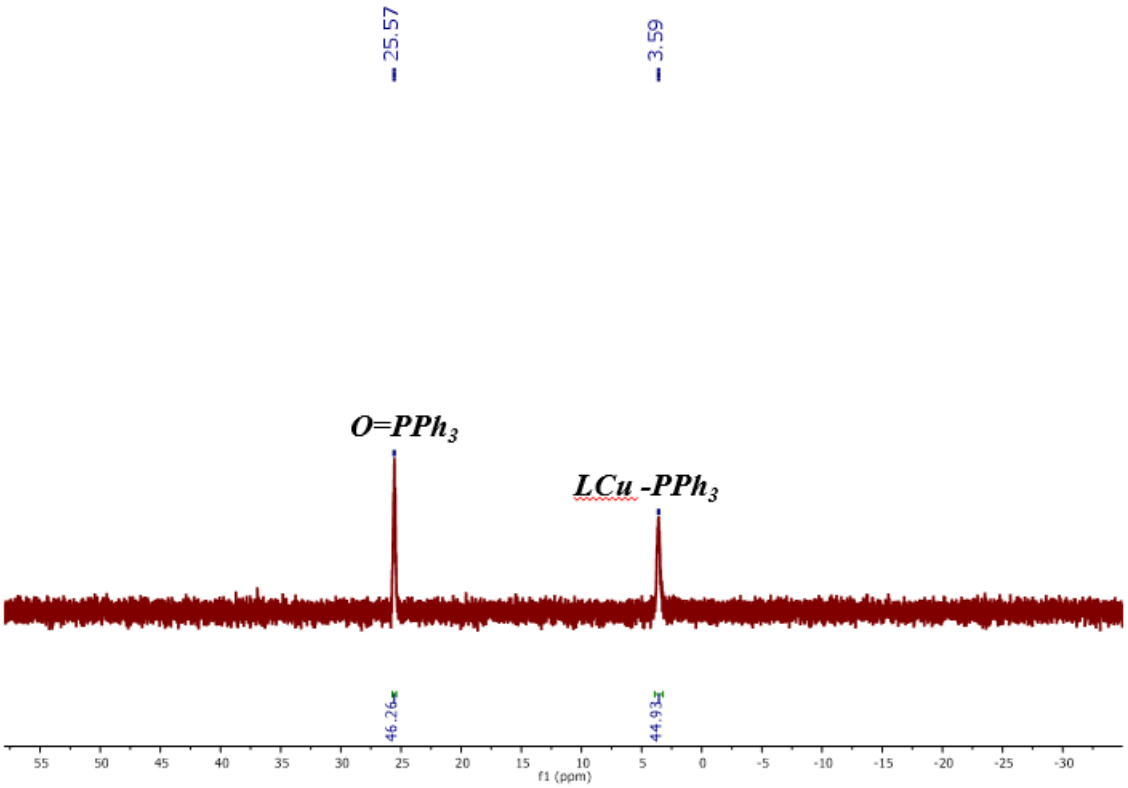
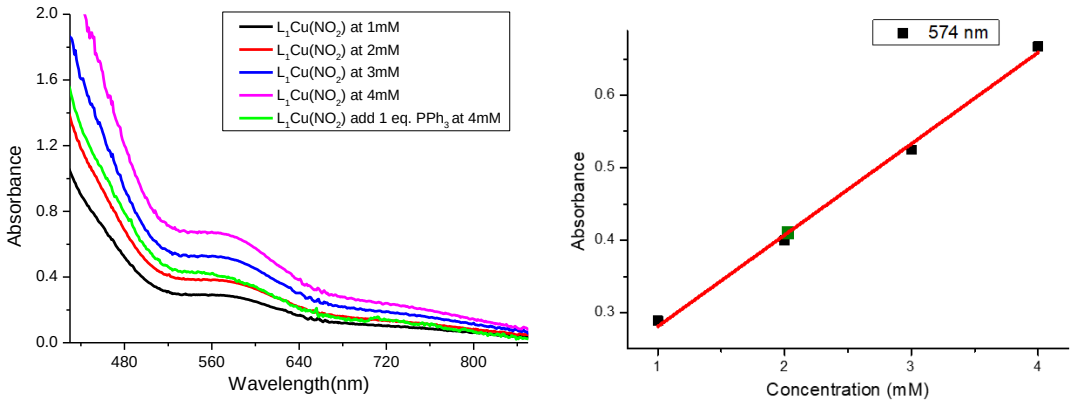


Figure S5. ^{31}P NMR spectrum (400 MHz, C_6D_6) obtained from 1 equivalent of $LCu^{II}ONO$ with 1 equivalent of PPh_3. The peak at +25.57 ppm is assigned as $O{=}PPh_3$, and the peak at +3.59 is assigned as $LCu^{I}PPh_3$, according to the reported literature.[1,3]

Analysis of the remaining unreacted species

Due to the detection of the low amount of phosphine adducts copper complex in this reaction, we explore the UV tracing experiment to predict the remaining amount of unreacted $LCu^{II}ONO$. To understand the remaining half the amount of the species, we have plotted the Beer's law plot for the $LCu^{II}ONO$ in different concentrations, as shown in **Figures S6**(A) and **S6**(B). We monitored this reaction by UV-Vis spectroscopy by adding 1 equivalent of PPh_3 (0.045, 0.174 mmol) in 4 mM solution of complex $LCu^{II}(ONO)$ (0.080 g, 0.174 mmol) in DCM forming green spectrum after 1 hr as shown in **Figure S6**(A) which is 51% remains unreacted of $LCu^{II}(ONO)$.



(A) (B)

Figure S6: (A) UV-Vis spectra of $LCu^{II}ONO$ in DCM at 25 °C at different concentrations, along with the spectra obtained after the reaction, indicated by the green line. (B) The calibration curve from Beer's plot for $LCu^{II}ONO$ at 574 nm, along with a green dot indicating that 51% of $LCu^{II}ONO$ remains unreacted.

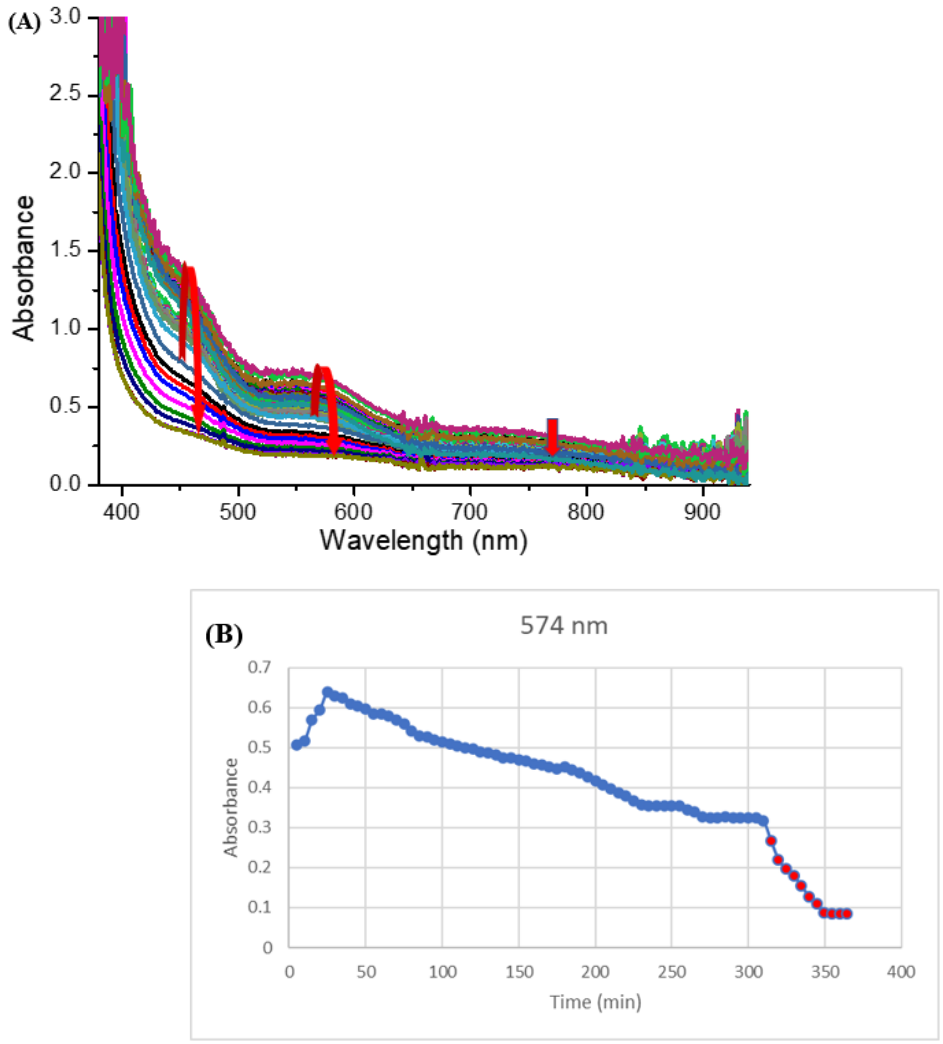


Figure S7: (A) UV-Vis spectra of $LCu^{II}ONO$ (2 mM) with two equivalents of PPh_3 at different time intervals at low temperature and room temperature. (B) Time trace plot of time (min) vs. absorbance at -40 °C (blue dots) and at room temperature (red dots). Red dotted line: absorbance at room temperature.

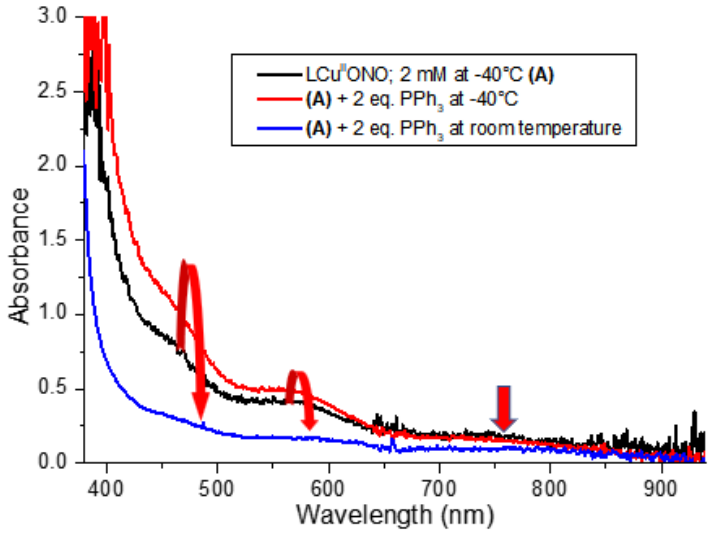


Figure S8: UV-Vis spectra of LCu^{II}ONO at -40 °C (black); after the addition of two equivalents of PPh_3 to LCu^{II}ONO at -40 °C (red) in 25 minutes; and the spectrum recorded after 365 minutes as the temperature returned to room temperature (blue).

