Supporting Information

Facile C_{sp}–C_{sp} Bond Formation Prompted by Electrophilic Fluorinating Reagent from bis(alkynyl) Platinum Complexes

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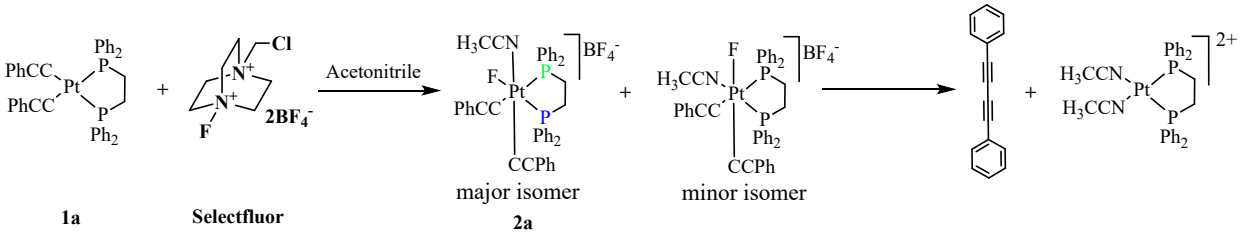
Contents

A. General techniques and procedures

Commercially available reagent (Selectfluor) was used as received. The NMR spectra were recorded on Bruker Avance DPX and Varian 300 & 500 MHz spectrometers. The ^{1}H NMR signals are reported in ppm downfield from TMS. The ^{1}H signals are referenced to the residual proton of a deuterated solvent 7.26 ppm for $CDCl_3$, 1.94 ppm for CD_3CN. The ^{31}P chemical shifts are reported in ppm downfield from H_3PO_4 and referenced to an external 85% phosphoric acid sample. The ^{19}F chemical shifts are reported in ppm downfield from $CFCl_3$. The [(dppe)Pt(C≡CPh)$_2$][1], **1a**, and [(bpy)Pt(C≡CPh)$_2$][2], **1b**, were synthesized based on the literature methods.

[1] *Journal of the Chemical Society, Dalton Transactions*, **1999**, 4287-4288.
[2] *Journal of Organometallic Chemistry*, **2019**, *897*, 95-106.

A1. Reaction of [(dppe)Pt(C≡CPh)$_2$], 1a, with Selectfluor



Selectfluor (3.5mg, 0.01 mmol) and [(dppe)Pt(C≡CPh)$_2$], **1a**, (5.6 mg, 0.01 mmol) were dissolved in CD_3CN in a NMR tube. The formation and decomposition of fluoro-Pt(IV) intermediate, **2a**, were monitored by ^{31}P & ^{19}F NMR spectroscopies. Moreover, 1,4-diphenylbutadiyne and Pt(II) byproduct formations as a result of reductive elimination reaction were demonstrated by ^{1}H & ^{31}P NMR.

$^{31}P\{^{1}H\}$-NMR (300 MHz, CD_3CN) of major isomer (**2a**): 30.00 (s, $^{1}J_{Pt\text{-}P}$ = 2483 Hz, P trans to phenylacetylene), 27.6 (d, $^{1}J_{Pt\text{-}P}$ = 1547 Hz, $^{2}J_{P\text{-}F}$ = 31 Hz, P trans to F); minor isomer: 22.7, 18.0.

$^{19}F\{^{1}H\}$-NMR (300 MHz, CD_3CN) of major isomer (**2a**): -314.9 (d, $^{1}J_{Pt\text{-}F}$ = 649 Hz, $^{2}J_{P\text{-}F}$ = 31 Hz); minor isomer: -299.0 (d, $^{1}J_{Pt\text{-}F}$ = 557 Hz, $^{2}J_{P\text{-}F}$ = 28 Hz)

^{1}H-NMR (300 MHz, CD_3CN) of 1,4-diphenyl-1,3-butadiyne: 7.38–7.47 (m), 7.56–7.59 (m).

$^{31}P\{^{1}H\}$-NMR (300 MHz, CD_3CN) of final Pt(II) byproduct: 39 (s, $^{1}J_{Pt\text{-}P}$ = 3589 Hz)

^{1}H-NMR (300 MHz, CD_3CN) of final Pt(II) byproduct: 7.62–7.81 (m, 20H, aryl), 2.80 (m, 4H, CH_2)

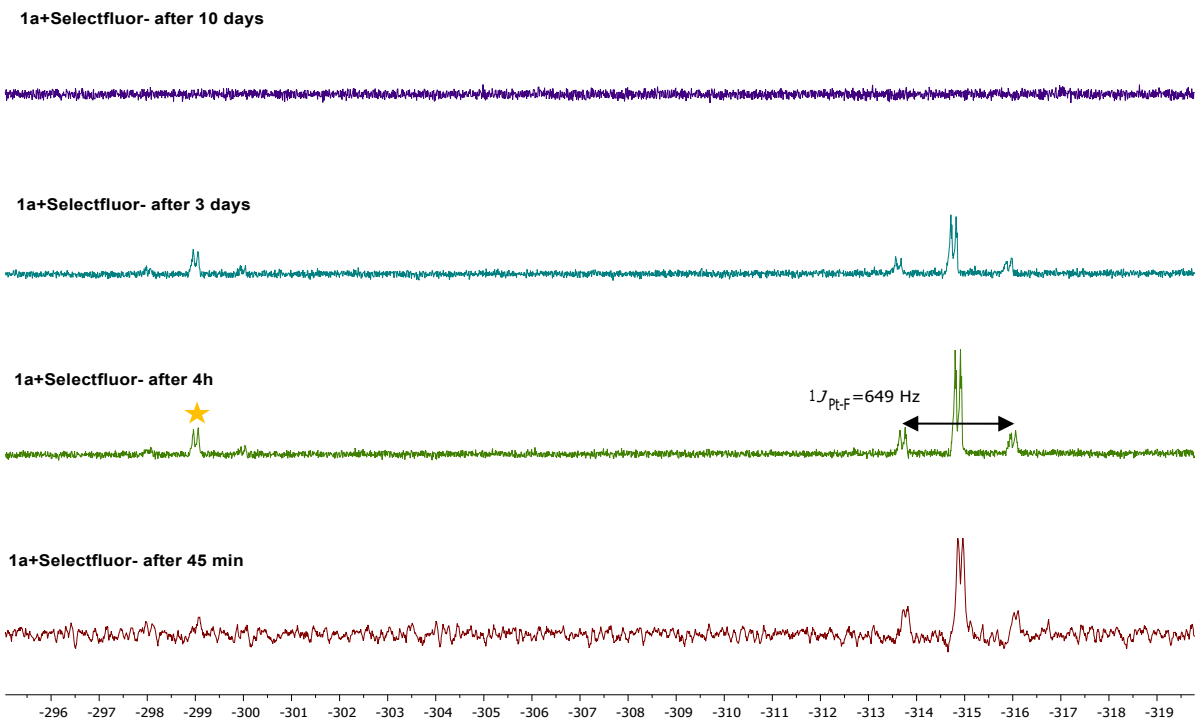


Figure S1. Monitoring the reaction of **1a** with 1 equiv. of Selectfluor by $^{19}F\{^1H\}$ NMR at RT in CD_3CN.

★ = minor isomer

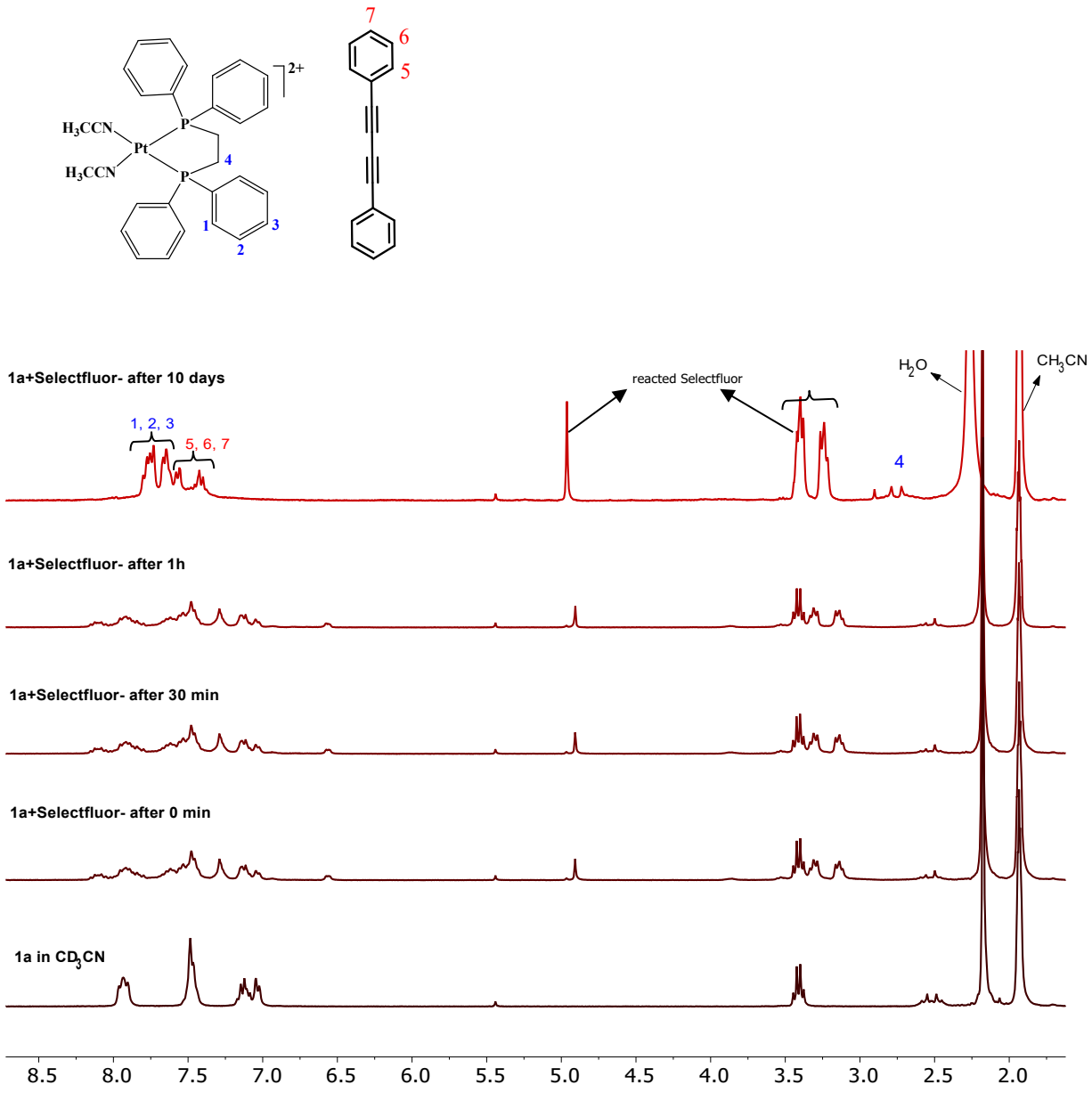
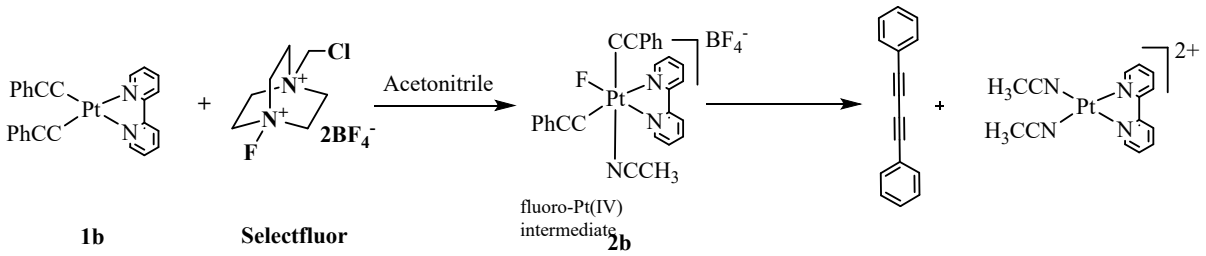


Figure S2. Monitoring the reaction of **1a** with 1 equiv. of Selectfluor by ^{1}H NMR at RT in CD_3CN.

A2. Reaction of [(bpy)Pt(C≡CPh)$_2$], 1b, with Selectfluor



Selectfluor (3.5mg, 0.01 mmol) and [(bpy)Pt(C≡CPh)$_2$], **1b**, (5.6 mg, 0.01 mmol) were dissolved in CD_3CN in a NMR tube. The formation of intermediate **2b** was monitored by ^{19}F & ^{1}H NMR spectroscopy. Moreover, the decomposition of **2b** and 1,4-diphenyl-1,3-butadiyne formation were demonstrated by ^{19}F & ^{1}H NMR:

$^{19}F\{^{1}H\}$-NMR (300 MHz, CD_3CN) of **2b**: -349.1 (s, Pt-F, $^{1}J_{Pt\text{-}F}$ = 1360 Hz), -151.56 (s, 4F, BF_4^-)

^{1}H-NMR (300 MHz, CD_3CN) of 1,4-diphenyl-1,3-butadiyne: 7.38–7.47 (m), 7.56–7.59 (m).

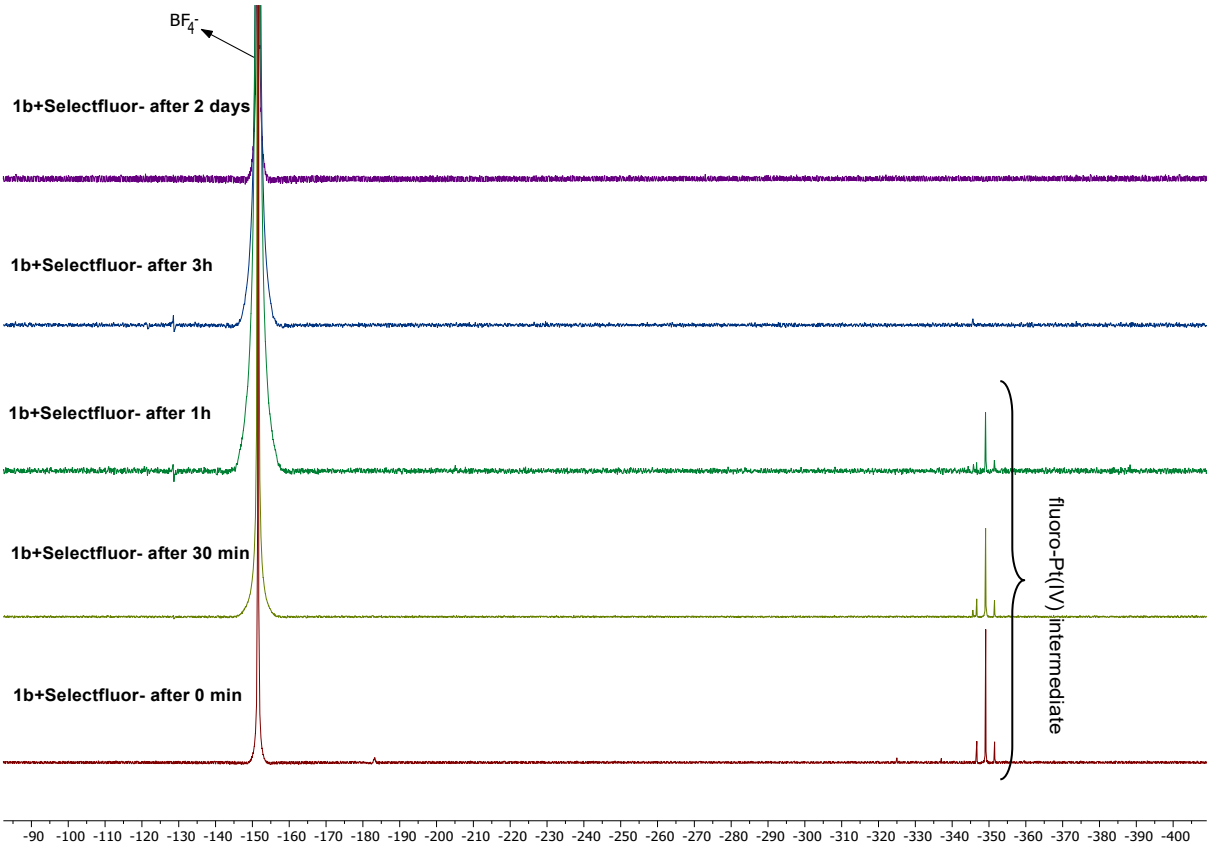


Figure S3. Monitoring the reaction of **1b** with 1 equiv. of Selectfluor by $^{19}F\{^{1}H\}$ NMR at RT in CD_3CN.