References

(1) Chand, K.; Chu, Y.-C.; Wang, T.-W.; Kao, C.-L.; Lin, Y.-F.; Tsai, M.-L.; Hsu, S. C. N. Nitric oxide generation study of unsymmetrical β-diketiminato copper(ii) nitrite complexes. *Dalton Trans.* **2022**, *51*, 3485-3496.

(2) Anju, B. S.; Nair, N. R.; Kundu, S. Nitrite and Nitric Oxide Interconversion at Mononuclear Copper (II): Insight into the Role of the Red Copper Site in Denitrification. *Angew. Chem. Int. Ed.* **2023**, *62*, e202311523 and the supporting information therein.

(3) Sakhaei, Z.; Kundu, S.; Donnelly, J. M.; Bertke, J. A.; Kim, W. Y.; Warren, T. H. Nitric oxide release via oxygen atom transfer from nitrite at copper(ii). *Chem. Commun.* **2017**, *53*, 549-552.

The coordinates of optimized structures.

Table S1.

Structure: **1-Cry**, Energy= -2904.961074 Hartree, Charge= 0, Multiplicity=2

The number of the imaginary frequencies: 0

Center Number	Coordinates (Angstroms) X	Y	Z
C	-2.01793100	-0.15895000	0.29564800
C	-2.27871600	-0.98811900	1.40647700
C	-1.33813400	-0.98477300	2.60400800
H	-0.90304000	0.01602100	2.68620100
C	-0.17450800	-1.96155200	2.35005800
H	-0.54525600	-2.98892700	2.25696200
H	0.55177800	-1.92849700	3.17080900
H	0.34749200	-1.71142900	1.42239800
C	-2.02883100	-1.29404700	3.93804100
H	-2.88634100	-0.63315900	4.10681700
H	-1.32293900	-1.15621100	4.76453200
H	-2.38554800	-2.32912500	3.98454700
C	-3.37596800	-1.85328800	1.34810300
H	-3.59867500	-2.49691900	2.19306400
C	-4.19051500	-1.90149200	0.21866600
H	-5.04499700	-2.57228500	0.19255400
C	-3.89759400	-1.10148600	-0.88333000
H	-4.52374200	-1.16344100	-1.76792600
C	-2.80235500	-0.23108300	-0.87380700

C	-2.45745700	0.60869700	-2.09656500
H	-1.39125900	0.84202400	-2.03202000
C	-2.67971300	-0.14711600	-3.41484700
H	-3.74459600	-0.30484300	-3.62149400
H	-2.18550400	-1.12310900	-3.40146500
H	-2.26719100	0.43260000	-4.24807700
C	-3.22200500	1.94452700	-2.11488700
H	-2.98242100	2.50776600	-3.02460900
H	-2.96334800	2.57132600	-1.25730000
H	-4.30526500	1.77334200	-2.09791400
C	-2.43643400	2.30770700	1.47287900
H	-3.26767700	1.99669900	0.83768600
H	-2.50587200	3.38225400	1.65354000
H	-2.56188600	1.79248800	2.43298000
C	-1.09098000	1.94894300	0.87193200
C	-0.08282800	2.92255300	0.96984200
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C	1.28198200	2.76927800	0.67984600
C	2.18934500	3.94857400	0.95862800
H	2.80979600	4.18502200	0.08716100
H	2.86974500	3.73414300	1.79198800
H	1.60678500	4.83369100	1.21948000
C	3.23003400	1.49416300	0.06246000
H	3.78280800	1.93745800	0.89982400
H	3.59194200	1.99834400	-0.84781000
C	3.59655000	0.03336600	-0.02563900
C	4.91665800	-0.41178100	0.04041000
H	5.72168900	0.30528600	0.16308700
C	5.17481800	-1.77573300	-0.04761200

H	6.19409600	-2.14461800	0.00711300
C	4.10657200	-2.66278400	-0.20329400
H	4.26538600	-3.73275100	-0.27414500
C	2.82124900	-2.14647800	-0.27099300
H	1.95052400	-2.77649200	-0.40755500
Cu	0.78678600	0.07840100	-0.30310900
N	0.32591500	-1.38553100	-2.50022300
N	-0.90699300	0.73966800	0.34027000
N	1.79007800	1.63643400	0.20827700
N	2.57540600	-0.82687600	-0.17831600
O	0.05518900	-1.51899200	-1.24697000
O	0.85024200	-0.29973200	-2.78977900

Table S2.

Structure: **1a**, Energy= -2904.958163 Hartree, Charge= 0, Multiplicity=2

The number of the imaginary frequencies: 0

Center	Coordinates (Angstroms)		
Number	X	Y	Z

C	-1.94545000	-0.08035000	0.38830800
C	-2.02759300	-0.77647800	1.61328300
C	-0.94187600	-0.62009900	2.66825400
H	-0.42152900	0.32259300	2.47691700
C	0.09035500	-1.75247700	2.51183200
H	-0.36260100	-2.72233000	2.74914500
H	0.94695800	-1.59921400	3.17889300
H	0.45437900	-1.80624600	1.48191200

C	-1.48312700	-0.55840500	4.10283500
H	-2.23467600	0.23175700	4.21044200
H	-0.66660300	-0.35074300	4.80362600
H	-1.94292200	-1.50471600	4.40886600
C	-3.08836400	-1.66559700	1.80765400
H	-3.16634100	-2.21067600	2.74340700
C	-4.04614000	-1.86468600	0.81590300
H	-4.87080200	-2.55183300	0.98445400
C	-3.93490900	-1.19180400	-0.39763500
H	-4.67563500	-1.36516800	-1.17235900
C	-2.88129900	-0.30360200	-0.64285900
C	-2.76717600	0.38974600	-1.99477400
H	-1.75248000	0.78931900	-2.07242800
C	-2.96573600	-0.58922800	-3.16387600
H	-3.99538800	-0.96208100	-3.21003400
H	-2.28740900	-1.44205200	-3.08269600
H	-2.75904300	-0.08007200	-4.11228000
C	-3.74915700	1.56884000	-2.11907100
H	-3.66390700	2.03278900	-3.10881600
H	-3.55591900	2.34197200	-1.36997100
H	-4.78405300	1.22794600	-1.99424000
C	-2.32287300	2.53186100	1.21594900
H	-3.19666400	2.11304400	0.71549200
H	-2.40595900	3.62035800	1.23564000
H	-2.34845600	2.17049000	2.25166100
C	-1.02226800	2.10224000	0.56680400
C	-0.01833700	3.08285800	0.47801700
H	-0.30812000	4.08738300	0.75954100
C	1.34107800	2.89031200	0.18956200

C	2.25718800	4.08926600	0.30532600
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H	2.93625600	3.98386800	1.16047900
H	1.68241000	5.00655400	0.44363900
C	3.27964900	1.52186200	-0.22897900
H	3.81699900	2.02147700	0.58730700
H	3.68009600	1.94338000	-1.16463000
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C	4.09371800	-2.65664100	-0.10561300
H	4.23777300	-3.73053200	-0.07486900
C	2.81516700	-2.13309000	-0.21981300
H	1.93628500	-2.76361800	-0.29221400
Cu	0.81263200	0.11112900	-0.44395000
N	-0.86147100	0.83327700	0.18862300
N	1.84055300	1.70256500	-0.13624300
N	2.58613600	-0.80617200	-0.25216400
N	0.11026900	-1.34476400	-1.54879600
O	0.15941200	-1.11469900	-2.77368200
O	-0.27936600	-2.44898300	-1.13579900

Table S3.

Structure: **1b**, Energy= -2904.95591 Hartree, Charge= 0, Multiplicity=2

The number of the imaginary frequencies: 0

Center Number		Coordinates (Angstroms) X	Y	Z
	C	-2.00326800	0.04042000	0.31356500
	C	-2.29062500	-0.28678500	1.65448100
	C	-1.36589600	0.17705100	2.77173300
	H	-0.92038000	1.12873900	2.46557600
	C	-0.21116400	-0.82923400	2.93704200
	H	-0.59382900	-1.80853200	3.24677300
	H	0.50598800	-0.48310700	3.69072600
	H	0.32417800	-0.96786800	1.99354300
	C	-2.07697300	0.41528700	4.10960500
	H	-2.92834300	1.09527600	3.99414900
	H	-1.37992100	0.85915800	4.82895100
	H	-2.44687600	-0.51793600	4.54893300
	C	-3.39824200	-1.09885800	1.91788100
	H	-3.64269800	-1.35912900	2.94270200
	C	-4.19405300	-1.58129200	0.88113600
	H	-5.05634100	-2.20440100	1.10234200
	C	-3.87209200	-1.28051000	-0.44036700
	H	-4.48227300	-1.68512700	-1.24135600
	C	-2.76735700	-0.48050800	-0.75127200
	C	-2.38403400	-0.19367100	-2.19699300
	H	-1.30205500	-0.02760400	-2.20554600
	C	-2.67731400	-1.37330200	-3.13583300
	H	-3.75384900	-1.51882200	-3.28299600
	H	-2.25148500	-2.30411700	-2.75162800
	H	-2.23882000	-1.17840400	-4.12102300
	C	-3.05016900	1.08581100	-2.73494400

H	-2.78857100	1.23499500	-3.78923600
H	-2.73034300	1.97396400	-2.18438500
H	-4.14232500	1.01421700	-2.66438100
C	-2.40769100	2.77569600	0.42292900
H	-3.23794800	2.24282600	-0.04377900
H	-2.46938800	3.83414000	0.16234500
H	-2.54160500	2.68346900	1.50756800
C	-1.06217700	2.20065700	0.02459500
C	-0.04816600	3.12666600	-0.27353800
H	-0.34075100	4.16894500	-0.28385800
C	1.31325900	2.86342800	-0.48345500
C	2.22467300	4.05087600	-0.70698800
H	2.84273900	3.91268600	-1.60092400
H	2.90759000	4.18859600	0.14041200
H	1.64550500	4.96819500	-0.82448800
C	3.26076100	1.45003200	-0.53017400
H	3.80140500	2.17501800	0.09108800
H	3.63649400	1.58369500	-1.55676000
C	3.62816600	0.06436200	-0.06165700
C	4.94962600	-0.33459500	0.13827100
H	5.75860100	0.36335600	-0.05073100
C	5.20366900	-1.62715200	0.58479200
H	6.22390600	-1.95728000	0.75241100
C	4.13097300	-2.49209200	0.81798100
H	4.28743800	-3.50547400	1.16950800
C	2.84483800	-2.03009700	0.58430200
H	1.97001100	-2.65244800	0.72893400
Cu	0.81386900	0.01134600	-0.26051100
N	-0.88243000	0.87944800	0.02399600

N	1.81861100	1.63319900	-0.46237400
N	2.60393300	-0.77679900	0.15796000
O	0.06964600	-1.76677900	-0.55222900
N	0.47759400	-2.12700600	-1.74727500
O	0.11176400	-3.24151900	-2.08759900

Table S4.

Structure: **2a**, Energy= -2829.707678 Hartree, Charge= 0, Multiplicity=2

The number of the imaginary frequencies: 0

Center	Coordinates (Angstroms)		
Number	X	Y	Z

C	-1.95348500	-0.18931900	0.25469700
C	-2.04966700	-1.25606500	1.17410900
C	-1.04034300	-1.39714900	2.30510600
H	-0.58670900	-0.41443300	2.46540300
C	0.09077400	-2.35876700	1.90151100
H	-0.30302600	-3.36359100	1.70941100
H	0.84442800	-2.42953000	2.69509300
H	0.58485300	-2.01476600	0.98998500
C	-1.67800000	-1.82769500	3.63378600
H	-2.50362800	-1.16338100	3.91259000
H	-0.93075100	-1.79940000	4.43500800
H	-2.06915200	-2.85035500	3.58907100
C	-3.07106800	-2.19655300	1.00806300
H	-3.15278300	-3.02671900	1.70325400
C	-3.98663000	-2.08524500	-0.03592600

H	-4.77373300	-2.82520700	-0.15317700
C	-3.89057800	-1.01826500	-0.92498400
H	-4.60888800	-0.93186900	-1.73586700
C	-2.88251900	-0.05594900	-0.79983700
C	-2.81430700	1.09153800	-1.79891800
H	-1.99559800	1.75015900	-1.49627200
C	-2.50083700	0.58766100	-3.21845500
H	-3.29417500	-0.07528100	-3.58447100
H	-1.55913200	0.03321200	-3.22799700
H	-2.42269900	1.43167900	-3.91461700
C	-4.11021100	1.92255600	-1.80713900
H	-4.00658300	2.78105900	-2.48087100
H	-4.35943400	2.30310300	-0.81094900
H	-4.96143400	1.32706000	-2.15687600
C	-2.34394500	2.15853300	1.66036500
H	-3.15994700	2.14527500	0.93366400
H	-2.33230100	3.13100800	2.15585300
H	-2.57589300	1.38902300	2.40533100
C	-1.00934500	1.86606600	1.00370300
C	-0.00820600	2.84053500	1.15801900
H	-0.30259600	3.74139500	1.68185800
C	1.34741100	2.75682300	0.79126100
C	2.24871200	3.90785400	1.18635400
H	2.83945000	4.25862500	0.33275100
H	2.95821700	3.60155600	1.96528300
H	1.66699300	4.74613100	1.57413500
C	3.27704200	1.57377200	-0.02652500
H	3.84564200	1.90388600	0.85281400
H	3.64159000	2.18151400	-0.87087700

C	3.63074400	0.12865700	-0.29758200
C	4.95432300	-0.31001200	-0.34473800
H	5.76071100	0.39783500	-0.18247000
C	5.21637400	-1.65258700	-0.59540700
H	6.23913500	-2.01449300	-0.62928700
C	4.14580400	-2.52582300	-0.80256800
H	4.30503100	-3.57918600	-1.00376600
C	2.85646900	-2.01736400	-0.75319500
H	1.98370700	-2.63703100	-0.92907900
Cu	0.81789900	0.17290700	-0.44671500
N	-0.84733600	0.70861500	0.35761600
N	1.84394300	1.70594500	0.15348300
N	2.60526300	-0.72070600	-0.49532200
N	0.07054600	-0.99864400	-1.74570300
O	-0.12319800	-2.19914000	-1.61960700

Table S5.

Structure: **2b**, Energy= -2829.69101 Hartree, Charge= 0, Multiplicity=2

The number of the imaginary frequencies: 0

Center	Coordinates (Angstroms)		
Number	X	Y	Z

C	-1.95624200	-0.18506600	0.24753300
C	-2.05654000	-1.23541300	1.18514600
C	-1.05345900	-1.35593900	2.32420700
H	-0.60783300	-0.36810900	2.47619200
C	0.08649100	-2.31491100	1.93952000

H	-0.29851200	-3.32518200	1.76019400
H	0.83880700	-2.36696500	2.73574600
H	0.58064100	-1.98326900	1.02282500
C	-1.69543000	-1.77537500	3.65431100
H	-2.52822200	-1.11467500	3.91982900
H	-0.95310000	-1.73053100	4.45928100
H	-2.07730500	-2.80187800	3.62018900
C	-3.07857400	-2.17744800	1.03157300
H	-3.16447700	-2.99510800	1.74075000
C	-3.98918800	-2.08306600	-0.01796800
H	-4.77667800	-2.82405200	-0.12558300
C	-3.88771200	-1.03269400	-0.92615500
H	-4.60161500	-0.96092000	-1.74223800
C	-2.87937100	-0.06975700	-0.81344900
C	-2.79858400	1.05398200	-1.83778900
H	-1.99200400	1.72698200	-1.53387600
C	-2.44800900	0.51323800	-3.23504500
H	-3.23337900	-0.15812200	-3.60286300
H	-1.50887800	-0.04358800	-3.20711400
H	-2.35138900	1.33862600	-3.95091700
C	-4.09931200	1.87463400	-1.89768700
H	-3.98449400	2.71773500	-2.58880000
H	-4.37592300	2.27650200	-0.91712300
H	-4.93769800	1.26541100	-2.25450700
C	-2.37583100	2.20080400	1.58785600
H	-3.17180700	2.19869600	0.83886800
H	-2.36376100	3.17390700	2.08202700
H	-2.63861500	1.43523700	2.32634000
C	-1.02945300	1.88961000	0.96672000

C	-0.02564000	2.86196400	1.11691200
H	-0.32265800	3.77716400	1.61355200
C	1.33298600	2.76099800	0.77171500
C	2.23439600	3.91994000	1.14093400
H	2.82793900	4.24886300	0.28055500
H	2.94147400	3.63204700	1.92891900
H	1.65226100	4.76815600	1.50545800
C	3.27297500	1.56156300	0.00622900
H	3.82733000	1.87631300	0.90048500
H	3.64640400	2.18749200	-0.82009400
C	3.63498500	0.12386200	-0.28621600
C	4.96041700	-0.30522600	-0.35467900
H	5.76468600	0.40628900	-0.19816500
C	5.22648400	-1.64451300	-0.61924300
H	6.25088500	-1.99967100	-0.67080700
C	4.15865100	-2.52355800	-0.81576200
H	4.32226000	-3.57448800	-1.02591500
C	2.86655000	-2.02471600	-0.74310700
H	1.99269000	-2.64895300	-0.90702800
Cu	0.82327500	0.14623000	-0.38824300
N	-0.85497600	0.72006900	0.34767800
N	1.83655200	1.68954500	0.17120900
N	2.61276100	-0.73067300	-0.47512800
O	0.07925700	-1.04717100	-1.72689400
N	-0.13692000	-2.27643800	-1.62181200

Table S6.

Structure: **3a**, Energy= -3941.575485 Hartree, Charge= 0, Multiplicity=2

The number of the imaginary frequencies: 0

Center Number	Coordinates (Angstroms) X	Y	Z
C	-1.52549100	-0.38366600	1.23069800
C	-1.38609100	-1.06900100	2.45614900
C	-0.15268800	-0.87323900	3.32908100
H	0.30710900	0.07972000	3.05533100
C	0.88763900	-1.96981800	3.03566200
H	0.50353800	-2.95406200	3.33079400
H	1.81377800	-1.78235400	3.59284600
H	1.11219100	-2.01469100	1.96765400
C	-0.47555900	-0.80824400	4.82881000
H	-1.23509100	-0.04771100	5.04329900
H	0.42762800	-0.55796500	5.39693100
H	-0.84464500	-1.76717900	5.20965700
C	-2.38073900	-1.97979200	2.82418900
H	-2.29207300	-2.52141200	3.76123100
C	-3.48098400	-2.21025500	2.00184200
H	-4.24781200	-2.91860700	2.30405600
C	-3.59056400	-1.54221200	0.78413600
H	-4.44196900	-1.74522600	0.14341900
C	-2.61519800	-0.62888700	0.36915600
C	-2.71121400	0.07617000	-0.97896300
H	-1.68799800	0.20128800	-1.34380200
C	-3.46551400	-0.74286300	-2.03192900
H	-4.53037000	-0.84027100	-1.78796400
H	-3.03584700	-1.74415200	-2.12816900

H	-3.39328200	-0.24817400	-3.00308800
C	-3.32860000	1.48089200	-0.86400600
H	-3.39148000	1.94226400	-1.85644400
H	-2.73177400	2.13767200	-0.22578900
H	-4.34178000	1.43042000	-0.44649900
C	-1.65273100	2.15008000	2.31090100
H	-2.62103100	1.77478900	1.97511900
H	-1.70405800	3.23653800	2.41160600
H	-1.47457100	1.72822100	3.30679800
C	-0.52918800	1.75666200	1.36866600
C	0.46805100	2.72372500	1.16782500
H	0.29063500	3.69624600	1.60897100
C	1.69910800	2.55182000	0.51748900
C	2.64066700	3.73592100	0.48847300
H	2.95370800	3.95571900	-0.53687300
H	3.54344500	3.54152900	1.08037200
H	2.15484400	4.62431900	0.89460700
C	3.36854300	1.26382900	-0.63780400
H	4.14266700	1.81314900	-0.09100300
H	3.38342100	1.65511500	-1.66889900
C	3.75548800	-0.19150700	-0.67578700
C	5.06027800	-0.60397600	-0.94321200
H	5.83337300	0.13732800	-1.11656100
C	5.34491100	-1.96469000	-0.98530100
H	6.35292700	-2.30845600	-1.19451000
C	4.31699200	-2.87898000	-0.74467800
H	4.49614200	-3.94809200	-0.75578700
C	3.04175100	-2.39430000	-0.48956200
H	2.20330100	-3.05345800	-0.29943500