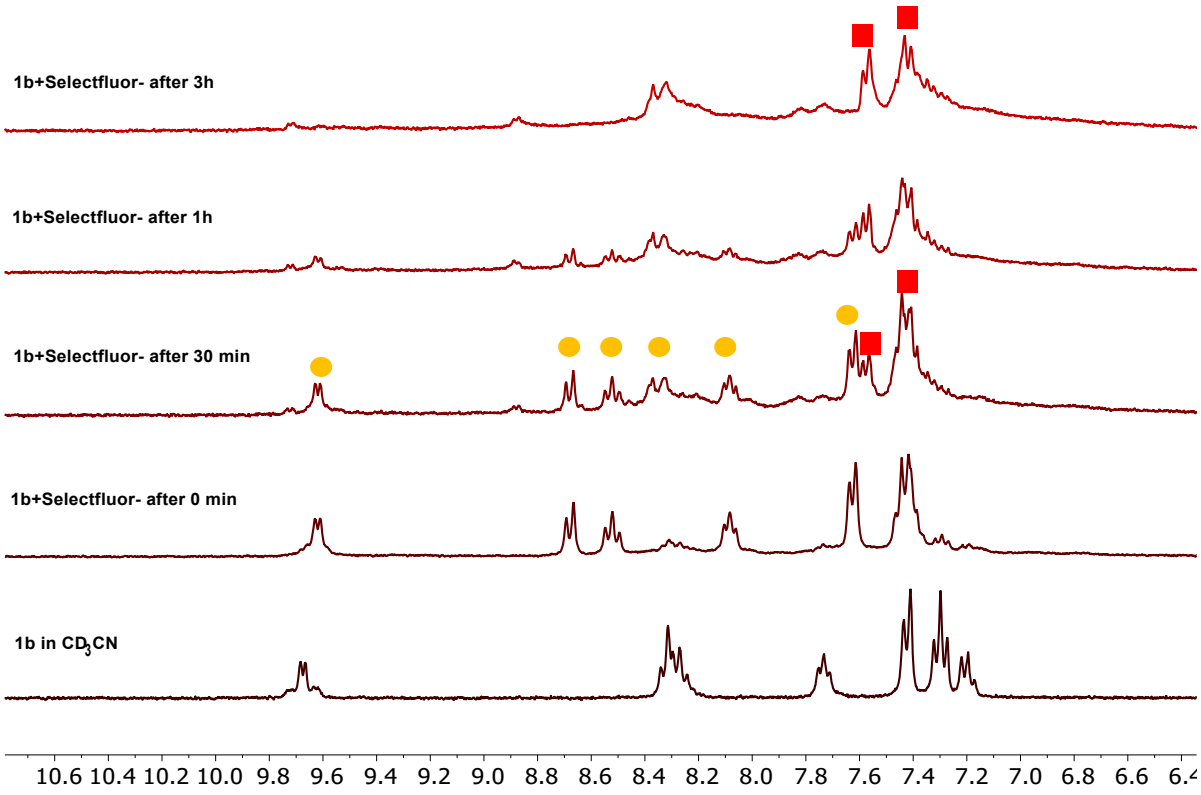


Figure S4. Monitoring the reaction of **1b** with 1 equiv. of Selectfluor by ^{1}H NMR at RT in CD_3CN.

● = fluoro-Pt(IV) intermediate

■ = 1,4-diphenylbutadiyne

A3. NMR spectra of Precursors

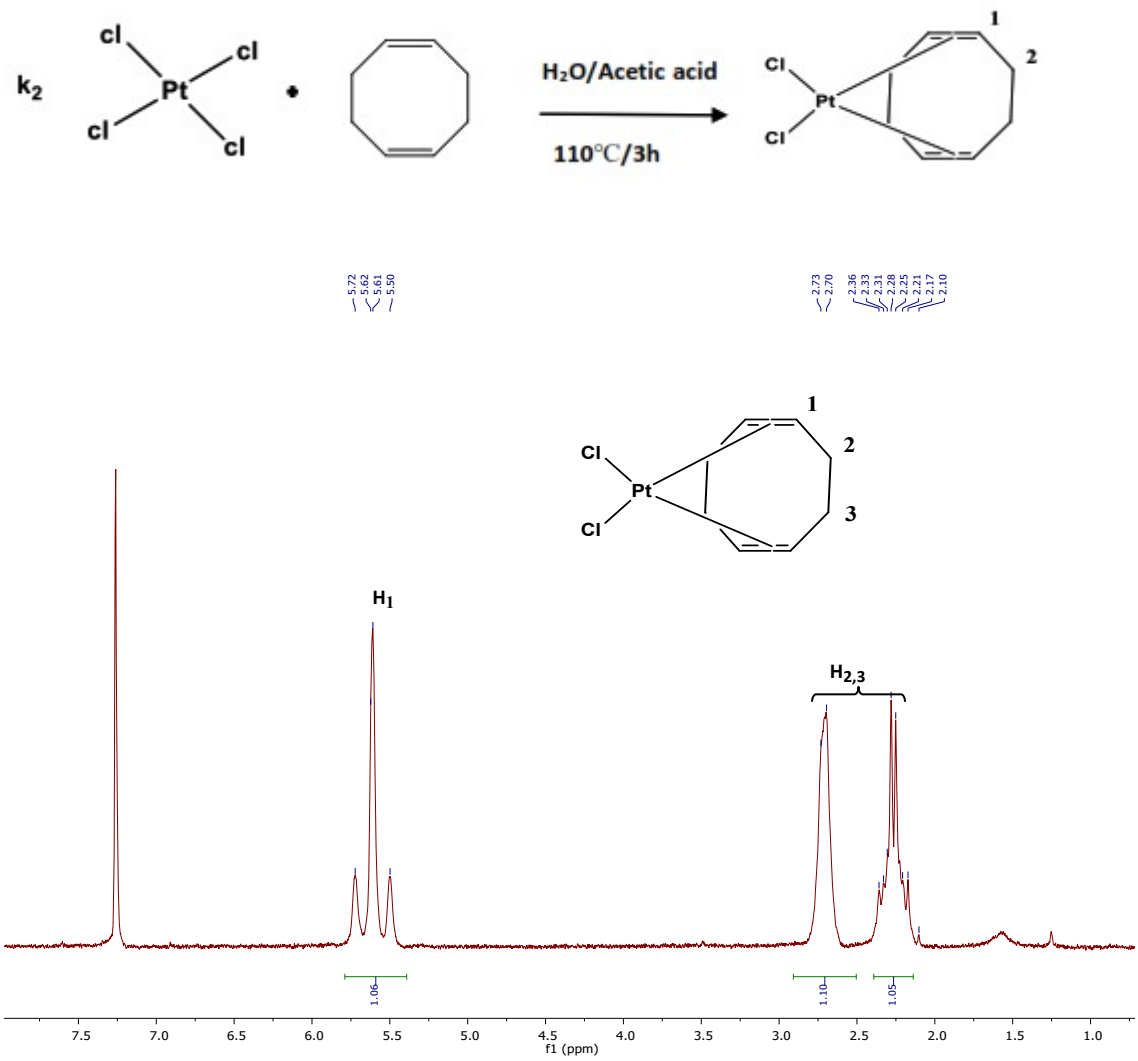


Figure S5. The ^{1}H NMR spectrum of $[Pt(COD)(Cl)_2]$ in $CDCl_3$.

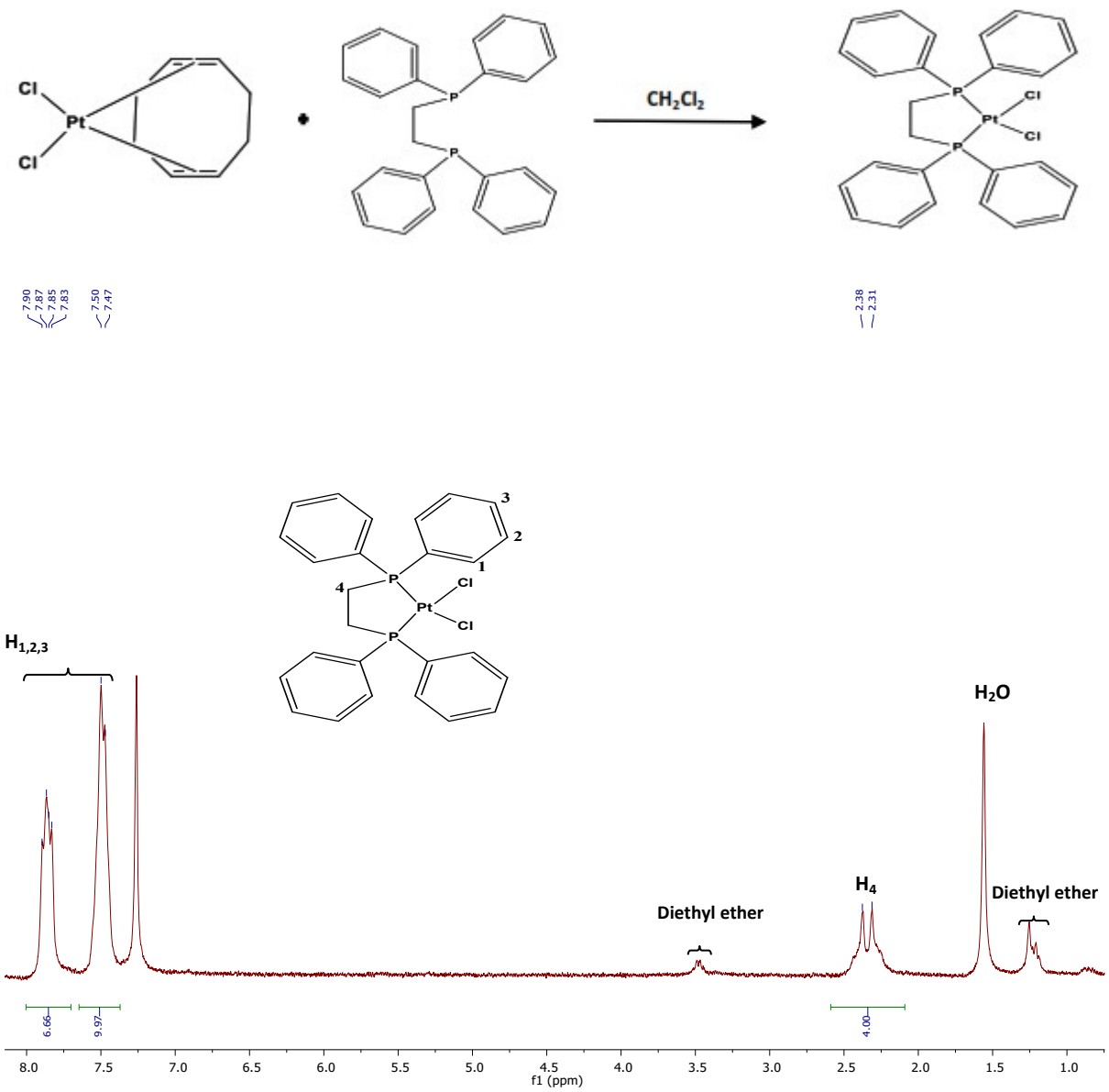


Figure S6. The ^{1}H NMR spectrum of $[Pt(dppe)(Cl)_2]$ in $CDCl_3$.

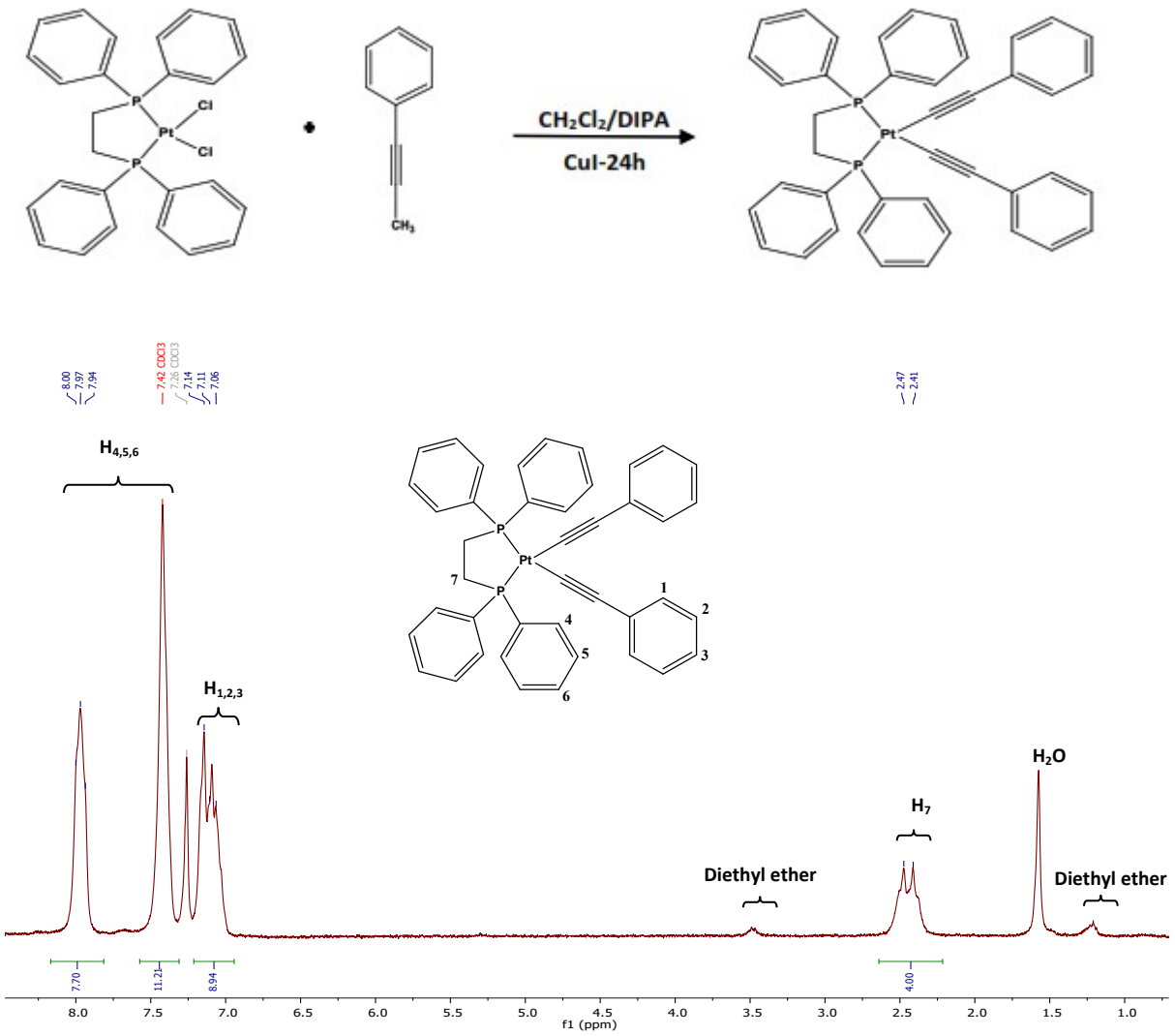


Figure S7. The ^{1}H NMR spectrum of $[Pt(dppe)(C{\equiv}CPh)_2]$ in $CDCl_3$.