Cu	0.92095000	-0.14524800	-0.32758200
N	-0.51165900	0.53709100	0.82965700
N	2.05164200	1.40636700	-0.04755700
N	2.76465300	-1.07684700	-0.46691900
N	0.04435300	-1.84443700	-0.88729900
O	-0.34450500	-2.01802100	-2.05543600
O	-0.00269800	-2.79415400	-0.08106300
P	0.64417800	0.84297100	-3.03296700
C	-0.84001800	0.74650400	-4.13057600
C	-1.11294100	-0.49415700	-4.73080600
C	-1.71111600	1.81646000	-4.36989900
C	-2.22116300	-0.65376800	-5.55882200
H	-0.45568400	-1.33574400	-4.54322100
C	-2.82934600	1.65093300	-5.19167000
H	-1.51767300	2.78759000	-3.92873300
C	-3.08723800	0.41833600	-5.79112200
H	-2.41367500	-1.61949000	-6.01792000
H	-3.49257200	2.49338900	-5.36813800
H	-3.95445900	0.29235100	-6.43298700
C	0.92558100	2.65596900	-2.89015200
C	1.99262900	3.35296000	-3.47355900
C	0.03563700	3.36153900	-2.06241000
C	2.14501500	4.72565300	-3.26124500
H	2.70748100	2.82929600	-4.09835200
C	0.17679100	4.73336500	-1.86567000
H	-0.76116300	2.82884900	-1.55299600
C	1.23196800	5.42196200	-2.46821300
H	2.97758100	5.24992500	-3.72215300
H	-0.52524100	5.25838300	-1.22458700

H	1.34952800	6.48985800	-2.30862400
C	1.92562800	0.27252700	-4.22648100
C	2.77194200	-0.78050200	-3.85936500
C	2.05001000	0.82351800	-5.51348900
C	3.74838200	-1.25175200	-4.74043000
H	2.65170500	-1.25130300	-2.89305000
C	3.02527700	0.35750200	-6.39210700
H	1.37567400	1.61496000	-5.82645000
C	3.88209300	-0.67812200	-6.00392700
H	4.39623200	-2.06872600	-4.43629800
H	3.11469000	0.79565700	-7.38214200
H	4.64088600	-1.04155500	-6.69101500

Table S7.

Structure: **4a**, Energy= -4978.185758 Hartree, Charge= 0, Multiplicity=2

The number of the imaginary frequencies: 0

Center Number	Coordinates (Angstroms) X	Y	Z
C	-2.21801300	0.93843400	1.55424200
C	-2.17621800	0.70892500	2.94550300
C	-1.16741300	1.41906300	3.83959800
H	-0.75068500	2.25899400	3.27818600
C	0.00580600	0.48433900	4.18530200
H	-0.34326600	-0.37048000	4.77763100
H	0.76185400	1.01910900	4.77342800
H	0.46668800	0.08817300	3.27734400

C	-1.80467900	1.99020700	5.11613100
H	-2.65674100	2.63972200	4.88582700
H	-1.06810900	2.57903500	5.67479000
H	-2.16156200	1.19601000	5.78156100
C	-3.05399800	-0.23267200	3.49143400
H	-3.02984700	-0.43012700	4.55931400
C	-3.94922700	-0.93014500	2.68550500
H	-4.62501200	-1.65914500	3.12483200
C	-3.97040800	-0.69931400	1.31145800
H	-4.66233700	-1.25917500	0.69193800
C	-3.10577900	0.22703000	0.71807100
C	-3.10824600	0.45353600	-0.78959000
H	-2.07004800	0.63373800	-1.08407600
C	-3.59123900	-0.76652100	-1.58042600
H	-4.65671100	-0.96538500	-1.41176300
H	-3.01870000	-1.65775200	-1.31021300
H	-3.45446800	-0.58774400	-2.64899600
C	-3.92619700	1.69235200	-1.19571400
H	-3.90953900	1.80856900	-2.28593000
H	-3.52931900	2.61036400	-0.75540900
H	-4.97183100	1.58967100	-0.88052500
C	-2.86300900	3.62098900	1.68366000
H	-3.70091300	2.96719700	1.43705100
H	-3.09868400	4.64053700	1.37006700
H	-2.76602000	3.62047500	2.77527600
C	-1.56520000	3.15733300	1.04746600
C	-0.70029300	4.17331500	0.61500300

H	-1.08253700	5.18473000	0.66717400
C	0.62181200	4.03109600	0.17112800
C	1.36231900	5.29225800	-0.21583700
H	1.76507500	5.20475900	-1.23006600
H	2.20235800	5.48810400	0.46148400
H	0.69545400	6.15519700	-0.18739300
C	2.61969200	2.79653800	-0.30773400
H	3.21912600	3.60242300	0.13061800
H	2.72221100	2.89623900	-1.40196400
C	3.22183600	1.47807300	0.09748900
C	4.59708700	1.24841600	0.05411100
H	5.26684900	2.05370700	-0.22900400
C	5.08211600	-0.02099600	0.35483800
H	6.14755400	-0.22456200	0.31489600
C	4.17733100	-1.02449300	0.70711700
H	4.50393500	-2.03170100	0.94195900
C	2.82443500	-0.71493900	0.75433400
H	2.08708700	-1.45798100	1.02598200
Cu	0.39557600	1.11286900	0.28238600
N	-1.28914300	1.85441900	0.96987700
N	1.22551500	2.85279500	0.08875100
N	2.35561800	0.50982700	0.44769300
N	-0.18672900	-0.78635300	0.35536700
O	-0.51149400	-1.41573400	-0.66446500
O	-0.14890700	-1.37080700	1.45482100
P	0.49374500	0.96939600	-2.74239500
C	-0.82122200	0.19690300	-3.78264100

C	-0.88581900	-1.20622500	-3.78877200
C	-1.73353300	0.92170500	-4.56098700
C	-1.83070300	-1.86427700	-4.57300300
H	-0.20346500	-1.78291000	-3.17600500
C	-2.69075500	0.25821300	-5.33290100
H	-1.69845400	2.00529500	-4.57280400
C	-2.73858100	-1.13618200	-5.34583800
H	-1.85996700	-2.94905000	-4.56943300
H	-3.39155600	0.83505200	-5.93050200
H	-3.48015400	-1.65200700	-5.94955800
C	0.32200500	2.75805200	-3.14945500
C	1.25759300	3.49633200	-3.88737200
C	-0.79363500	3.42570500	-2.61863700
C	1.06822700	4.86328800	-4.10722800
H	2.13300400	3.00589300	-4.29861500
C	-0.99204800	4.78408400	-2.85333300
H	-1.50394600	2.88072700	-2.00591600
C	-0.06069600	5.50880600	-3.60069400
H	1.80304400	5.42095900	-4.68144700
H	-1.86317500	5.27853600	-2.43390100
H	-0.20826000	6.57047900	-3.77652800
C	1.98753700	0.48810100	-3.71240800
C	3.15131800	0.12519400	-3.02555300
C	2.00475200	0.49119800	-5.11624800
C	4.32027400	-0.19818800	-3.71742300
H	3.13887900	0.07326100	-1.94585800
C	3.16823900	0.16490800	-5.81087100

H	1.10336400	0.75120200	-5.66285500
C	4.33217300	-0.17384800	-5.11227800
H	5.21312500	-0.47605700	-3.16460500
H	3.16945600	0.17392400	-6.89721800
H	5.23841200	-0.42634700	-5.65528400
P	1.50867500	-4.00615300	-0.19563000
C	0.11393200	-5.10740000	0.30529400
C	-1.10219500	-4.49061800	0.64486300
C	0.20722500	-6.50582000	0.36036700
C	-2.20366500	-5.26255700	1.01627100
H	-1.16987400	-3.40824400	0.62133100
C	-0.89454600	-7.27412600	0.74042900
H	1.14175700	-6.99585800	0.10569300
C	-2.10349900	-6.65477900	1.06607500
H	-3.13840600	-4.77224900	1.27550200
H	-0.80896400	-8.35686200	0.78032500
H	-2.96018400	-7.25446000	1.36153600
C	2.97467400	-5.11408100	0.00929300
C	3.46210100	-5.97893400	-0.98173700
C	3.65309900	-5.04837700	1.23726500
C	4.59453600	-6.76113100	-0.74787300
H	2.95505400	-6.03751200	-1.93963700
C	4.78033100	-5.83529500	1.47559800
H	3.29328800	-4.37318800	2.01054200
C	5.25535600	-6.69288100	0.48065200
H	4.96036600	-7.42600000	-1.52575400
H	5.29129600	-5.77355700	2.43247800

H	6.13771200	-7.30070400	0.65988300
C	1.35015000	-3.99191900	-2.03309700
C	2.25451200	-3.18946800	-2.74712700
C	0.38606800	-4.71735100	-2.74587000
C	2.21091700	-3.12677400	-4.13846000
H	2.99495900	-2.60442600	-2.20893600
C	0.34063400	-4.65372400	-4.14062200
H	-0.32519300	-5.33817900	-2.21163200
C	1.25187500	-3.86090100	-4.83976300
H	2.91068700	-2.49070100	-4.66958900
H	-0.40991300	-5.22548900	-4.68013800
H	1.20753900	-3.80475100	-5.92366900

Table S8.

Structure: **5a**, Energy= -3866.326764 Hartree, Charge= 0, Multiplicity=2

The number of the imaginary frequencies: 0

Center	Coordinates (Angstroms)		
Number	X	Y	Z

C	11.63153700	-1.83141700	5.84510500
C	11.63402200	-3.23544300	5.73240500
C	11.18458900	-4.12173300	6.88045300
H	10.75653800	-3.47236600	7.64394700
C	12.39184100	-4.83655100	7.51032400
H	12.82768800	-5.55911400	6.80897400
H	12.08875700	-5.37797700	8.41342000

H	13.16959600	-4.11769400	7.77622600
C	10.10937700	-5.14245900	6.47761400
H	9.24206800	-4.65903700	6.01495700
H	9.76044700	-5.68601900	7.36200700
H	10.50049300	-5.87630100	5.76283300
C	12.10882700	-3.81142300	4.54812900
H	12.10853300	-4.89367200	4.44822600
C	12.58316300	-3.02498100	3.50216200
H	12.93977500	-3.48921000	2.58642200
C	12.61627700	-1.63839600	3.64369800
H	13.01150300	-1.02840400	2.83674200
C	12.16174400	-1.02336900	4.81328800
C	12.23214300	0.48689100	4.98348100
H	12.20990400	0.67759900	6.06012300
C	13.53600100	1.08627900	4.43973400
H	14.40460400	0.57210000	4.86368400
H	13.59940700	2.14811400	4.70521500
H	13.59768100	1.01990400	3.34716000
C	11.00788800	1.18451800	4.36590900
H	10.94360400	0.97796000	3.29047400
H	11.07475600	2.27121900	4.49889100
H	10.07815100	0.84569600	4.83268400
C	8.89883100	-1.48874300	6.04348900
H	8.80495700	-2.56603600	6.21455200
H	9.27140800	-1.35957200	5.02442600
H	7.90516300	-1.04204400	6.11538800
C	9.84248100	-0.87971100	7.06473500
C	9.24686300	-0.03292400	8.01608900
H	8.17361800	0.08758600	7.93655100

C	9.88657800	0.76176800	8.98695300
C	9.02124500	1.71942300	9.77802400
H	7.97700300	1.65618000	9.46654100
H	9.35781100	2.75445400	9.64441800
H	9.07745600	1.49774800	10.84973300
C	11.77680700	1.58145200	10.19371500
H	11.25438400	1.52975200	11.15890000
H	11.73681400	2.63621000	9.87769500
C	13.21359300	1.20988100	10.44496900
C	13.98238100	1.88471700	11.39587700
H	13.55013700	2.72125300	11.93508100
C	15.27492800	1.45056600	11.65700700
H	15.88371400	1.95223900	12.40266300
C	15.77347000	0.35134600	10.95153700
H	16.77298800	-0.02937700	11.12932400
C	14.96550100	-0.24840500	9.99787300
H	15.30470000	-1.08807500	9.40360900
Cu	12.42596700	-0.59200000	8.38480400
N	13.91573800	-1.21372400	7.30541400
N	11.14252500	-1.17611800	7.01876600
N	11.18872400	0.69961800	9.20583800
N	13.71078300	0.17424500	9.74782100
O	14.64198800	-2.15661400	7.61659200
P	11.81796700	-2.50768100	10.47922000
C	11.33490300	-1.40460100	11.87906500
C	10.00643300	-1.02440500	12.11601500
C	12.34659300	-0.82111900	12.65875800
C	9.69839600	-0.09015000	13.10599200
H	9.20353200	-1.45992100	11.53226700

C	12.03849300	0.11161300	13.64835900
H	13.38343300	-1.09553100	12.49292900
C	10.71281000	0.48543400	13.87466400
H	8.66135000	0.18495000	13.27777700
H	12.83914700	0.55159500	14.23586000
H	10.47149500	1.21346700	14.64359100
C	13.13260700	-3.51728000	11.27073000
C	13.02627700	-4.02058400	12.57837700
C	14.29749200	-3.77374100	10.53547600
C	14.05911400	-4.77448400	13.13168500
H	12.13597500	-3.81306800	13.16418100
C	15.33343800	-4.52842000	11.09176900
H	14.39715000	-3.37274200	9.53228700
C	15.21523900	-5.03078100	12.38746400
H	13.96527700	-5.16061700	14.14277800
H	16.23243000	-4.71810400	10.51221100
H	16.02114800	-5.61612400	12.82107800
C	10.38267500	-3.65234000	10.33790800
C	9.23499400	-3.16775000	9.68650000
C	10.40512800	-4.98942400	10.75652500
C	8.12647600	-3.99013800	9.49204100
H	9.21469600	-2.14824100	9.31106100
C	9.29921100	-5.81624800	10.54604100
H	11.28640900	-5.39229700	11.24299300
C	8.15493900	-5.31927200	9.92023800
H	7.24770900	-3.59527200	8.98971200
H	9.33434700	-6.85137700	10.87433100
H	7.29667800	-5.96500000	9.75813800

Table S9.

Structure: **6a**, Energy= -3866.324476 Hartree, Charge= 0, Multiplicity=2

The number of the imaginary frequencies: 0

Center Number	Coordinates (Angstroms) X	Y	Z
C	11.91428500	-2.24238800	6.16506400
C	11.48783700	-3.58966900	6.28307100
C	10.27415400	-3.94757300	7.12902700
H	10.16597000	-3.15861500	7.87684800
C	10.42858500	-5.27720000	7.88062800
H	10.40209200	-6.13557500	7.19916300
H	9.60609600	-5.39471000	8.59288700
H	11.36771900	-5.31506400	8.43972700
C	8.97696500	-3.96109300	6.30144900
H	8.78146900	-2.99145500	5.83781200
H	8.12267700	-4.20724100	6.94349400
H	9.03267700	-4.71351300	5.50528300
C	12.21341300	-4.58619300	5.62375800
H	11.89398600	-5.62032900	5.70451900
C	13.35178100	-4.27749700	4.88194600
H	13.90759100	-5.06478200	4.37993200
C	13.77307200	-2.95428900	4.79104100
H	14.66105400	-2.71580900	4.21246100
C	13.07078000	-1.91903400	5.42041900
C	13.54685100	-0.48338500	5.25013100
H	12.96072500	0.14080000	5.93016900

C	15.03188700	-0.31239200	5.61208000
H	15.24647600	-0.69004400	6.61348200
H	15.30562900	0.74884800	5.57798800
H	15.67845900	-0.83955300	4.90052600
C	13.30814200	0.01038800	3.81048600
H	13.91159300	-0.56657400	3.09921800
H	13.59367500	1.06467400	3.71475000
H	12.26097100	-0.08814300	3.51334200
C	9.87927900	-0.80946800	4.81955700
H	8.79929400	-0.86701500	4.65741200
H	10.34627700	-1.70718600	4.41504000
H	10.24545400	0.05084400	4.24839100
C	10.18464100	-0.60390300	6.29509100
C	9.34101500	0.31890400	6.94376700
H	8.59128900	0.77439500	6.30722400
C	9.32075600	0.72765300	8.28953600
C	8.27099300	1.76304800	8.65261300
H	7.71835400	2.07843900	7.76581800
H	8.74375700	2.64351700	9.09875500
H	7.54715100	1.36761100	9.37528500
C	10.08006700	0.75629600	10.57397600
H	10.24507000	-0.07157600	11.27005300
H	9.09209400	1.16328500	10.82046400
C	11.12630900	1.82301400	10.85013300
C	11.79567200	1.85639200	12.07666400
H	11.58365200	1.10812200	12.83135400
C	12.74687700	2.84796900	12.30214300
H	13.29000300	2.88229800	13.24209600
C	12.99797300	3.77854000	11.29501000

H	13.73483400	4.56550200	11.41953300
C	12.27565100	3.66926000	10.10653600
H	12.44114000	4.37736100	9.29658100
Cu	11.69260400	-0.84674200	8.75656800
N	13.50177200	-0.40730400	8.58899900
N	11.19514700	-1.23995100	6.87950900
N	10.14706700	0.24643000	9.21346200
N	11.36082000	2.71845600	9.87755100
O	14.55739400	-0.88941500	8.89247300
P	11.97362900	-2.36831400	10.43057300
C	12.40707200	-1.65359500	12.05930400
C	11.55032300	-1.71451700	13.16537100
C	13.64656000	-1.00416900	12.18352100
C	11.92928200	-1.13832000	14.38040000
H	10.59132900	-2.21468400	13.08226900
C	14.02508200	-0.44189400	13.40012400
H	14.31426500	-0.94753300	11.32950400
C	13.16761900	-0.50581600	14.50197300
H	11.25778800	-1.19204400	15.23239100
H	14.98744900	0.05380800	13.48650700
H	13.46285800	-0.06348100	15.44884300
C	13.30511200	-3.59489000	10.17444400
C	13.93925700	-4.24707700	11.24334800
C	13.69171100	-3.89649100	8.86232200
C	14.92291100	-5.20403900	10.99700300
H	13.67158300	-4.00093400	12.26598400
C	14.67283900	-4.85693600	8.61741000
H	13.22849900	-3.38136300	8.03102100
C	15.28835700	-5.51354100	9.68382200

H	15.40572900	-5.70658000	11.83010500
H	14.95333700	-5.07993300	7.59254600
H	16.05664600	-6.25793700	9.49553400
C	10.45870800	-3.34243700	10.75567000
C	9.22772000	-2.81503900	10.33845900
C	10.49126900	-4.58745400	11.39914200
C	8.04757500	-3.52444700	10.56351700
H	9.19986500	-1.85924400	9.82329900
C	9.31027600	-5.29316700	11.62338700
H	11.43891400	-5.01286100	11.71189800
C	8.08675800	-4.76386300	11.20474700
H	7.09993400	-3.11074000	10.23129800
H	9.34575500	-6.25936700	12.11809700
H	7.16839800	-5.31831400	11.37455800

Table S10.