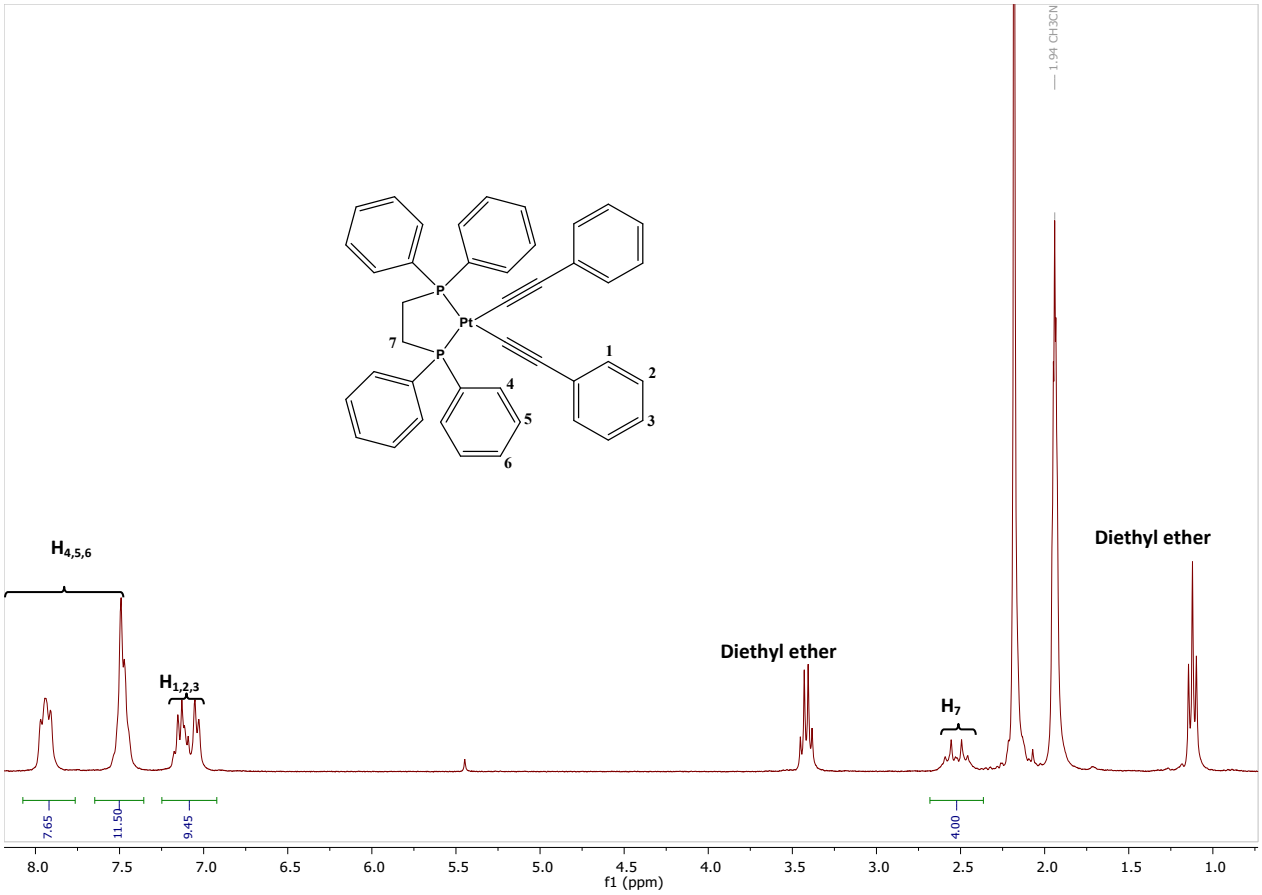


Figure S8. The ^{1}H NMR spectrum of [Pt(dppe)(C≡CPh)$_2$] in CD_3CN.

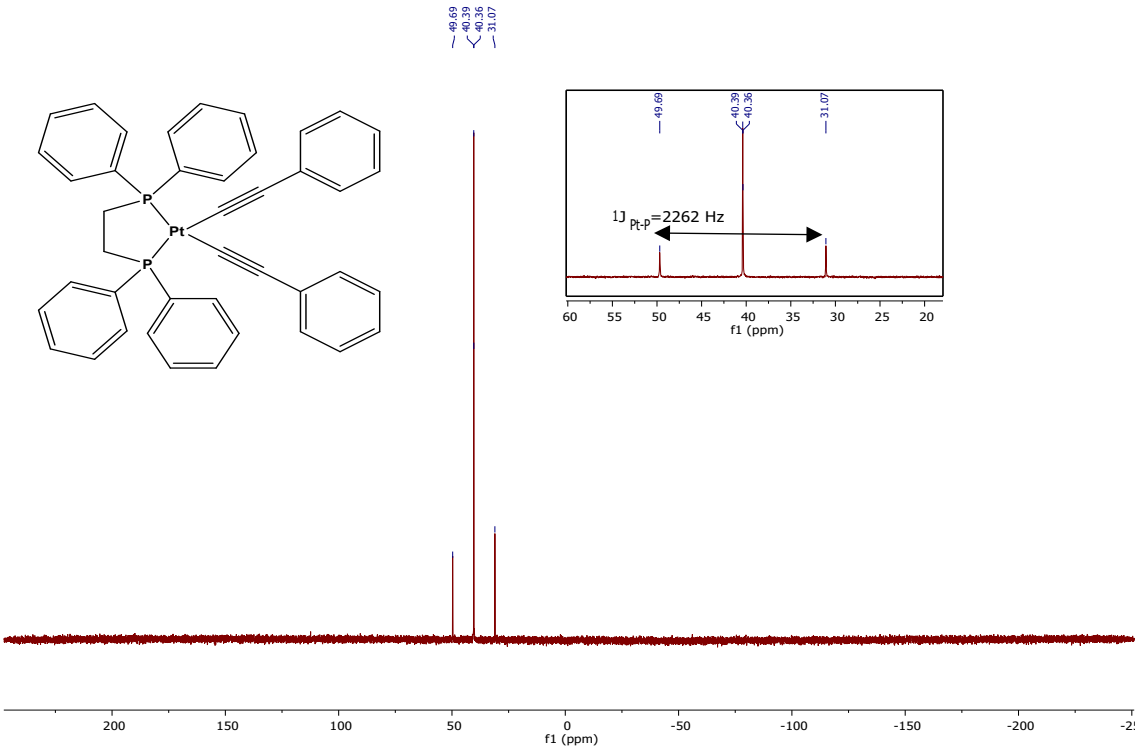


Figure S9. The ^{31}P NMR spectrum of [Pt(dppe)(C≡CPh)$_2$] in CD_3CN.

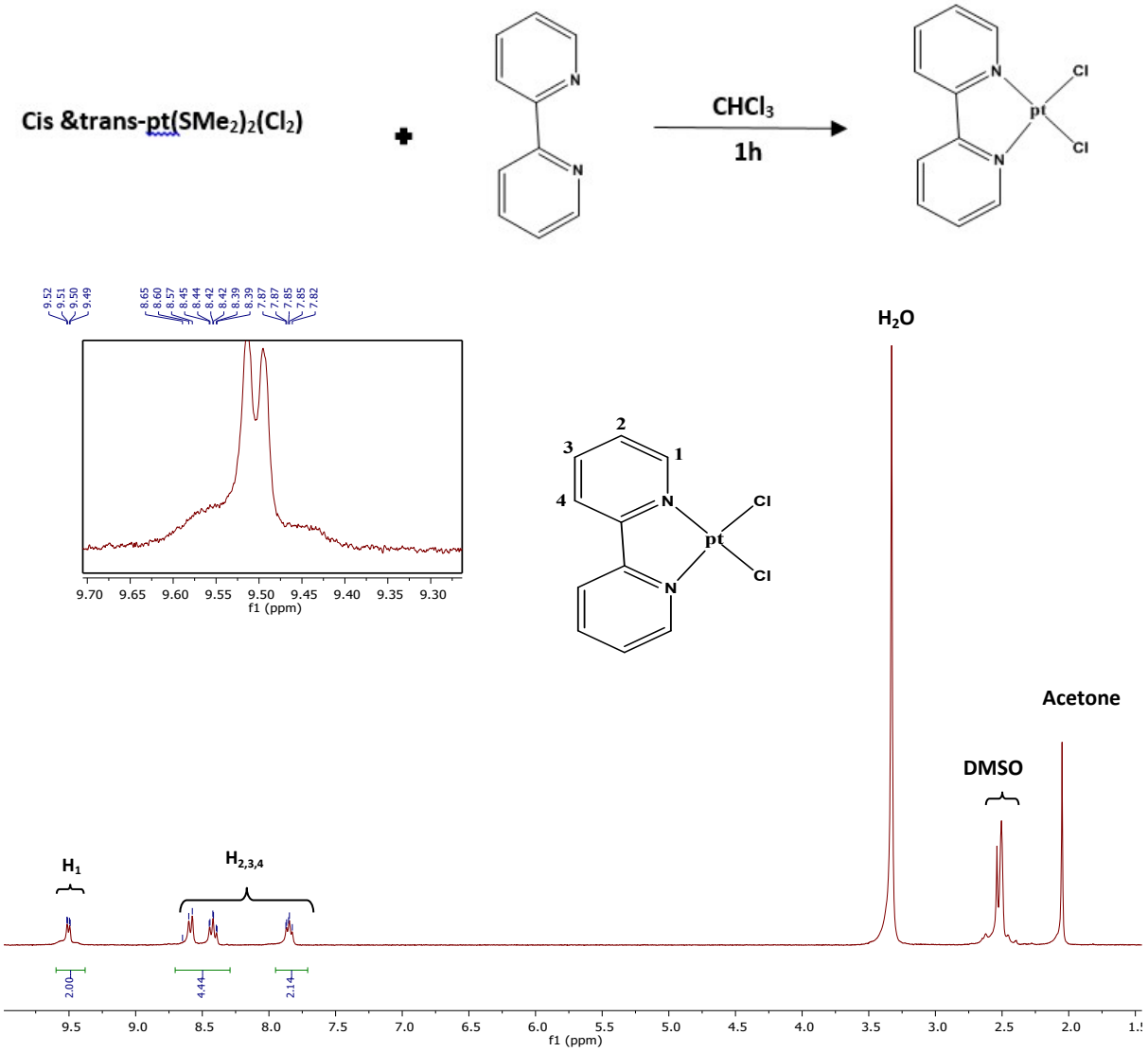


Figure S10. The ^{1}H NMR spectrum of [Pt(bipy)Cl_2] in dmso-d_6.

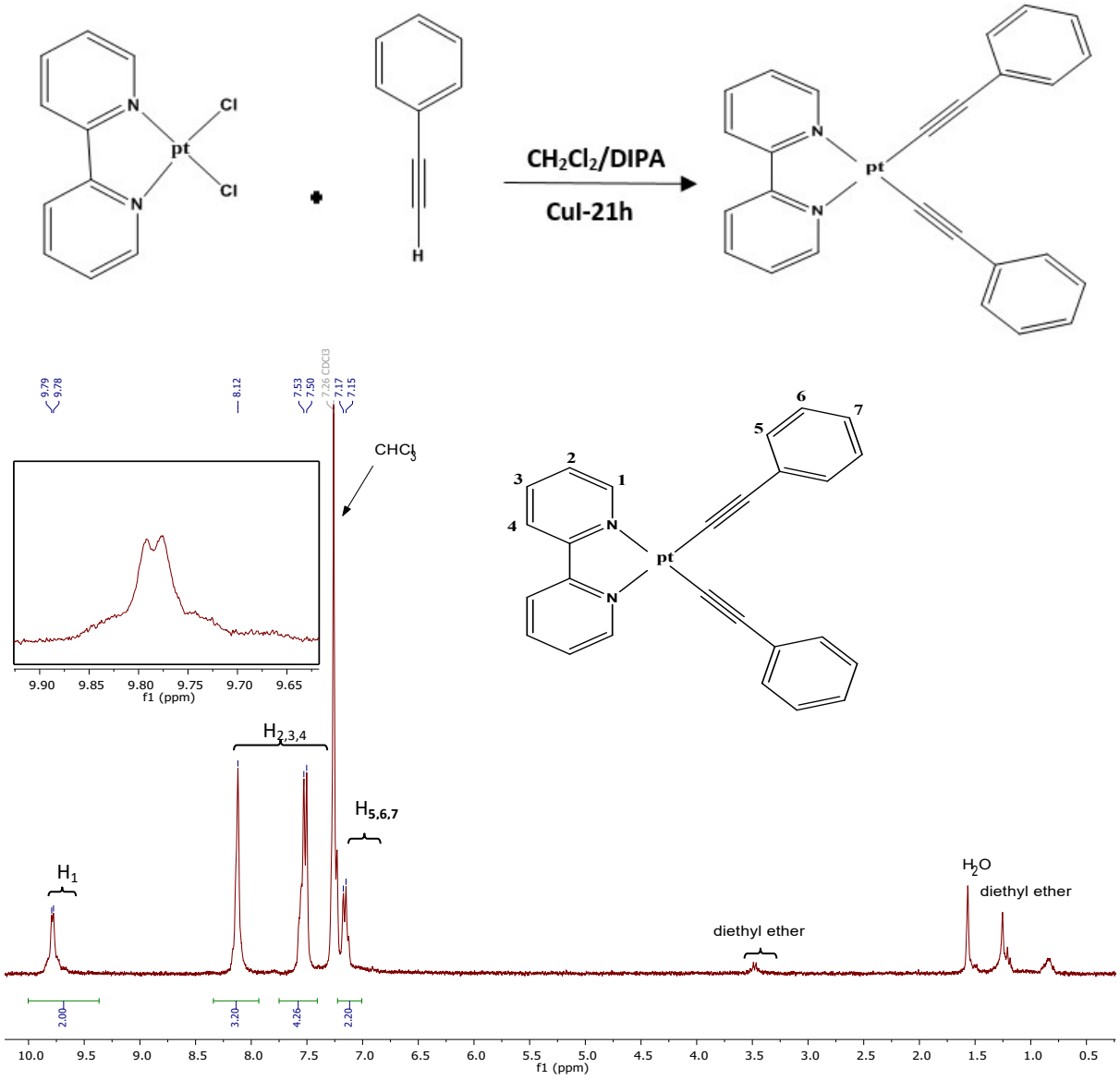


Figure S11. The ^{1}H NMR spectrum of [Pt(bipy)(C≡CPh)$_2$] in $CDCl_3$.