Structure: **[LCu^{I}PPh$_3$]**, Energy= -3736.383981 Hartree, Charge= 0, Multiplicity=1

The number of the imaginary frequencies: 0

Center	Coordinates (Angstroms)		
Number	X	Y	Z

C	2.71961000	-1.25731600	0.09740200
C	3.72654300	-0.44691200	-0.47483900
C	3.63675900	-0.05105200	-1.94386900
H	3.24485800	-0.91658800	-2.49069400
C	2.62153800	1.08931700	-2.13159300
H	2.48678100	1.32577000	-3.19378700

H	2.94276000	1.99488500	-1.60649300
H	1.65596100	0.78719200	-1.71805700
C	4.98571000	0.31488000	-2.57315200
H	4.86434000	0.46328700	-3.65183800
H	5.73177300	-0.47279300	-2.41838200
H	5.38711000	1.24757400	-2.16005800
C	4.76960800	-0.00276000	0.34290400
H	5.54989300	0.62414500	-0.07581500
C	4.82434100	-0.34630000	1.69249000
H	5.64260600	0.00996500	2.31251700
C	3.83027600	-1.15351500	2.24312400
H	3.88528000	-1.42305300	3.29303600
C	2.77162200	-1.62765000	1.46109200
C	1.65998500	-2.48293500	2.05785900
H	1.32856800	-3.17869900	1.27871800
C	2.09742800	-3.32010300	3.26516000
H	1.28915500	-3.99870300	3.55961100
H	2.32745700	-2.69336600	4.13449800
H	2.98425100	-3.92247800	3.03821600
C	0.45108900	-1.60046000	2.41096700
H	-0.39440600	-2.19916600	2.76906600
H	0.12746900	-1.05133900	1.52234600
H	0.70850700	-0.86823200	3.18454500
C	2.88947700	-3.64123300	-1.30801400
H	3.76465300	-3.07233700	-1.63960300
H	2.79242800	-4.52975100	-1.93502600
H	3.09583500	-3.96163600	-0.28038800
C	1.63418200	-2.79101700	-1.36102900
C	0.55733500	-3.29109500	-2.11702000

H	0.74013600	-4.23889900	-2.60878300
C	-0.74707400	-2.77327900	-2.26663000
C	-1.72419000	-3.65147200	-3.03091100
H	-2.58322200	-3.92226800	-2.40634500
H	-1.24129400	-4.57317300	-3.36006400
H	-2.11697200	-3.13974500	-3.91731300
C	-2.54505700	-1.24962900	-1.82612600
H	-3.04638000	-1.61411100	-2.73199100
H	-2.62750200	-0.15908700	-1.86062800
C	-3.34258800	-1.72605900	-0.62192500
C	-2.78859300	-2.54050800	0.37053100
H	-1.76080200	-2.87253300	0.28835100
C	-3.57797000	-2.90685000	1.45949900
H	-3.16811100	-3.53254200	2.24730400
C	-4.89436900	-2.45581200	1.52148700
H	-5.54492600	-2.71252100	2.35116700
C	-5.36114400	-1.65434400	0.47877300
H	-6.38457500	-1.28270000	0.48861900
C	-1.45093000	2.38656700	-1.14144400
C	-1.27077000	2.07025500	-2.49523900
H	-0.63317600	1.23067700	-2.75925900
C	-1.92915300	2.79868600	-3.48556900
H	-1.78524900	2.54292800	-4.53120000
C	-2.78112900	3.84581400	-3.12864800
H	-3.30023300	4.41053400	-3.89758700
C	-2.97432600	4.16073900	-1.78087400
H	-3.64228500	4.97039400	-1.50146100
C	-2.31116500	3.43633300	-0.79043400
H	-2.46575100	3.68044300	0.25601500

C	-1.57834400	1.37372500	1.56517500
C	-2.91938000	0.98916300	1.41316500
H	-3.32495200	0.80444500	0.42484200
C	-3.74341000	0.84636900	2.52748400
H	-4.77785000	0.54742900	2.39256100
C	-3.23748300	1.07710700	3.80906700
H	-3.87860800	0.96032600	4.67806300
C	-1.90516700	1.46080300	3.96693000
H	-1.50516600	1.64788400	4.95953000
C	-1.07909400	1.61146700	2.85168800
H	-0.04654700	1.91446200	2.98626500
C	0.87363900	2.53034800	0.54900300
C	0.93891600	3.87291000	0.15416900
H	0.14072000	4.30489900	-0.43904900
C	2.03544500	4.66040800	0.50907900
H	2.07777700	5.69779300	0.18895500
C	3.07231600	4.11932300	1.27145300
H	3.92528200	4.73362100	1.54569000
C	3.01366100	2.78229000	1.66965300
H	3.82161800	2.34223000	2.24473600
C	1.92837200	1.98951800	1.30053800
H	1.91830900	0.94065800	1.57687500
N	1.59708400	-1.64245800	-0.68460200
N	-1.13662500	-1.60244600	-1.76503200
N	-4.61367700	-1.28882900	-0.56964300
P	-0.50286900	1.40768200	0.08075200
Cu	0.03904900	-0.51483900	-0.68167700

Table S11.

Structure: **TS-1a**, Energy= -3941.494531 Hartree, Charge= 0, Multiplicity=2

The number of the imaginary frequencies: 1, ν = -203.7 cm^{-1}

Center Number	Coordinates (Angstroms) X	Y	Z
C	-2.56590200	0.36455700	-0.42415300
C	-2.80963200	-0.25946900	0.81897600
C	-1.77343800	-0.17587100	1.93191900
H	-1.16567500	0.71473200	1.74455800
C	-0.82362600	-1.38394200	1.90143100
H	-1.37120700	-2.30538600	2.11768600
H	-0.02618700	-1.26954800	2.64579500
H	-0.36476900	-1.49621500	0.91648300
C	-2.39901400	-0.01718800	3.32496400
H	-3.10077300	0.82384800	3.35453600
H	-1.61566200	0.16404600	4.06976900
H	-2.94001700	-0.91873100	3.63413600
C	-4.00423200	-0.96118800	0.99453100
H	-4.19564700	-1.47162000	1.93345500
C	-4.95120000	-1.03142200	-0.02602100
H	-5.86836300	-1.59533200	0.12061900
C	-4.72363900	-0.36283300	-1.22575300
H	-5.47844100	-0.39454400	-2.00758200
C	-3.53595600	0.34411500	-1.44967400
C	-3.34234400	1.09801000	-2.76017400
H	-2.36644700	1.58961100	-2.72039300

C	-3.34248600	0.17319300	-3.98827000
H	-4.31035600	-0.32820200	-4.10283200
H	-2.57053200	-0.59407700	-3.91385500
H	-3.16668900	0.75894400	-4.89879400
C	-4.41552400	2.18920700	-2.93653400
H	-4.21632700	2.77794000	-3.83962300
H	-4.44823700	2.87644300	-2.08487700
H	-5.41259700	1.74554000	-3.04116500
C	-2.18370500	3.06943400	0.09860300
H	-3.07989300	3.03468400	-0.52555400
H	-1.87354600	4.11049300	0.20676000
H	-2.47301100	2.68650700	1.08374300
C	-1.07043000	2.22416400	-0.48747100
C	0.13745500	2.88424400	-0.77649400
H	0.15058000	3.95123000	-0.59182900
C	1.34459200	2.32158000	-1.22752500
C	2.52780000	3.25321600	-1.39132200
H	2.99150400	3.13444800	-2.37695900
H	3.30172300	3.04212600	-0.64274100
H	2.22402700	4.29509300	-1.27436700
C	2.77855000	0.46479800	-1.78184200
H	3.58377000	0.92899700	-1.19781600
H	3.04685400	0.60673800	-2.84105900
C	2.78145200	-1.01791400	-1.48114200
C	3.93847800	-1.79210100	-1.55827100
H	4.87561200	-1.33012500	-1.85192700
C	3.86881800	-3.14963800	-1.25798900
H	4.75822600	-3.76910200	-1.31865600
C	2.64492600	-3.70235100	-0.87555600

H	2.53724200	-4.75491600	-0.64401800
C	1.53738000	-2.87111900	-0.82197800
H	0.55923100	-3.24083000	-0.54794000
Cu	0.08396000	-0.31985900	-1.32630000
N	-1.27681900	0.92064200	-0.67342900
N	1.47281300	1.02605300	-1.48207000
N	1.60263500	-1.56255400	-1.12413800
N	-1.13365800	-1.61569900	-2.15173000
O	-0.70725900	-2.17161600	-3.18394500
O	-1.75079300	-2.57272700	-1.19308200
P	-1.82241800	-4.26937200	-1.56076700
C	-0.53242100	-5.45407300	-1.79013800
C	0.23656700	-5.40347200	-2.99875700
C	-0.05089900	-6.30817600	-0.74866600
C	1.36568400	-6.18579600	-3.15915000
H	-0.06913000	-4.72818500	-3.79072900
C	1.08996300	-7.07615900	-0.92932200
H	-0.60700200	-6.39801200	0.17702000
C	1.81672900	-7.03329000	-2.13046800
H	1.91606200	-6.13262200	-4.09547600
H	1.41001600	-7.73755900	-0.12730700
H	2.70925400	-7.63709000	-2.26054300
C	-2.77233500	-4.67773800	-0.07535100
C	-4.15251900	-4.91633700	-0.16036200
C	-2.15767200	-4.67451100	1.18877700
C	-4.89953900	-5.14850400	0.99395300
H	-4.64371900	-4.91053200	-1.12695000
C	-2.90579100	-4.91893400	2.33837900
H	-1.09776000	-4.46315200	1.27696000

C	-4.28049100	-5.15165200	2.24558200
H	-5.96774000	-5.32779600	0.91371200
H	-2.41664100	-4.91256300	3.30807800
H	-4.86446100	-5.33187400	3.14321600
C	-2.90564900	-4.31583100	-3.00063000
C	-3.82162100	-3.26932600	-3.20166200
C	-2.92755500	-5.42494500	-3.86194700
C	-4.73909400	-3.33511400	-4.24858600
H	-3.81151800	-2.41496900	-2.53618400
C	-3.83416800	-5.47385800	-4.91856700
H	-2.23442100	-6.24352600	-3.70373900
C	-4.74557600	-4.43133200	-5.11340800
H	-5.44599100	-2.52301900	-4.39299300
H	-3.83582900	-6.33143300	-5.58514700
H	-5.45755900	-4.47630800	-5.93244400

Table S12.