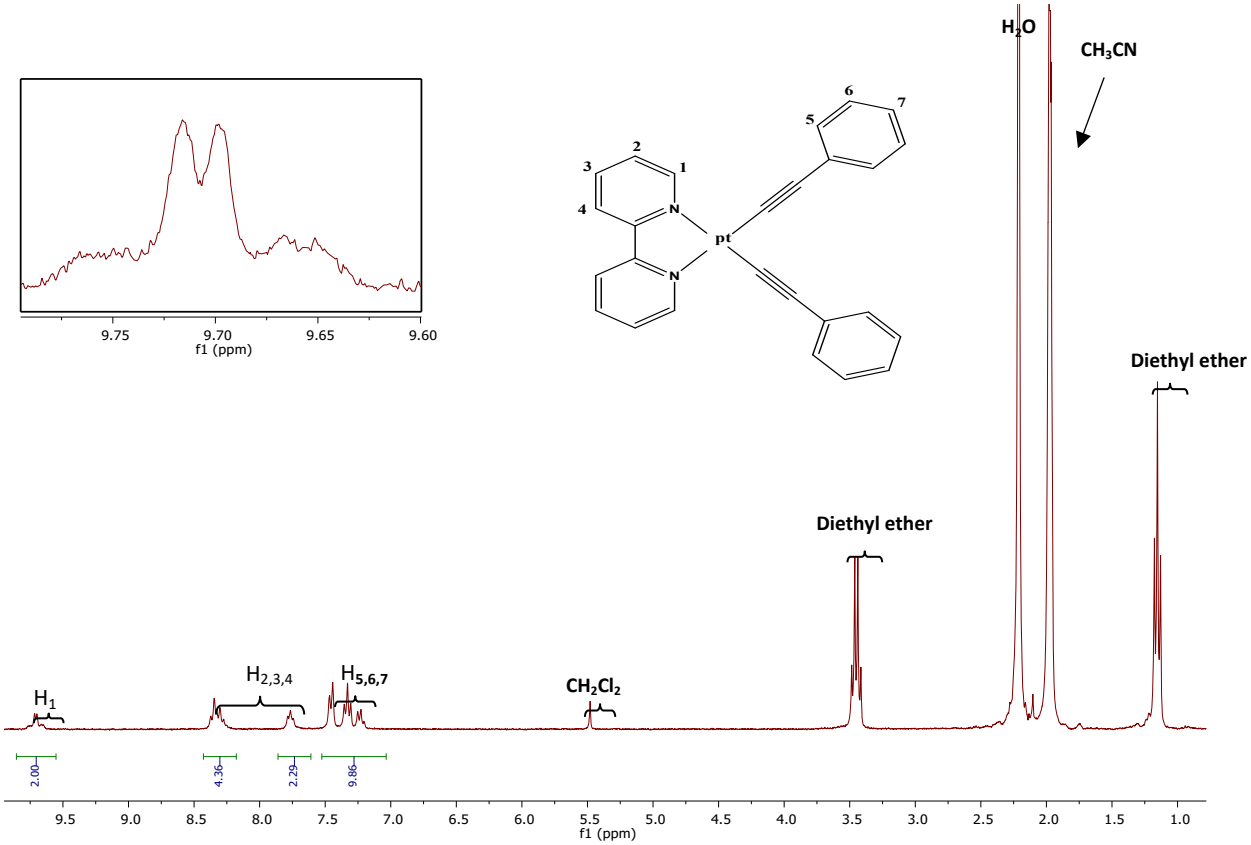


Figure S12. The ^{1}H NMR spectrum of [Pt(bipy)(C≡CPh)$_2$] in CD_3CN.

B. Computational Details

Density functional calculations were performed with the program suite Gaussian 09[3] using the B3LYP[4] (Becke, 3 parameter, Lee-Yang-Parr) level of theory with D3 dispersion correction[5]. The LANL2DZ basis set[6] was chosen to describe Pt and The 6-31G(d)[7] basis set was used for other atoms. The geometries of complexes were fully optimized by employing the density functional theory without imposing any symmetry constraints. To evaluate and ensure the optimized structures of the molecules, frequency calculations were carried out using analytical second derivatives. In all cases only real frequencies were obtained for the optimized structures. The stationary points and transition states were characterized by full vibration frequency calculations, with no imaginary frequency for minima (stationary point) and one imaginary frequency for transition states. Solvent effects have been taken into account using the PCM model.[8] The connectivity between transition structures and minima was confirmed through Intrinsic Reaction Coordinate (IRC) calculations.[9] Single-point calculations were performed using the some selected functionals, and the results are summarized in the Table S1. Natural bond orbitals (NBOs) and wiberg bond index (WBI)[10] analysis was calculated at studied level of B3LYP theory by using the NBO 3.1[11] program. The Multiwfn[12] software is used for the atoms-in-molecules (AIM) analysis.[13]

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[3] M. J. Frisch, G. W. T., H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox; Gaussian, Inc., Wallingford CT, **2009**.

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[7] Yang, Y.; Weaver, M. N.; Merz, K. M., Jr. *J Phys Chem A* **2009**, *113*.

[8] (a) Cossi, M.; Scalmani, G.; Rega, N.; Barone, V. *J. Chem. Phys.* **2002**, *117*, 43(b) Barone, V.; Cossi, M.; Tomasi, J. *J. Chem. Phys.* **1997**, *107*, 3210.

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[10] Mayer, I. *J. Comput. Chem.* **2007**, *28*.

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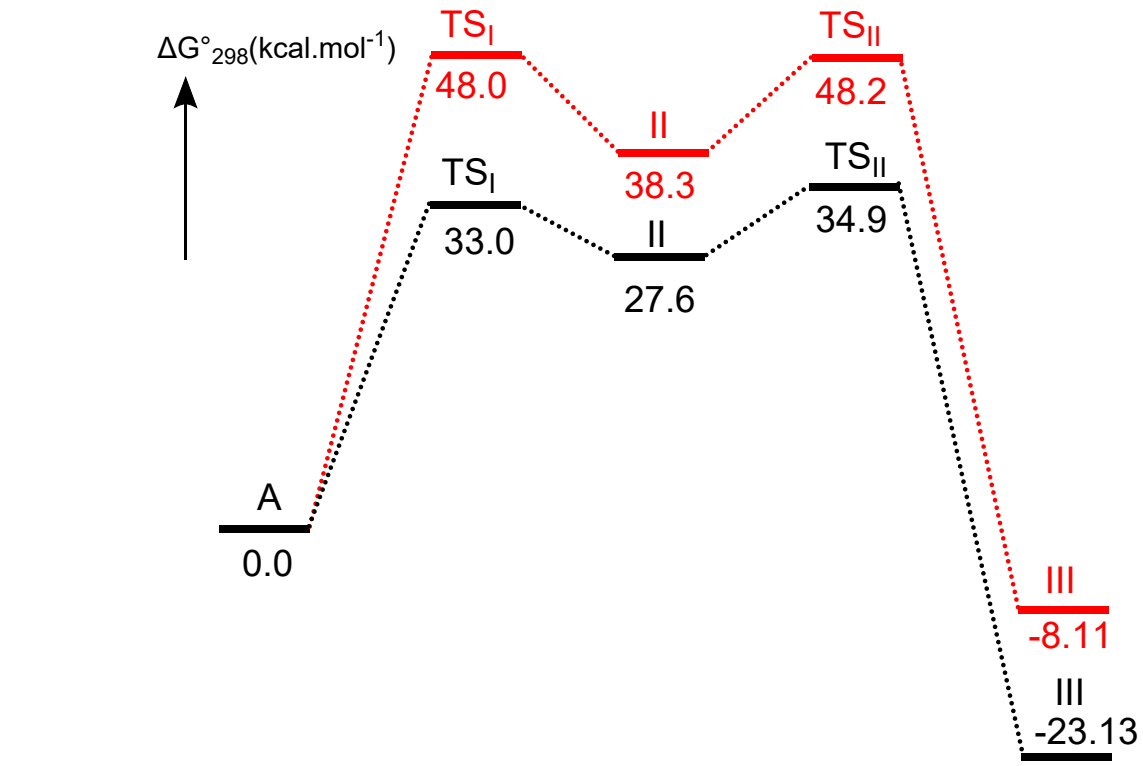
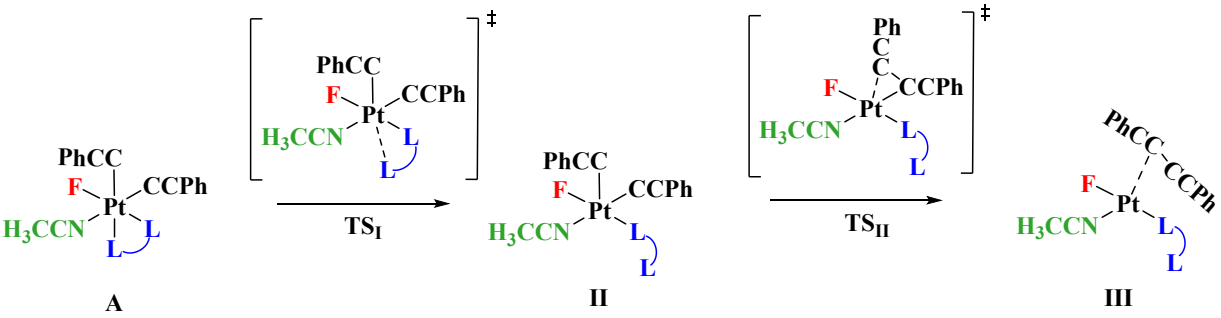
[13] Bader, R. F.; Molecules, A. I. A quantum theory. *Clarendon: Oxford, UK* **1990**.

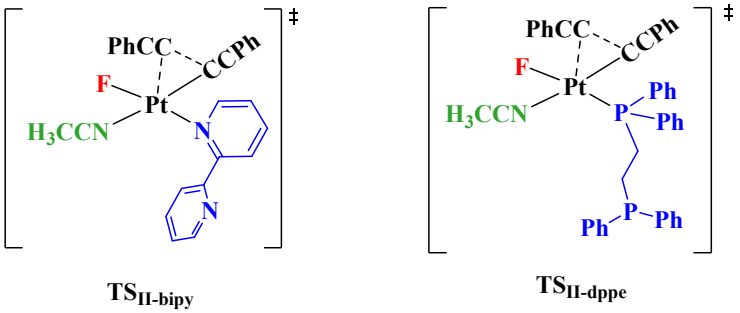
B1. Potential energy surfaces for possible mechanisms



A



B



C

Figure S13. Standard Gibbs free energy (in kcal.mol^{-1}) diagram for the chelate opening mechanism: A) The potential energy surface (PES) changes for the two-step reaction mechanism of Path I. (The energy related to TS_I extrapolated from L–L dihedral angle's relaxed scan related of the A in Scheme 3. B) The structures of the intermediate and transition states related to the investigated reaction mechanism. C) The structure of TS_{II} associated to the bipy and dppe ligands. The red diagram is corresponding to the dppe ligand, and the black diagram is corresponding to the bipy ligand.

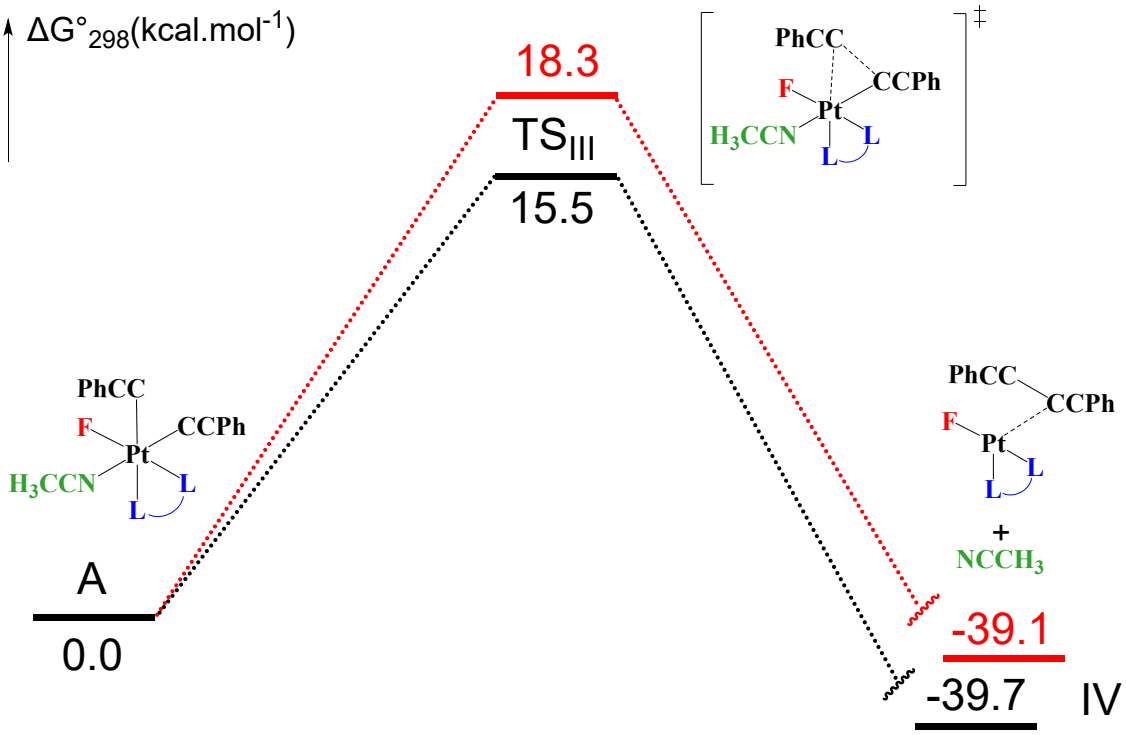


Figure S14. Standard Gibbs free energy (in kcal.mol^{-1}) diagram for path II as the direct path by six-coordinate complex. The red diagram is corresponding to the dppe ligand, and the black diagram is corresponding to the bipy ligand.

Path III. Our main mechanistic discussion in this work focuses on this pathway, which is deliberated in detail in the primary literature in Figure 2. In the Supporting Information, we compare the results of the calculated single point energy for the optimized structures in path III using B3LYP-D3BJ. We employed various functionals and basis sets for refine the energy and method validation to identify the most effective approach that accurately reflects the time differences observed in the detection of products in experimental section. All methods used for single-point energy calculations are summarized in Table S1. For better comparison, the PES for PBE0-D3/6311G+(2d,p)/def2-TZVPP is depicted in Figure S15. As shown in this figure, the single point energy does not affect the overall relative energy; therefore, our discussion throughout the article will remain based on the methods used for optimizing structures.

Table S1. Calculated ΔG°(ΔH°) in kcal.mol^{-1} by single point calculation for optimized structure by PCM/B3LYP-D3/631G(d),LANL2DZ.

Functional	Basis Set	compound	dppe	bipy
B3LYP-D3	*631G(d)/LANL2DZ*	*2*	*0 (0)*	*0 (0)*
		TS_{diss}	*15.8 (13.5)*	*12.1 (9.8)*
		3	*16.2 (14.2)*	*7.9 (8.4)*
		4	*6.5 (18.1)*	*3.1 (14.4)*
		TS_{C-C}	*16.4 (27.9)*	*12.4 (23.6)*
		5	*-45.9 (-33.3)*	*-43.5 (-32.5)*
B3LYP-D3	*6311G+(2d,p)/LANL2TZ(f)*	*2*	*0 (0)*	*0 (0)*
		TS_{diss}	*19.1 (16.9)*	*15.8 (13.6)*
		3	*19.5 (17.5)*	*9.7 (10.2)*
		4	*6.0 (17.5)*	*5.8 (17.2)*
		TS_{C-C}	*17.5 (29.1)*	*15.1 (26.4)*
		5	*-40.2 (-27.7)*	*-36.1 (-25.1)*
B3LYP-D3	*6311G+(2d,p)/def2-TZVPP*	*2*	*0 (0)*	*0 (0)*
		TS_{diss}	*18.6 (16.3)*	*15.5 (13.2)*
		3	*18.9 (17.0)*	*9.3 (9.8)*
		4	*5.4 (16.9)*	*5.3 (16.7)*
		TS_{C-C}	*16.2 (27.8)*	*13.8 (25.0)*
		5	*-44.2 (-31.6)*	*-39.3 (-28.3)*
M06-2X	*6311G+(2d,p)/def2-TZVPP*	*2*	*0 (0)*	*0 (0)*
		TS_{diss}	*16.0 (13.8)*	*14.0 (11.7)*
		3	*16.5 (14.5)*	*9.6 (10.1)*
		4	*69.1 (80.7)*	*69.3 (80.7)*
		TS_{C-C}	*80.5 (92.0)*	*77.3 (88.6)*
		5	*17.5 (30.0)*	*25.5 (36.5)*
PBE0-D3	*6311G+(2d,p)/def2-TZVPP*	*2*	*0 (0)*	*0 (0)*
		TS_{diss}	*21.5 (19.3)*	*17.6 (15.3)*
		3	*22.0 (20.1)*	*12.3 (12.8)*
		4	*7.5 (19.1)*	*7.7 (19.1)*
		TS_{C-C}	*17.0 (28.5)*	*14.6 (25.9)*
		5	*-41.2 (-28.7)*	*-37.6 (-26.6)*

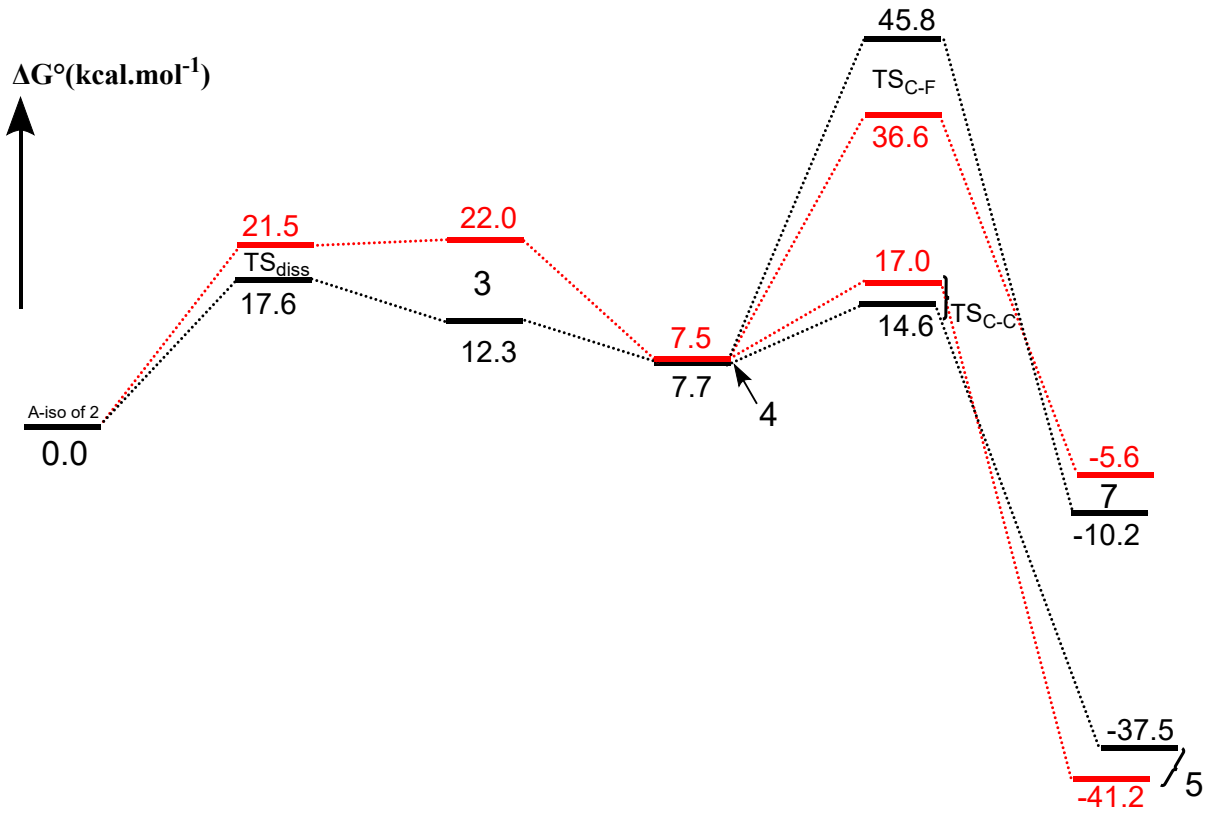


Figure S15. Standard Gibbs free energy (in kcal.mol^{-1}) diagram for path III, obtained through single point calculations using the PCM/PBE0-D3/6-311G+(2d,p),def2-TZVPP method. The red diagram is corresponding to the dppe ligand, and the black diagram is corresponding to the bipy ligand.

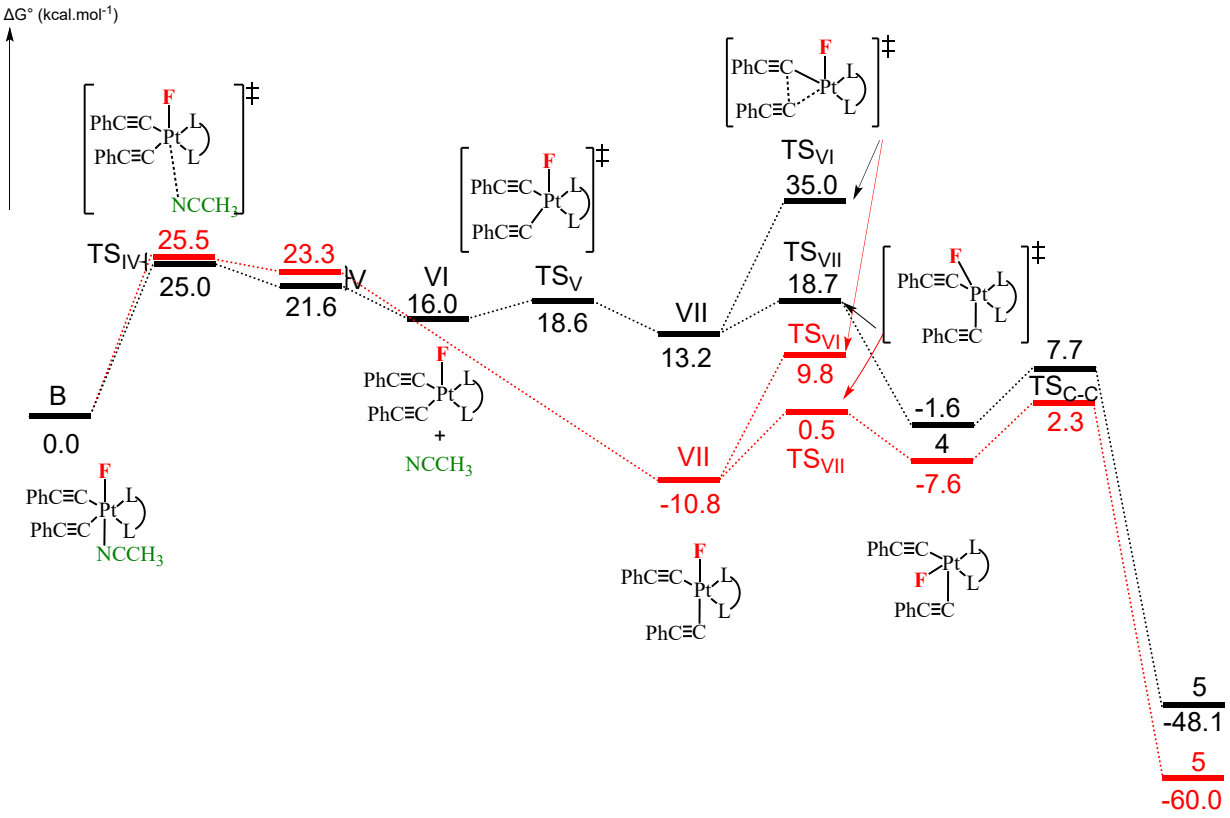
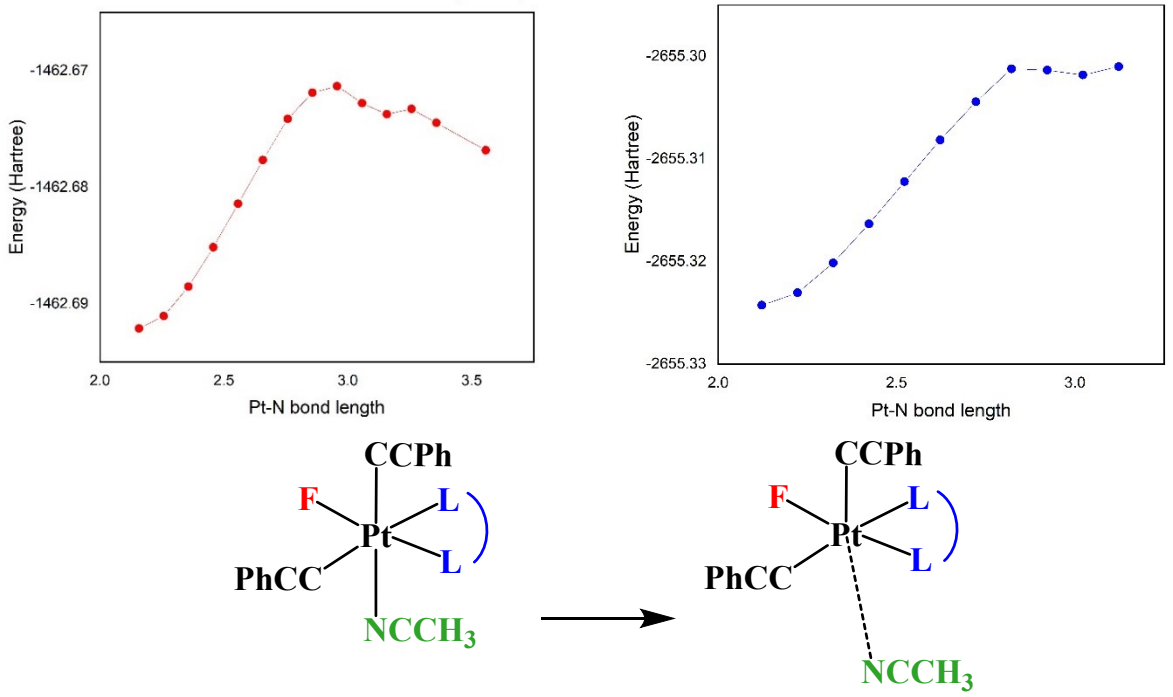
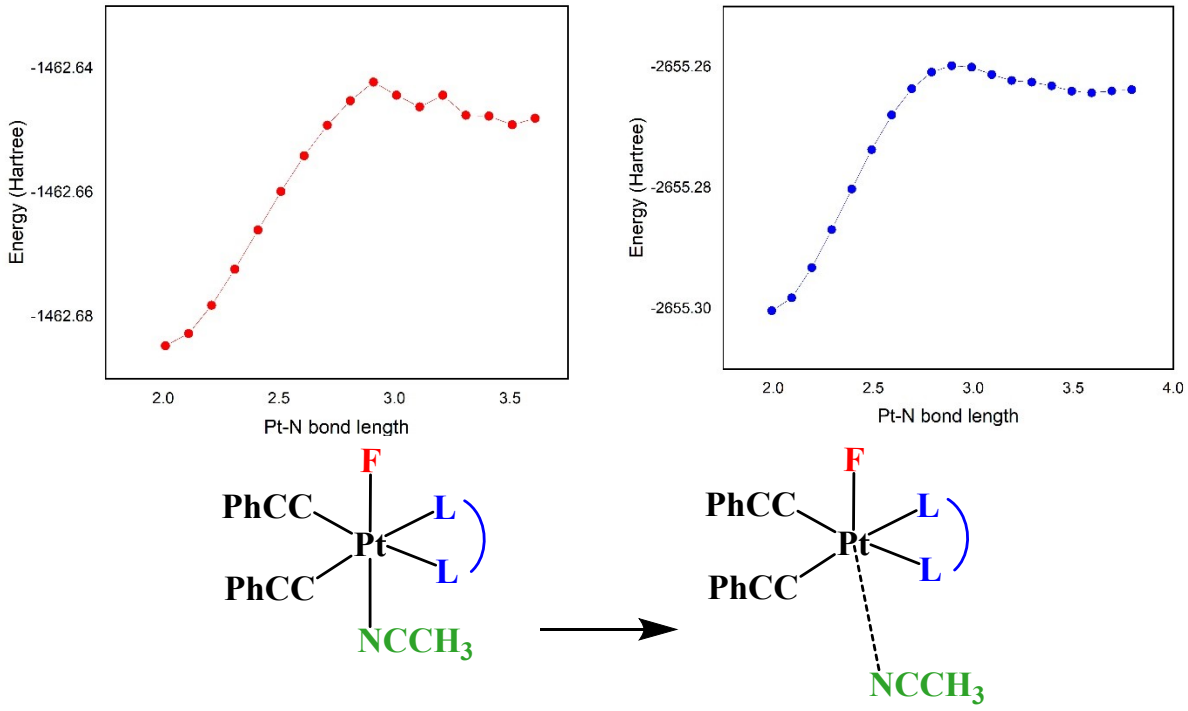


Figure S16. Calculated reaction mechanism for isomer B of intermediate 2 based on Gibbs free energy changes in kcal.mol^{-1} (path IV). The red diagram is corresponding to the dppe ligand, and the black diagram is corresponding to the bipy ligand.

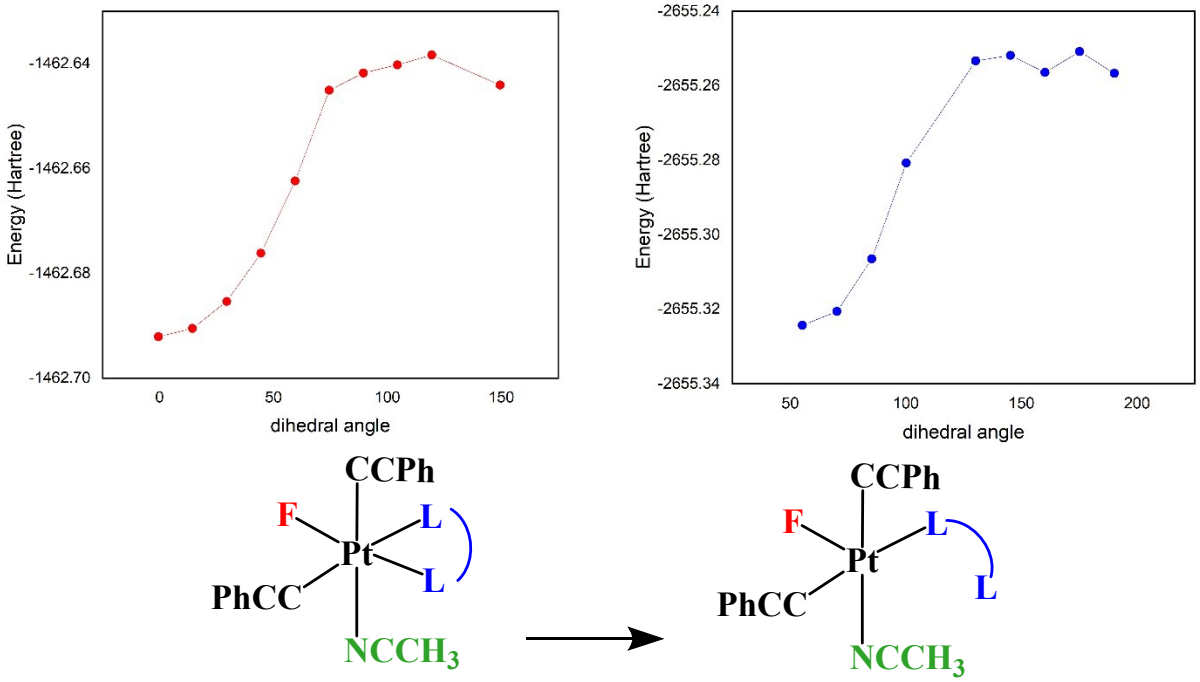
B2. PES Scan coordinated of some investigated complexes:



A)