Structure: **TS-1b**, Energy= -3941.497894 Hartree, Charge= 0, Multiplicity=2

The number of the imaginary frequencies: 1, ν = -226.9 cm^{-1}

Center	Coordinates (Angstroms)		
Number	X	Y	Z

C	1.25307800	2.95791600	-0.00702700
C	1.16355200	1.59456900	-0.36017500
C	0.78800200	0.55087600	0.68464800
H	1.26508900	0.87989700	1.61203000
C	1.32476800	-0.84691300	0.35496300

H	0.81044100	-1.28566800	-0.50890000
H	1.16292300	-1.51797300	1.20459100
H	2.39784500	-0.82287000	0.15359500
C	-0.72770100	0.46567600	0.94532500
H	-1.12104800	1.37965400	1.39393800
H	-0.94286800	-0.35881200	1.63623700
H	-1.27523500	0.27077900	0.01498600
C	1.46653800	1.23368300	-1.67703600
H	1.40219300	0.19297900	-1.97625700
C	1.86909800	2.18578700	-2.61216500
H	2.10059300	1.88388100	-3.63028100
C	1.98928400	3.52107400	-2.23579400
H	2.32051100	4.25297900	-2.96575700
C	1.68660400	3.92919600	-0.93239600
C	1.86577800	5.37825400	-0.49831500
H	1.14987000	5.57592600	0.30526800
C	3.27252300	5.58088100	0.09452800
H	3.45889800	4.86687000	0.90082200
H	3.38729200	6.59847000	0.48757600
H	4.03974700	5.42071700	-0.67272300
C	1.59077900	6.39676400	-1.61214700
H	2.34370000	6.34832000	-2.40706200
H	1.61543900	7.41323400	-1.20347000
H	0.60751700	6.23598700	-2.06876200
C	-1.30098300	3.85632900	0.33561300
H	-1.27001300	2.95330400	-0.27601500
H	-1.03552700	4.69360000	-0.32077000
H	-2.32251500	4.01397200	0.68840700
C	-0.33500800	3.79443300	1.50665500

C	-0.83256600	4.27007800	2.72984200
H	-1.88398500	4.52681800	2.75499500
C	-0.09153800	4.55874100	3.88273200
C	-0.83409300	5.19394200	5.03907200
H	-1.89359600	5.31112700	4.80505600
H	-0.42544100	6.18175300	5.28249700
H	-0.74659700	4.57666000	5.94068800
C	1.90921400	4.82830500	5.13941100
H	1.43570200	4.50957300	6.07573300
H	1.91954000	5.93021000	5.16032600
C	3.32997100	4.34805600	5.15310100
C	4.16038000	4.57683500	6.25006300
H	3.77079000	5.11131400	7.11053800
C	5.46485500	4.09674700	6.22893600
H	6.12185700	4.24997200	7.07945600
C	5.90693700	3.40730700	5.09931000
H	6.90585100	2.99193700	5.03980800
C	5.02725100	3.22750900	4.04156900
H	5.30692800	2.67359300	3.15050100
Cu	2.31166100	3.33670700	2.70559200
N	4.45363100	1.64188200	1.65687400
N	0.91466800	3.36372500	1.32166300
N	1.21347600	4.32963700	3.97179900
N	3.76044100	3.68095000	4.06543100
O	3.45231300	2.41781300	1.42720900
O	3.96179400	0.33823500	1.98394600
P	3.55981200	-0.13964500	3.66394700
C	2.26300700	0.43768400	4.74246300
C	0.91056700	0.23869500	4.33442300

C	2.48939200	1.31678100	5.83721500
C	-0.13929200	0.83320600	5.01734900
H	0.69658700	-0.39426100	3.48041200
C	1.42472200	1.87974800	6.52701600
H	3.50039300	1.54445500	6.15097300
C	0.10119300	1.65065100	6.13072100
H	-1.15746200	0.65540600	4.68208000
H	1.63225300	2.51034500	7.38777500
H	-0.72390800	2.10180600	6.67264200
C	5.15200500	-0.08519600	4.51733100
C	5.26042600	-0.28553200	5.90520000
C	6.32256300	0.11414600	3.76359300
C	6.50351000	-0.23257700	6.52973100
H	4.37396100	-0.48948200	6.49540200
C	7.56601900	0.15156000	4.39440100
H	6.25169400	0.25337500	2.69216700
C	7.66116100	-0.00841800	5.77770400
H	6.57084100	-0.38210000	7.60343500
H	8.46188300	0.31069300	3.80112100
H	8.63015600	0.02813800	6.26670900
C	3.19454800	-1.86461400	3.24275400
C	3.87338100	-2.48200000	2.17706400
C	2.31455800	-2.63129900	4.02453100
C	3.64995100	-3.82617700	1.88578400
H	4.55924100	-1.90095100	1.57343300
C	2.08532900	-3.97151300	3.71945700
H	1.80492500	-2.17873400	4.86746100
C	2.74985500	-4.57373000	2.64798900
H	4.17653200	-4.28865800	1.05587700

H	1.39209000	-4.54767700	4.32549700
H	2.57207800	-5.61924900	2.41377200

Table S13.

Structure: **TS-3a**, Energy= -3941.507181 Hartree, Charge= 0, Multiplicity=2

The number of the imaginary frequencies: 1, ν = -323.8 cm^{-1}

Center	Coordinates (Angstroms)		
Number	X	Y	Z

C	-1.55945600	-0.27245100	1.23038400
C	-1.38722200	-1.08348500	2.37364400
C	-0.10491500	-1.00196200	3.19005400
H	0.33495900	-0.01421900	3.02703100
C	0.90687700	-2.03634000	2.66419600
H	0.53743800	-3.05577700	2.82711400
H	1.87345400	-1.93388500	3.17252400
H	1.06385900	-1.90679800	1.59104300
C	-0.32389400	-1.16122200	4.70033800
H	-1.06778600	-0.44789500	5.07309900
H	0.61581800	-0.98592200	5.23638800
H	-0.66423600	-2.16956600	4.96181400
C	-2.38592900	-2.00612200	2.69791700
H	-2.27022800	-2.63725500	3.57396400
C	-3.52841900	-2.12966900	1.91086200
H	-4.30073900	-2.84590100	2.17859900
C	-3.67054400	-1.34454300	0.76893800
H	-4.55367500	-1.46668600	0.15086800

C	-2.69082200	-0.41626700	0.39785200
C	-2.82901400	0.40682500	-0.87727100
H	-1.81651900	0.52323300	-1.27465800
C	-3.66482400	-0.29570800	-1.95339700
H	-4.72297600	-0.35545800	-1.67126000
H	-3.30227000	-1.31066200	-2.14124800
H	-3.60625000	0.26267600	-2.89082300
C	-3.39096200	1.81809500	-0.62823700
H	-3.50744400	2.34763100	-1.58185000
H	-2.73132100	2.41557100	0.00517200
H	-4.37553100	1.76839000	-0.14723200
C	-1.65252900	2.18931600	2.47692400
H	-2.63257500	1.82861800	2.15979600
H	-1.70658700	3.26658200	2.65023300
H	-1.43044000	1.70465500	3.43570900
C	-0.56224100	1.85879800	1.47155000
C	0.41618700	2.85313900	1.28221300
H	0.22646200	3.80248900	1.76815000
C	1.66470400	2.72512600	0.64777200
C	2.60080400	3.91410100	0.70808300
H	2.97572800	4.16321400	-0.28938000
H	3.46767900	3.70332600	1.34691600
H	2.09125900	4.79084200	1.11248000
C	3.38703000	1.45359500	-0.45109600
H	4.13773100	1.95621900	0.17086200
H	3.49036700	1.87746700	-1.46434500
C	3.73369300	-0.01661500	-0.52164600
C	5.04052000	-0.46224400	-0.72287200
H	5.84668300	0.25923300	-0.80819900

C	5.28496800	-1.82871900	-0.81607700
H	6.29462100	-2.19600600	-0.97108600
C	4.21284400	-2.71858200	-0.71038600
H	4.35827800	-3.79068800	-0.78114400
C	2.93896300	-2.20159500	-0.52076700
H	2.05779500	-2.83492300	-0.46934200
Cu	0.91474600	0.05080900	-0.29788900
N	-0.54469400	0.66292400	0.88309900
N	2.03804600	1.60823400	0.04592100
N	2.70763000	-0.88169800	-0.42448800
N	-0.05499600	-1.38423000	-1.23337500
O	0.58985900	-1.37965500	-2.50309000
O	-0.11198400	-2.54100200	-0.79340000
P	0.65706700	0.46628300	-3.11399500
C	-0.89139900	0.37233400	-4.09523800
C	-1.35719900	-0.88789300	-4.51107300
C	-1.57689100	1.51774000	-4.53068800
C	-2.47627900	-0.99529200	-5.33302100
H	-0.83739800	-1.77842000	-4.18196800
C	-2.70530600	1.40449000	-5.34409400
H	-1.23223000	2.50295600	-4.24435700
C	-3.15874400	0.14919800	-5.75031000
H	-2.81858600	-1.97809000	-5.64423000
H	-3.22364400	2.30343500	-5.66533300
H	-4.03422500	0.06330400	-6.38738300
C	0.91869100	2.31697300	-2.97264900
C	2.03887900	2.98696000	-3.48776100
C	0.01866200	3.03239200	-2.16383500
C	2.22066000	4.35059300	-3.24275700

H	2.76171600	2.45398200	-4.09516700
C	0.19144100	4.39395800	-1.93511000
H	-0.81488500	2.51599200	-1.69821900
C	1.29422400	5.06044000	-2.47724500
H	3.08639600	4.85863700	-3.65918800
H	-0.52111100	4.92818200	-1.31398800
H	1.43795900	6.12065700	-2.29026100
C	1.97821200	0.01244100	-4.29684600
C	3.09431400	-0.72583400	-3.88567600
C	1.90322200	0.45610500	-5.62534100
C	4.12604200	-1.00327600	-4.78282000
H	3.14743200	-1.09779700	-2.87351800
C	2.93220800	0.17301100	-6.52284300
H	1.03904900	1.02339200	-5.95724800
C	4.04861200	-0.55383300	-6.10181000
H	4.98624400	-1.57579800	-4.44792600
H	2.86148100	0.51847500	-7.55017800
H	4.85055600	-0.77280100	-6.80094300

Table S14.