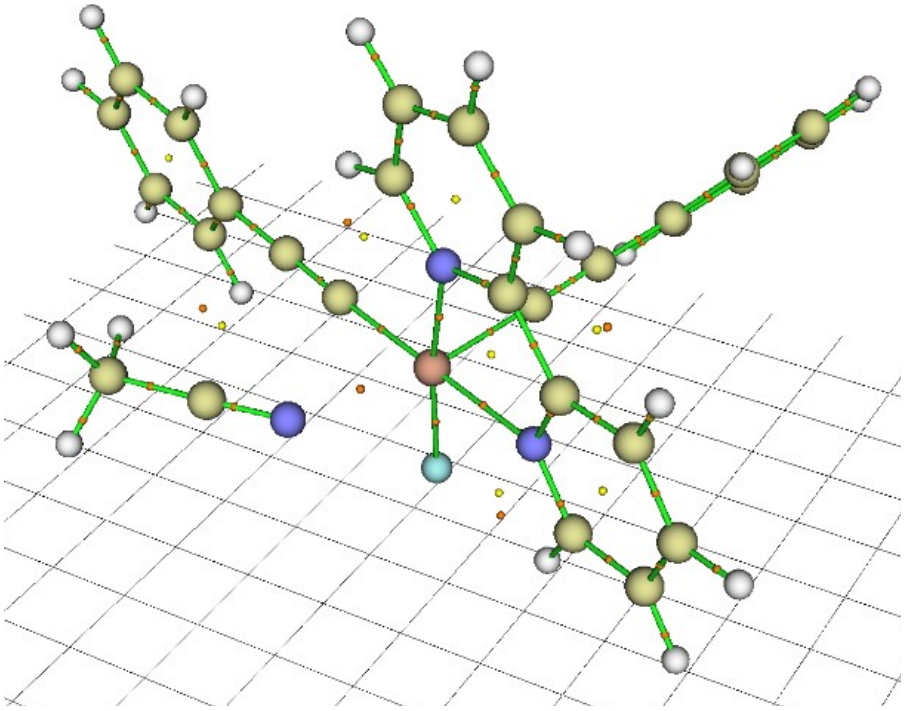
B)



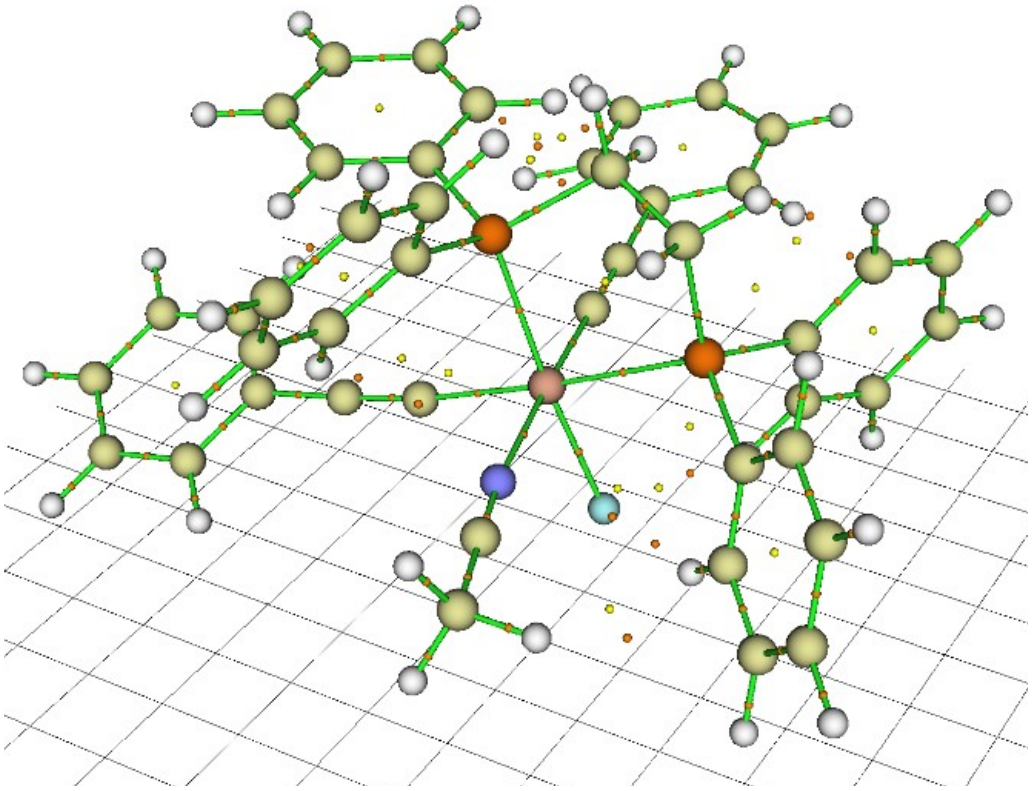
C)

Figure S17. Relaxed PES scans A) for isomer A between the Pt atom of complex and nitrogen atom of acetonitrile ligand along the Pt–N bond B) for isomer B between the Pt atom of complex and nitrogen atom of acetonitrile ligand along the Pt–N bond C) for the dihedral angle of ancillary ligand related to chelate opening of isomer A. In all PES scans, the red diagram is corresponding to the bipy ligand, while the blue diagram is representing the dppe ligand.

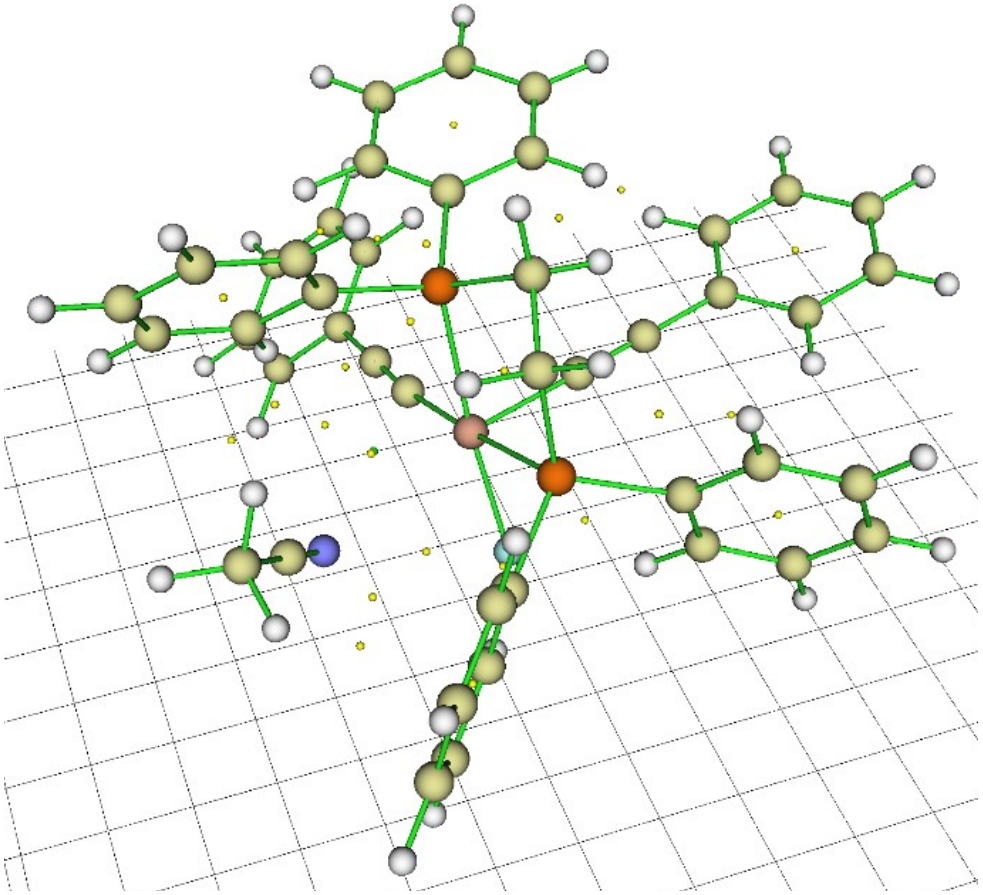
B3. Atoms-in-molecules (AIM) analysis results:



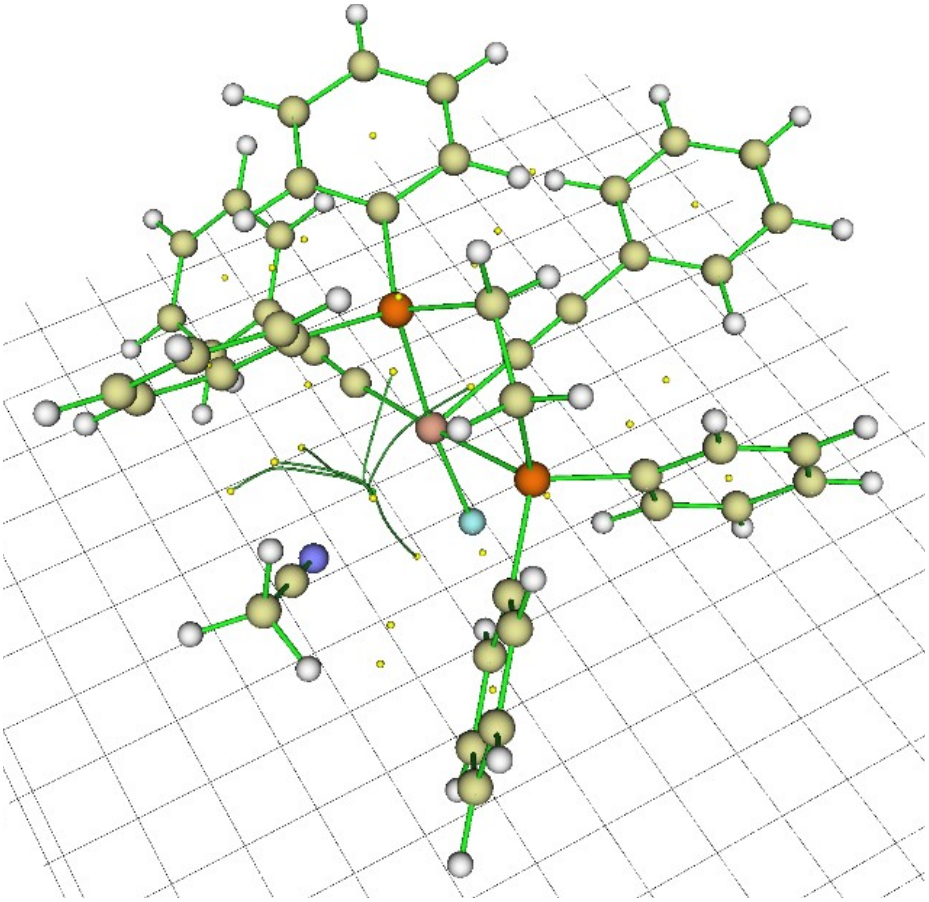
A) TS_{diss} of $[(bipy)Pt(C{\equiv}CPh)_2F]^+$



B) **2** of $[(dppe)Pt(C{\equiv}CPh)_2F]^+$



C) TS_{diss} of $[(dppe)Pt(C{\equiv}CPh)_2F]^+$



D) The cage critical point for the $[(dppe)Pt(C{\equiv}CPh)_2F]^+$ complex which exists between acetonitrile and the ring critical points associated with the groups in dppe ligand.

Figure S18. AIM topological analysis diagrams for A) TS_{diss} of $[(bipy)Pt(C{\equiv}CPh)_2F]^+$ complex; B) **2** of $[(dppe)Pt(C{\equiv}CPh)_2F]^+$ complex; C)TS_{diss} of $[(dppe)Pt(C{\equiv}CPh)_2F]^+$ complex; and D) Cage critical point for the TS_{diss} of $[(dppe)Pt(C{\equiv}CPh)_2F]^+$ complex.

B4. XYZ Cartesian coordinates of stereoisomers

A_{bipy}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.692097 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.245865 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.343965 hartrees

C	4.35730100	-1.37180400	-1.72627500
C	4.98020000	-1.52476700	-0.48774700
C	4.22634500	-1.45008300	0.68449300
C	2.85414600	-1.22136300	0.59235200
C	2.98468700	-1.14432500	-1.75798800
C	1.93315800	-1.11631900	1.74179500
C	2.32771900	-1.24883700	3.07142700
C	1.38279000	-1.12948500	4.08919000
H	1.68842000	-1.23059600	5.12480000
C	0.05181900	-0.87904500	3.76281200
C	-0.29926400	-0.75522900	2.42417200
H	4.91646400	-1.42444100	-2.65284600
H	6.04880200	-1.70087400	-0.42852000
H	2.41504700	-1.01044800	-2.67094700
H	-0.71274300	-0.77735700	4.52369400
H	-1.31302900	-0.55829100	2.10057700
H	3.36479000	-1.44314300	3.31267300
H	4.70650700	-1.56699300	1.64757400
N	0.62003600	-0.87663600	1.45188700
N	2.27701200	-1.07622500	-0.62512200
Pt	0.19661000	-0.70615600	-0.55728300
C	-1.74156300	-0.35041300	-0.38750300
C	-2.92943400	-0.12828100	-0.24554200
C	-4.32635600	0.12544700	-0.08214400

C	-5.15958400	0.29267100	-1.20649700
C	-4.89196500	0.21409900	1.20575600
C	-6.52111800	0.54213200	-1.04276400
H	-4.72926000	0.22552100	-2.20122300
C	-6.25453500	0.46354800	1.36051300
H	-4.25581200	0.08646700	2.07664200
C	-7.07344700	0.62833200	0.23902900
H	-7.15239100	0.66957400	-1.91768600
H	-6.67815100	0.52962500	2.35874100
H	-8.13495300	0.82277300	0.36317900
F	0.07655300	-0.61280800	-2.52198800
C	1.10431400	3.78374900	-0.22714900
C	2.44474800	4.21810500	-0.21611200
C	2.74317500	5.57436300	-0.09666100
C	1.71467300	6.51547900	0.01328700
C	0.38164600	6.09304500	0.00363900
C	0.07422900	4.73865400	-0.11528200
H	3.24160000	3.48528200	-0.30160300
H	3.78037600	5.89746400	-0.08955600
H	1.95058400	7.57176600	0.10613700
H	-0.42085200	6.82031000	0.08892500
H	-0.96014300	4.40819000	-0.12277500
C	0.79574000	2.39327800	-0.34600700
C	0.53299800	1.21277600	-0.45862100
N	-0.14859600	-2.83277800	-0.67383200
C	-0.32919600	-3.97187200	-0.70319400
C	-0.55832000	-5.40592900	-0.74695800
H	0.40204100	-5.92973100	-0.73921100
H	-1.14581300	-5.70817100	0.12489600
H	-1.10460600	-5.65958900	-1.66017500

A_{dppe}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2655.324269 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.593726 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.726584 hartrees

P	2.48094000	-0.02883000	0.29603000
P	-0.51591900	-0.48022500	1.54758500
C	0.83509600	0.31293500	2.52644300
H	0.76994400	1.38579500	2.32494500
H	0.65164200	0.16931700	3.59521400
C	2.21440200	-0.22944000	2.11536500
H	2.99869200	0.26409800	2.69465100
H	2.28794900	-1.30237600	2.31861500
C	3.16153500	1.61263200	-0.07641900
C	3.04631000	2.06328600	-1.40352000
C	3.81791900	2.39569000	0.88201100
C	3.60365300	3.28869300	-1.76349700
H	2.50293300	1.46360100	-2.12814200
C	4.36259900	3.62810300	0.51217200
H	3.91291400	2.06334000	1.91030600
C	4.26150500	4.07161200	-0.80853700
H	3.51336000	3.63944200	-2.78724600
H	4.86538300	4.23718300	1.25725100
H	4.68720100	5.02967900	-1.09217600
C	3.69033300	-1.27530000	-0.23586800
C	4.59425900	-1.85556400	0.66609700
C	3.69969900	-1.64987100	-1.59065600
C	5.49798000	-2.81931500	0.21406200
H	4.60229100	-1.56702200	1.71255300

C	4.60862500	-2.61209500	-2.03075400
H	2.97484500	-1.21556800	-2.27350900
C	5.50452800	-3.19900100	-1.13053500
H	6.19369400	-3.27247900	0.91377000
H	4.61047100	-2.91029200	-3.07496200
H	6.20600100	-3.95227400	-1.47703500
C	-2.07171100	0.39153000	1.86702100
C	-3.28740500	-0.31067600	1.81980700
C	-2.07478100	1.77626500	2.10643200
C	-4.49045000	0.36950700	2.00257100
H	-3.30492500	-1.37885100	1.64086300
C	-3.28284900	2.44679700	2.29083300
H	-1.15331500	2.34314700	2.13481800
C	-4.49123000	1.74743200	2.23340900
H	-5.42578400	-0.17889600	1.95493500
H	-3.27444600	3.51748200	2.46871200
H	-5.43075600	2.27467900	2.36940000
C	-0.68419800	-2.21696400	2.03800100
C	-0.10211200	-2.69027500	3.22429900
C	-1.40179300	-3.09708500	1.20818000
C	-0.23199400	-4.03627200	3.57092200
H	0.44800700	-2.02850800	3.88402500
C	-1.53545200	-4.43612100	1.56953700
H	-1.83497600	-2.74088500	0.27865700
C	-0.94585400	-4.90843100	2.74665100
H	0.22605800	-4.39870500	4.48583600
H	-2.09114500	-5.11118600	0.92618400
H	-1.04253300	-5.95500900	3.01923400
Pt	0.28131900	-0.36693900	-0.66413300
F	1.09162000	-0.16454000	-2.56618600

C	-1.59965700	-0.64530600	-1.34667500
C	-2.77813500	-0.80749600	-1.61476500
C	-4.17008200	-0.98023000	-1.88220100
C	-5.09723800	-0.01426800	-1.43922700
C	-4.64443300	-2.11771200	-2.56525900
C	-6.46017800	-0.18702600	-1.67295700
H	-4.73704800	0.85876600	-0.90475800
C	-6.00933000	-2.28214100	-2.79636100
H	-3.93514300	-2.86554800	-2.90753100
C	-6.92132700	-1.31956800	-2.35179800
H	-7.16397100	0.56335600	-1.32351400
H	-6.36246900	-3.16399100	-3.32366400
H	-7.98434200	-1.45165100	-2.53265600
C	-0.06765400	1.55449600	-0.55658900
C	-0.25468100	2.74593800	-0.40766600
C	-0.45596500	4.13988000	-0.17859400
C	-1.75723500	4.67962000	-0.13734800
C	0.64794600	4.98732000	0.04422600
C	-1.94560000	6.03657600	0.12055000
H	-2.60839600	4.02587600	-0.30031600
C	0.44929800	6.34311100	0.29816200
H	1.64987200	4.57208900	0.01806700
C	-0.84506100	6.87200300	0.33752400
H	-2.95269700	6.44275300	0.15211000
H	1.30693200	6.98814000	0.46807700
H	-0.99556400	7.92910200	0.53756700
N	0.72038200	-2.43505800	-0.85190600
C	1.09700300	-3.52285400	-0.91313100
C	1.58996300	-4.88636000	-0.96159200
H	1.23806200	-5.42692100	-0.07754500

H	1.22386800	-5.38295600	-1.86451500
H	2.68444000	-4.86569800	-0.97303400

B_{bipy}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.684693 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.237448 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.336531 hartrees

C	-3.22645400	-3.50370800	-0.30100700
C	-4.48512500	-2.90990200	-0.37125200
C	-4.59084300	-1.51978600	-0.36680600
C	-3.43411900	-0.74302300	-0.29083900
C	-2.10664100	-2.68202400	-0.23151400
C	-3.43643000	0.73693600	-0.27163200
C	-4.59670900	1.51153900	-0.30255700
C	-4.49470000	2.90176800	-0.28048500
H	-5.39316300	3.50900900	-0.30417700
C	-3.23629200	3.49788500	-0.22690300
C	-2.11328600	2.67828800	-0.19399500
H	-3.10375400	-4.58027600	-0.30161300
H	-5.38088800	-3.51879800	-0.42956300
H	-1.09761700	-3.07380600	-0.17968100
H	-3.11641500	4.57461700	-0.20869300
H	-1.10458000	3.07188100	-0.15014900
H	-5.57166500	1.04343300	-0.34027600
H	-5.56566100	-1.05335400	-0.42428000
N	-2.22066700	1.34171500	-0.21614200
N	-2.21759500	-1.34557300	-0.22818100
Pt	-0.54846500	-0.00030500	-0.17186500
F	-0.57353800	0.00182800	-2.11574000

C	0.86863100	-1.37445900	-0.18167500
C	1.71618400	-2.24638700	-0.16774400
C	2.71338000	-3.27015300	-0.15596700
C	4.08116700	-2.93074100	-0.14187900
C	2.34671200	-4.63064700	-0.15470000
C	5.05345300	-3.92931500	-0.12669200
H	4.36889600	-1.88354000	-0.14280200
C	3.32556300	-5.62286900	-0.13924300
H	1.29430000	-4.89848600	-0.16559700
C	4.68042100	-5.27701900	-0.12520700
H	6.10456500	-3.65492500	-0.11590700
H	3.03018600	-6.66834000	-0.13818900
H	5.44067300	-6.05281600	-0.11318100
C	0.86581600	1.37671800	-0.18123700
C	1.71217400	2.24987800	-0.17411000
C	2.70836200	3.27469700	-0.17258900
C	4.07652500	2.93653200	-0.16640400
C	2.34050200	4.63485600	-0.17572800
C	5.04801300	3.93598500	-0.16371400
H	4.36515600	1.88958100	-0.16400000
C	3.31857300	5.62797300	-0.17284300
H	1.28781100	4.90176600	-0.18050400
C	4.67380300	5.28336000	-0.16690900
H	6.09941700	3.66254200	-0.15918000
H	3.02228400	6.67318300	-0.17541400
H	5.43343600	6.05985400	-0.16486500
N	-0.58987200	-0.00190500	1.83731800
C	-0.62388300	-0.00064900	2.98910400
C	-0.67183800	0.00114300	4.43938100
H	-1.19895100	-0.89273800	4.78575700

H	0.34765100	0.00251900	4.83600900
H	-1.20040000	0.89512100	4.78331900

B_{dppe}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2655.300334 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.570184 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.704111 hartrees

P	1.63614500	-1.44080700	0.84348700
P	-1.65721000	-1.37222100	0.89222900
C	-0.72508800	-2.30402700	2.18795600
H	-0.63580700	-1.59913000	3.02059200
H	-1.31833700	-3.15244000	2.54355400
C	0.65483000	-2.77483400	1.70056600
H	1.24195900	-3.16046000	2.53874800
H	0.53766400	-3.58474600	0.97641400
C	2.81422100	-0.73503400	2.03013900
C	4.18555400	-0.68043100	1.73762300
C	2.33303400	-0.20808600	3.24149400
C	5.06813600	-0.10332700	2.65269400
H	4.56683600	-1.08239600	0.80535200
C	3.22383200	0.36056300	4.15051700
H	1.27252500	-0.20920700	3.45780700
C	4.58979400	0.41667900	3.85764700
H	6.12841500	-0.06369100	2.42149400
H	2.84873200	0.76562900	5.08561300
H	5.27909100	0.86490000	4.56715600
C	2.57225600	-2.21310600	-0.50887200
C	2.79838200	-3.59780600	-0.55548900
C	3.08118400	-1.38963400	-1.52928300

C	3.50494900	-4.15295400	-1.62372600
H	2.43930300	-4.25141100	0.23202300
C	3.78930700	-1.95264800	-2.59069600
H	2.91810900	-0.31742600	-1.49573300
C	3.99563400	-3.33474100	-2.64349700
H	3.67121200	-5.22533400	-1.65491100
H	4.17579000	-1.31080800	-3.37658700
H	4.54095300	-3.77116600	-3.47496100
C	-3.12486200	-0.64312200	1.67205700
C	-4.39715900	-1.19327600	1.45036300
C	-2.97699800	0.47811700	2.50686800
C	-5.51491300	-0.62446200	2.06433100
H	-4.52110400	-2.05373500	0.80161800
C	-4.10020900	1.03662000	3.11455000
H	-1.99580000	0.91216800	2.65688700
C	-5.36812200	0.48940500	2.89421300
H	-6.49782800	-1.05091100	1.88841700
H	-3.98570900	1.90707200	3.75357500
H	-6.24040100	0.93400300	3.36430100
C	-2.21597700	-2.48475600	-0.42125500
C	-2.04340500	-3.87443000	-0.36654200
C	-2.81046400	-1.89373400	-1.55152100
C	-2.44925100	-4.66671900	-1.44306700
H	-1.60514000	-4.34925500	0.50481200
C	-3.22153900	-2.69236800	-2.61679200
H	-2.93992300	-0.81530900	-1.59726700
C	-3.03419900	-4.07877900	-2.56627900
H	-2.31026400	-5.74244300	-1.39881100
H	-3.68222000	-2.23375900	-3.48643600
H	-3.34791800	-4.69817800	-3.40115600

Pt	-0.00108700	0.19536700	0.08237800
C	-1.48678100	1.46966500	-0.43800600
C	-2.48008900	2.12706600	-0.69315900
C	-3.69800400	2.83795800	-0.92277400
C	-4.90568900	2.32535900	-0.40444200
C	-3.72449800	4.04476100	-1.64824700
C	-6.10405600	3.00639400	-0.60802800
H	-4.88887100	1.39676600	0.15669500
C	-4.92853700	4.71939100	-1.84820200
H	-2.79780400	4.44522700	-2.04881400
C	-6.12086900	4.20480500	-1.32943200
H	-7.02662200	2.60133000	-0.20102900
H	-4.93612200	5.64970700	-2.40947000
H	-7.05652200	4.73415200	-1.48640300
N	0.02550600	-0.56173200	-1.76048700
C	0.08258800	-1.07743000	-2.78876600
C	0.16621900	-1.76994000	-4.05920300
H	0.05608600	-1.05711200	-4.88107800
H	1.14135300	-2.26340700	-4.12523000
H	-0.63304100	-2.51636600	-4.10735800
C	1.48822000	1.48840400	-0.39977600
C	2.44482400	2.20959800	-0.62347800
F	-0.00508700	0.91539200	1.92474200
C	3.60987400	3.00803100	-0.84290000
C	3.62162200	4.03468200	-1.80750200
C	4.77833400	2.76505500	-0.09132800
C	4.77218500	4.79488500	-2.01360700
H	2.72520700	4.22722500	-2.38965900
C	5.92375000	3.52998500	-0.30297000
H	4.77425500	1.97463400	0.65337600

C	5.92603100	4.54654100	-1.26372200
H	4.76802400	5.58340000	-2.76109600
H	6.81706600	3.33191500	0.28313100
H	6.82058500	5.14099700	-1.42683000

C_{bipy}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.683010 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.235624 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.335692 hartrees

C	-4.49612400	-1.37644600	1.55527300
C	-5.10624500	-1.54306100	0.31347300
C	-4.33011200	-1.51093500	-0.84458300
C	-2.95416100	-1.31336900	-0.73500800
C	-3.11910600	-1.18191400	1.60134300
C	-2.02763400	-1.25001000	-1.87897600
C	-2.41951600	-1.38696400	-3.20901700
C	-1.47067000	-1.29739900	-4.22521900
H	-1.77549200	-1.40199000	-5.26067100
C	-0.13661900	-1.07051800	-3.89597200
C	0.21396800	-0.94284100	-2.55837200
H	-5.06676100	-1.39393200	2.47614000
H	-6.17753000	-1.69564200	0.24091900
H	-2.58846600	-1.04436700	2.53472400
H	0.63332100	-0.99055000	-4.65392900
H	1.23116000	-0.76693100	-2.23565800
H	-3.45962000	-1.56041800	-3.45198900
H	-4.79619200	-1.63727200	-1.81314100
N	-0.71121500	-1.03674800	-1.58621000
N	-2.38157800	-1.15512000	0.48415000

Pt	-0.27160600	-0.89270500	0.38841700
F	-0.10649800	-2.90254000	0.44428800
C	1.67911100	-0.69585900	0.14524700
C	2.87745600	-0.55561900	-0.00590100
C	4.28320400	-0.38547900	-0.20025400
C	4.78693600	0.82742900	-0.71149000
C	5.18424400	-1.42136100	0.11596100
C	6.15761300	0.99578500	-0.89992900
H	4.09546000	1.62824700	-0.95617000
C	6.55370200	-1.24441800	-0.07517700
H	4.80079000	-2.35784100	0.50981800
C	7.04487500	-0.03759200	-0.58282300
H	6.53410000	1.93533800	-1.29455800
H	7.23894700	-2.05018600	0.17253200
H	8.11267000	0.09681700	-0.73039600
C	-0.48619800	1.08096500	0.29372300
C	-0.64252800	2.28279400	0.19237900
C	-0.82511300	3.69578400	0.07784600
C	-2.10077600	4.23383600	-0.18546300
C	0.26867000	4.57260200	0.22300000
C	-2.27367200	5.61223900	-0.30013600
H	-2.94693300	3.56249900	-0.29833100
C	0.08725400	5.94983300	0.10729700
H	1.25398800	4.16304000	0.42498100
C	-1.18239100	6.47448500	-0.15426000
H	-3.26218800	6.01448700	-0.50359700
H	0.93860900	6.61506700	0.22124600
H	-1.32045800	7.54824600	-0.24394500
N	0.04570900	-0.82370500	2.38511300
C	0.26765500	-0.76641700	3.51472000

C	0.53590200	-0.70264800	4.93926100
H	-0.22346700	-0.08153000	5.42352000
H	1.52544100	-0.26511600	5.10136600
H	0.50762500	-1.71250100	5.35897500

C_{dppe}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2655.318122 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.587984 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.723470 hartrees

Pt	-0.27075300	-0.58138000	0.59031800
F	-0.53193900	-2.58274200	0.94295400
C	1.59759500	-0.76538100	1.32169800
C	2.75239300	-0.86254800	1.69805800
C	4.12026900	-0.95800100	2.09607700
C	5.02180100	0.07913800	1.77858300
C	4.59851700	-2.08687100	2.79093800
C	6.36313000	-0.01595200	2.14522200
H	4.65962300	0.94780400	1.23806700
C	5.94132800	-2.17381000	3.15490800
H	3.90951100	-2.88925500	3.03777100
C	6.82789200	-1.14089600	2.83400200
H	7.04708200	0.78955900	1.89251800
H	6.29720100	-3.05012300	3.68958400
H	7.87383900	-1.21239600	3.11864900
C	0.01506300	1.36603600	0.40007800
C	0.22950400	2.55261300	0.24321500
C	0.49901500	3.93661500	0.02244100
C	-0.55402000	4.84790400	-0.19073800
C	1.82813400	4.40602200	-0.00702900

C	-0.28048700	6.19421100	-0.42609100
H	-1.57703200	4.48880900	-0.17150000
C	2.09228800	5.75364500	-0.24551800
H	2.64163400	3.70480700	0.14915600
C	1.04077800	6.65194100	-0.45473400
H	-1.10107000	6.88753600	-0.58910300
H	3.12063600	6.10355400	-0.26775100
H	1.25008600	7.70180300	-0.63965300
P	-2.47720800	-0.34905800	-0.43537600
C	-2.12341100	-0.70675200	-2.21467400
C	-3.13069900	1.34594300	-0.33257200
C	-3.81098200	-1.44353600	0.13011500
C	-0.80069700	-0.03858900	-2.61787100
H	-2.94573400	-0.37128100	-2.85228500
H	-2.06405600	-1.79608700	-2.31109300
C	-3.42328600	2.11578900	-1.46669700
C	-3.36973300	1.87662500	0.94664300
C	-3.50067300	-2.66770200	0.74471400
C	-5.15153500	-1.07260400	-0.07558100
P	0.57898600	-0.70801600	-1.58565700
H	-0.84624100	1.04261100	-2.46071600
H	-0.55929800	-0.23056000	-3.66760700
C	-3.95972900	3.39795000	-1.32117300
H	-3.24646700	1.73509400	-2.46649200
C	-3.90946900	3.15283800	1.08569200
H	-3.13596500	1.29494700	1.83208900
C	-4.53558600	-3.51627000	1.14259200
H	-2.46266900	-2.93263200	0.91562300
C	-6.17465600	-1.93158300	0.32330000
H	-5.39600400	-0.12110900	-0.53743100