Structure: **TS-4a**, Energy= -4978.120717 Hartree, Charge= 0, Multiplicity=2

The number of the imaginary frequencies: 1, ν = -115.6 cm^{-1}

Center	Coordinates (Angstroms)		
Number	X	Y	Z

C	-1.92357200	0.51957900	1.60821700
C	-1.81353700	0.15648600	2.96685700

C	-0.77945400	0.79441800	3.88633900
H	-0.32475900	1.63080400	3.34881300
C	0.35072800	-0.19154200	4.23116200
H	-0.04311100	-1.05926300	4.77488700
H	1.09937100	0.29442700	4.86930000
H	0.83338800	-0.55930000	3.32341700
C	-1.41337900	1.35382500	5.17162200
H	-2.23907900	2.03940300	4.95211100
H	-0.66447100	1.89823000	5.75863300
H	-1.80856200	0.55174800	5.80561900
C	-2.67209600	-0.82743600	3.46998100
H	-2.59194000	-1.12290400	4.51256500
C	-3.62261600	-1.43447000	2.65606300
H	-4.28329200	-2.19675900	3.06034700
C	-3.71999400	-1.06716000	1.31505200
H	-4.46157000	-1.55055200	0.68842000
C	-2.87157300	-0.10312500	0.76189000
C	-2.96124900	0.26960000	-0.71432400
H	-1.93163700	0.39901200	-1.06584500
C	-3.61778400	-0.80726200	-1.58701200
H	-4.68069300	-0.92839600	-1.34508600
H	-3.13217900	-1.78041400	-1.48263800
H	-3.55073000	-0.51628200	-2.63745100
C	-3.70407800	1.59910700	-0.94672700
H	-3.76473000	1.80833800	-2.02138300
H	-3.20421200	2.44383800	-0.47019300
H	-4.72699600	1.54292900	-0.55468400
C	-2.55208300	3.18720500	1.98084900
H	-3.39721800	2.52131700	1.80025000

H	-2.84036700	4.20881900	1.72197500
H	-2.34568100	3.16115900	3.05663300
C	-1.31173400	2.76995400	1.20816900
C	-0.51605000	3.82686100	0.73469200
H	-0.91424800	4.82399300	0.87600800
C	0.75783500	3.74645500	0.14999400
C	1.42347400	5.04748400	-0.24641900
H	1.74065100	5.01416300	-1.29372500
H	2.31217400	5.24541600	0.36547500
H	0.73645000	5.88664600	-0.12491800
C	2.73065600	2.57340200	-0.55018300
H	3.33342900	3.41858600	-0.19904000
H	2.74829400	2.62248000	-1.65274400
C	3.40746200	1.29619200	-0.12018300
C	4.78807800	1.11859800	-0.20022500
H	5.41289400	1.92941500	-0.56037500
C	5.33844100	-0.10450600	0.17613500
H	6.41063100	-0.26389500	0.11422100
C	4.49501700	-1.11277600	0.64542000
H	4.87325000	-2.07797300	0.96172500
C	3.13041900	-0.85956200	0.70229000
H	2.42512600	-1.59060500	1.07648100
Cu	0.63572500	0.79096200	0.19493100
N	-1.02271500	1.47681300	1.05502000
N	1.37193500	2.59117300	-0.04808500
N	2.59741500	0.31165100	0.31409500
N	0.04091100	-1.09406400	0.29529700
O	0.43529400	-1.81401800	-0.89400400
O	0.37713100	-1.70725400	1.34516400

P	0.45427600	0.84047000	-2.82958200
C	-0.90823300	0.09002300	-3.82543800
C	-0.97707900	-1.31285500	-3.84862600
C	-1.85124500	0.82714000	-4.55329500
C	-1.95295700	-1.96104400	-4.60191300
H	-0.26682600	-1.89288500	-3.27393000
C	-2.83897300	0.17392600	-5.29581400
H	-1.81519600	1.91099200	-4.54919200
C	-2.88944400	-1.22034900	-5.32787100
H	-1.98204400	-3.04646600	-4.61303300
H	-3.56314700	0.75916900	-5.85619400
H	-3.65463100	-1.72575600	-5.91044200
C	0.27886400	2.63268800	-3.21338300
C	1.15126400	3.35940700	-4.03497500
C	-0.77422700	3.31290500	-2.58089900
C	0.96109800	4.72949700	-4.23400900
H	1.97842000	2.85796300	-4.52550000
C	-0.97600200	4.67411800	-2.79511300
H	-1.42872500	2.77595600	-1.90373200
C	-0.10743500	5.38835300	-3.62410500
H	1.64707900	5.27916600	-4.87278100
H	-1.79767800	5.17938100	-2.29598800
H	-0.25598100	6.45248300	-3.78386700
C	1.89831500	0.35443300	-3.87144100
C	3.10595300	0.03008800	-3.24272500
C	1.83601600	0.31299800	-5.27326300
C	4.23734000	-0.30264500	-3.99034800
H	3.15750000	0.01205600	-2.16273500
C	2.96204400	-0.02240800	-6.02339400

H	0.90191500	0.54455200	-5.77565600
C	4.16835900	-0.32587800	-5.38364300
H	5.16424500	-0.55057300	-3.48088700
H	2.90026700	-0.04843300	-7.10772500
H	5.04514300	-0.58574700	-5.96989700
P	1.05840200	-3.52111100	-0.58430500
C	-0.40019000	-4.37856100	0.05636800
C	-1.65840900	-3.75935500	0.01082500
C	-0.29854800	-5.68864800	0.55408700
C	-2.79199000	-4.43873900	0.45133100
H	-1.73874300	-2.74208700	-0.34645900
C	-1.43510400	-6.36056200	1.00089900
H	0.66875400	-6.17758400	0.59053700
C	-2.68578000	-5.73946000	0.94743200
H	-3.75654900	-3.94222800	0.41913300
H	-1.34387600	-7.37219800	1.38592200
H	-3.57077000	-6.26579400	1.29338000
C	2.48498600	-4.25027300	0.20993600
C	3.69967700	-4.51719900	-0.48061300
C	2.52076700	-4.26985100	1.63606300
C	4.86477900	-4.81096800	0.21582500
H	3.71372400	-4.51900300	-1.56488600
C	3.69287100	-4.56669800	2.31490400
H	1.61753900	-4.03922100	2.19207600
C	4.88180000	-4.83618700	1.61787800
H	5.77175500	-5.03538600	-0.34053900
H	3.68645400	-4.58637700	3.40190800
H	5.79730000	-5.06293300	2.15552600
C	1.18061500	-3.86614300	-2.35967500

C	2.15466700	-3.20769800	-3.12659800
C	0.26572300	-4.71647800	-2.99768900
C	2.21720400	-3.39978100	-4.50506900
H	2.84759700	-2.52444800	-2.65129300
C	0.32932000	-4.90443100	-4.37872100
H	-0.49913800	-5.22114700	-2.41739500
C	1.30167800	-4.24582600	-5.13459800
H	2.96448300	-2.86748500	-5.08377100
H	-0.38498800	-5.56323900	-4.86423800
H	1.34122600	-4.38640000	-6.21083000

Table S15.

Structure: **PPh_3**, Energy= -1036.585477 Hartree, Charge= 0, Multiplicity=1

The number of the imaginary frequencies: 0

Center	Coordinates (Angstroms)		
Number	X	Y	Z

P	-0.00356400	-0.00242500	-1.26640800
C	-1.64234600	0.20189800	-0.44119300
C	-2.54189500	1.11370600	-1.01634800
H	-2.25918900	1.65050200	-1.91874300
C	-3.79256800	1.33918700	-0.44218900
H	-4.47558100	2.05147700	-0.89643100
C	-4.16895200	0.64188700	0.70825600
H	-5.14588100	0.80994400	1.15245000
C	-3.28678200	-0.27592700	1.28141300
H	-3.57475600	-0.82243200	2.17528500

C	-2.03027400	-0.49332200	0.71288100
H	-1.34866600	-1.20344400	1.16946600
C	0.64360500	-1.52292500	-0.44335000
C	0.32480500	-2.75747500	-1.03086200
H	-0.26772000	-2.78148200	-1.94228700
C	0.75910100	-3.95249000	-0.45782500
H	0.50053200	-4.90007100	-0.92197300
C	1.53366700	-3.92878600	0.70432900
H	1.87970200	-4.85803200	1.14785400
C	1.86605800	-2.70592600	1.29046200
H	2.46952900	-2.68146100	2.19369500
C	1.42228400	-1.51028000	0.72264700
H	1.67976600	-0.56482000	1.18872400
C	0.99396000	1.31758000	-0.44715500
C	0.58729500	2.00504000	0.70512800
H	-0.36806900	1.77143200	1.16345400
C	1.40473700	2.98612600	1.26957900
H	1.07667300	3.51172500	2.16217000
C	2.64015600	3.28889900	0.69408500
H	3.27493500	4.05211600	1.13510300
C	3.05436300	2.61036400	-0.45458800
H	4.01233600	2.84386800	-0.91063100
C	2.23287400	1.63833200	-1.02465000
H	2.55532100	1.12196800	-1.92565300

Table S16.

Structure: **$OPPh_3$**, Energy= -1111.875431 Hartree, Charge= 0, Multiplicity=1

The number of the imaginary frequencies: 0

Center Number	Coordinates (Angstroms) X	Y	Z
P	0.00509500	-0.03168600	0.95129700
C	-0.03067600	1.66797100	0.30391200
C	-1.22317100	2.40491700	0.38625400
H	-2.12532300	1.93536700	0.76730600
C	-1.25759100	3.73402400	-0.03015700
H	-2.18464000	4.29614500	0.03174200
C	-0.10140600	4.33980700	-0.52959500
H	-0.12967000	5.37505200	-0.85679200
C	1.08878900	3.61506600	-0.60922000
H	1.98806700	4.08436300	-0.99699500
C	1.12602000	2.28357600	-0.19345800
H	2.05252600	1.72296400	-0.26063900
C	1.45865600	-0.82076300	0.18877700
C	2.50621700	-1.21517600	1.02956000
H	2.41478100	-1.05200700	2.09846600
C	3.64695700	-1.81469500	0.49303300
H	4.45686900	-2.11979500	1.14912200
C	3.74429000	-2.02183800	-0.88368700
H	4.63148600	-2.48882200	-1.30144400
C	2.69918400	-1.63202700	-1.72659700
H	2.77266900	-1.79634200	-2.79756800
C	1.55880500	-1.03456500	-1.19349500
H	0.74876600	-0.74004600	-1.85353100
C	-1.44942200	-0.85026700	0.22599000
C	-1.94198200	-0.53193400	-1.04803200

H	-1.49298600	0.27267800	-1.62198800
C	-3.02699400	-1.23291200	-1.57390800
H	-3.40636800	-0.98003100	-2.55954900
C	-3.62889700	-2.25082300	-0.83046500
H	-4.47573300	-2.79345200	-1.24041800
C	-3.14735800	-2.56611300	0.44207100
H	-3.61971000	-3.35189700	1.02417900
C	-2.06060000	-1.86897200	0.96940900
H	-1.68562300	-2.10025500	1.96145900
O	0.03629300	-0.13243400	2.45828200

Table S17.

Structure: **NO**, Energy= -129.932018 Hartree, Charge= 0, Multiplicity=2

The number of the imaginary frequencies: 0

Center	Coordinates (Angstroms)		
Number	X	Y	Z

N	0.58675200	-0.25121600	0.00710700
O	-0.57194500	-0.25121600	0.00710700