C	2.07389200	0.27096200	-1.84918900
C	0.90181300	-2.38103200	-2.21077000
C	-4.20837100	3.91523400	-0.04882200
H	-4.18323300	3.98734200	-2.20508700
H	-4.09337500	3.55378000	2.07775600
C	-5.86793300	-3.15262500	0.93214500
H	-4.29793000	-4.46145900	1.62212600
H	-7.20977000	-1.64494200	0.16313200
C	2.01043800	1.58634100	-2.33358100
C	3.31549000	-0.29838800	-1.51734700
C	1.67768200	-2.48439900	-3.38294400
C	0.30107800	-3.52378700	-1.65953900
H	-4.62702700	4.91122300	0.06058700
H	-6.66839800	-3.81662000	1.24580000
C	3.18468800	2.32201800	-2.49080500
H	1.06235600	2.05124400	-2.57419900
C	4.48245600	0.44641200	-1.67356000
H	3.37036200	-1.31038800	-1.13274500
C	1.84648800	-3.72567600	-3.99246200
H	2.14903000	-1.60904000	-3.81780300
C	0.48236300	-4.76066500	-2.28245500
H	-0.26157400	-3.44758000	-0.73714600
C	4.41813300	1.75621700	-2.15819600
H	3.13009300	3.34089100	-2.86026800
H	5.43760100	0.00614100	-1.40633900
C	1.24911700	-4.86467300	-3.44412000
H	2.44735100	-3.80122200	-4.89354700
H	0.02339100	-5.64510400	-1.85078600
H	5.32887300	2.33609800	-2.27461200
H	1.38572100	-5.83054600	-3.92162200

N	-1.10742800	-0.36722400	2.59045300
C	-1.54786100	-0.31580400	3.65615700
C	-2.11463900	-0.25141600	4.99320900
H	-3.19396900	-0.42168200	4.93879300
H	-1.92233600	0.73491400	5.42507700
H	-1.65617700	-1.02006800	5.62208100

D_{bipy}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.671326 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.223855 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.324338 hartrees

C	0.01015400	-0.00713300	3.92274100
C	0.01445900	1.38005400	4.05600300
C	0.01299300	2.18020100	2.91444900
C	0.00730200	1.57946600	1.65827900
C	0.00475800	-0.56051300	2.64740400
C	0.00474900	2.30434200	0.38022200
C	0.00589700	3.68896300	0.23307100
C	0.00242200	4.23997600	-1.04819400
H	0.00320200	5.31736700	-1.17062000
C	-0.00209600	3.40197300	-2.16286600
C	-0.00305300	2.02533300	-1.97119800
H	0.01102200	-0.66191600	4.78571700
H	0.01890000	1.83966900	5.03807000
H	0.00149600	-1.62877400	2.47997900
H	-0.00492100	3.79748300	-3.17128900
H	-0.00628800	1.29864200	-2.77417200
H	0.00913000	4.33036900	1.10492300
H	0.01628600	3.25898700	3.00284400

N	0.00032200	1.51905600	-0.73009500
N	0.00349400	0.22062800	1.55811400
Pt	-0.00113500	-0.46031400	-0.37811900
C	2.03803800	-0.43580200	-0.38531800
C	3.25378300	-0.35410600	-0.35848600
C	4.67949100	-0.25921600	-0.33115200
C	5.30760600	0.95760000	0.00439600
C	5.48336700	-1.37610000	-0.63677800
C	6.69809600	1.05086200	0.03221600
H	4.69481500	1.82253100	0.24118400
C	6.87341500	-1.27509100	-0.60691700
H	5.00734400	-2.31707900	-0.89643100
C	7.48622700	-0.06331800	-0.27293000
H	7.16779100	1.99540300	0.29257500
H	7.47999200	-2.14451900	-0.84506900
H	8.56970900	0.01215700	-0.25054300
N	-0.00357000	-2.45774000	0.00806800
C	-0.00685500	-3.59672500	0.18406500
C	-0.01117400	-5.03018000	0.41119300
H	0.78751800	-5.28896500	1.11250900
H	0.15496200	-5.54662600	-0.53890400
H	-0.97766100	-5.32958400	0.82711300
C	-2.04036300	-0.43247200	-0.38199900
C	-3.25602700	-0.34937400	-0.35496900
C	-4.68182200	-0.25501100	-0.33047800
C	-5.32240600	0.96893100	-0.61205300
C	-5.47344200	-1.37978100	-0.02155100
C	-6.71297400	1.06138200	-0.58460000
H	-4.71933500	1.84007800	-0.85089700
C	-6.86361400	-1.27956800	0.00400600

H	-4.98777600	-2.32638000	0.19657300
C	-7.48881700	-0.06067800	-0.27688700
H	-7.19235400	2.01144700	-0.80397000
H	-7.46059400	-2.15519800	0.24369100
H	-8.57237500	0.01420000	-0.25631000
F	-0.00386300	-0.88360900	-2.31070500

D_{dppe}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2655.319352 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.588904 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.720456 hartrees

Pt	0.04656200	-0.01177600	0.78443000
C	-1.97582500	-0.11790500	0.88701100
C	-3.19380800	-0.15456500	0.86946700
C	-4.61755100	-0.19075000	0.80558700
C	-5.33862700	-1.29881400	1.29517300
C	-5.32746600	0.88083600	0.22478300
C	-6.72947400	-1.33136200	1.20499900
H	-4.79814400	-2.12705400	1.74354800
C	-6.71790400	0.84017600	0.13920800
H	-4.77768200	1.73598100	-0.15491800
C	-7.42448800	-0.26387500	0.62770600
H	-7.27234400	-2.19211700	1.58594900
H	-7.25194300	1.67305300	-0.31033100
H	-8.50836600	-0.29221600	0.55915000
P	0.21150500	-1.41448800	-1.10422600
C	0.70583000	-0.21900800	-2.41589200
C	-1.36635200	-2.17957600	-1.56357600
C	1.45592900	-2.72321800	-0.93902300

C	-0.21923700	1.00714400	-2.35136800
H	0.67703200	-0.68889100	-3.40185400
H	1.74225400	0.06475800	-2.21357300
C	-1.82704600	-2.14376200	-2.88906600
C	-2.12498000	-2.83419000	-0.57774100
C	2.81166500	-2.45750700	-1.19572200
C	1.06944600	-3.99903300	-0.49185600
P	-0.15073400	1.78244100	-0.67824600
H	-1.26237200	0.72246500	-2.52049900
H	0.04796000	1.73273100	-3.12270300
C	-3.03793700	-2.75570000	-3.21946300
H	-1.26079700	-1.64907400	-3.67028300
C	-3.32360900	-3.45549000	-0.91983100
H	-1.79786300	-2.83693200	0.45523200
C	3.76530600	-3.45505600	-0.99963500
H	3.13659900	-1.48148000	-1.53116300
C	2.03267300	-4.98668400	-0.28672400
H	0.02631600	-4.23453200	-0.31478400
C	-1.64139600	2.77335100	-0.41278100
C	1.27286500	2.89942000	-0.55182900
C	-3.78425200	-3.41166500	-2.23895700
H	-3.39278600	-2.71785800	-4.24463500
H	-3.90502100	-3.95662800	-0.15273400
C	3.38089800	-4.71547000	-0.53517500
H	4.80962900	-3.23785600	-1.19999300
H	1.72530300	-5.96907000	0.05858900
C	-2.38440000	3.23043900	-1.51074500
C	-1.99986100	3.13599600	0.89625000
C	1.65282700	3.33970000	0.72841300
C	1.93756400	3.37213500	-1.69170800

H	-4.72591600	-3.88509100	-2.50022000
H	4.12857600	-5.48619300	-0.37395400
C	-3.49207100	4.05389700	-1.29507200
H	-2.11414500	2.96095400	-2.52650400
C	-3.10537700	3.95954100	1.09558200
H	-1.43615900	2.74252800	1.73566900
C	2.68923900	4.26055900	0.85543400
H	1.16194400	2.92869300	1.60473400
C	2.97953400	4.29215700	-1.54929600
H	1.66290800	3.04198200	-2.68727500
C	-3.85121400	4.41876200	0.00417900
H	-4.07139900	4.40475000	-2.14349100
H	-3.39288300	4.23445600	2.10589700
C	3.35215200	4.73935400	-0.28040900
H	2.98829200	4.59745000	1.84336600
H	3.49680000	4.65414800	-2.43241400
H	-4.71553300	5.05562400	0.16771700
H	4.16300800	5.45397200	-0.17465700
N	0.25291400	-1.71319300	2.11247600
C	0.49421500	-2.67803200	2.69876000
C	0.80966400	-3.90422700	3.41131100
H	1.29824200	-4.59707100	2.71879900
H	-0.10880600	-4.35737400	3.79487700
H	1.48461800	-3.68364400	4.24320800
C	2.07603800	0.12106600	0.72501400
C	3.28672300	0.19331400	0.60084500
C	4.69877600	0.26612400	0.41049900
C	5.28362700	1.42135300	-0.14789500
C	5.52763200	-0.82452200	0.74477100
C	6.65962100	1.47975400	-0.36195000

H	4.64920600	2.26141700	-0.41089400
C	6.90281500	-0.75795400	0.52547100
H	5.08120700	-1.71901500	1.16801900
C	7.47395900	0.39286000	-0.02720400
H	7.09766500	2.37593200	-0.79296200
H	7.52997400	-1.60604000	0.78626800
H	8.54589800	0.44174300	-0.19683000
F	0.00090900	1.30106400	2.38717500

B5. XYZ Cartesian coordinates of Reactant and Products in path I

II_{bipy}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.671326 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.223855 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.324338 hartrees

C	4.71109000	-1.55164700	-0.07502500
C	3.76268300	-2.47671400	-0.50420700
C	2.51468200	-2.49492300	0.12048400
C	2.26324900	-1.56850500	1.13803900
C	4.37771000	-0.69959400	0.98314300
C	0.95966300	-1.53577000	1.85475800
C	0.96030400	-1.61520300	3.24975700
C	-0.23643700	-1.66544400	3.95445500
H	-0.23477100	-1.73271400	5.03720500
C	-1.43438700	-1.64378800	3.24112500
C	-1.38913700	-1.52986400	1.86213600
H	5.69294000	-1.49523200	-0.53286900
H	3.98620200	-3.17829500	-1.30164800
H	5.09763800	0.02628600	1.35312400
H	-2.39746400	-1.69688800	3.73494500
H	-2.29732000	-1.46812700	1.28038800
H	1.91698400	-1.65169000	3.75626800
H	1.75794000	-3.21927400	-0.16788100
N	-0.21930200	-1.46254000	1.17844000
N	3.18768300	-0.70585700	1.59144300
Pt	-0.38009300	-1.02285500	-0.88481400

C	-1.70385200	0.31964000	-0.49621700
C	-2.47693800	1.20677000	-0.20353900
C	-3.40273600	2.22921900	0.16678200
C	-3.99036200	3.05563700	-0.81048500
C	-3.72280300	2.42762700	1.52453000
C	-4.87755200	4.06162700	-0.43189100
H	-3.74372500	2.90355800	-1.85677100
C	-4.61101500	3.43627300	1.89234300
H	-3.26892000	1.78960600	2.27688500
C	-5.18968700	4.25529600	0.91742300
H	-5.32501100	4.69644400	-1.19120400
H	-4.85106200	3.58452400	2.94124200
H	-5.88037700	5.04161900	1.20808500
F	-0.57337300	-0.66102800	-2.79340000
C	2.68651800	2.37014000	-0.53522200
C	3.30933500	2.60415700	0.70846400
C	4.27031800	3.60498900	0.83033600
C	4.62227200	4.38365400	-0.27764300
C	4.00696500	4.15862000	-1.51325400
C	3.04450500	3.15961200	-1.64623300
H	3.04258000	1.98211000	1.55644300
H	4.74837300	3.77677000	1.79051000
H	5.37391400	5.16161600	-0.17876300
H	4.27897800	4.76120700	-2.37506800
H	2.56597100	2.97948000	-2.60404500
C	1.71414900	1.33562700	-0.66219600
C	0.92572700	0.41268500	-0.74914500
N	-1.83234200	-2.59949100	-1.09399100
C	-2.66379000	-3.39238500	-1.20905300
C	-3.71126800	-4.38804300	-1.35246600
H	-4.60572700	-3.91641700	-1.77015700
H	-3.37075300	-5.18256400	-2.02286600
H	-3.94624300	-4.81301500	-0.37215300

$TS_{II,bipy}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.633417 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.188835 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.288271 hartrees

C	4.58293000	-1.70511200	0.11335300
C	3.63136400	-2.65744700	-0.24576400

C	2.36788500	-2.59735700	0.34363900
C	2.10680200	-1.57216900	1.25899300
C	4.23534800	-0.74430800	1.06781000
C	0.78429500	-1.44874200	1.93095900
C	0.72945900	-1.41128300	3.32622500
C	-0.49621600	-1.35108400	3.97958400
H	-0.54032100	-1.32852100	5.06334500
C	-1.66437200	-1.32908400	3.21708000
C	-1.55972100	-1.33411400	1.83620500
H	5.57653100	-1.70749200	-0.32220900
H	3.86447100	-3.43725800	-0.96388100
H	4.95427500	0.01015100	1.37784000
H	-2.64593800	-1.29006200	3.67440000
H	-2.43666600	-1.27249800	1.20653200
H	1.66264300	-1.44203300	3.87540500
H	1.60325100	-3.33057600	0.10438800
N	-0.36256700	-1.38920600	1.20404900
N	3.03011200	-0.67586600	1.64354700
Pt	-0.41610300	-1.11476500	-0.87801700
C	-1.26304600	0.64023800	-0.57414100
C	-2.09367100	1.48907300	-0.29923900
C	-3.04452300	2.48379500	0.06265200
C	-3.66024700	3.29093900	-0.91556700
C	-3.37893100	2.66823800	1.42107100
C	-4.58854100	4.25895200	-0.53811700
H	-3.40439400	3.15072300	-1.96127700
C	-4.30832100	3.63915500	1.78616300
H	-2.90596600	2.04473900	2.17396800
C	-4.91527000	4.43682000	0.81024000
H	-5.05833600	4.87674500	-1.29803500

H	-4.56000200	3.77417900	2.83418400
H	-5.63928500	5.19317700	1.09915900
F	-0.48149300	-0.90351800	-2.82029600
C	2.61788200	2.30189200	-0.59736900
C	3.22638700	2.56926000	0.64967200
C	4.22826600	3.53049800	0.74149700
C	4.63447100	4.23682900	-0.39684600
C	4.03539000	3.97852800	-1.63481600
C	3.03345000	3.01796900	-1.74109000
H	2.91545300	2.00080500	1.51962900
H	4.69576500	3.73007500	1.70122800
H	5.41714700	4.98593600	-0.31952300
H	4.35140800	4.52652000	-2.51751600
H	2.56475900	2.81141100	-2.69817200
C	1.59944500	1.32268200	-0.69225800
C	0.70889800	0.48343500	-0.74450300
N	-1.81825700	-2.73441300	-1.04981200
C	-2.60748700	-3.57265600	-1.14139500
C	-3.60755300	-4.61980200	-1.25798200
H	-4.52221000	-4.20253800	-1.68959100
H	-3.22932800	-5.41599500	-1.90585800
H	-3.82506800	-5.02861000	-0.26685200
C	4.71109000	-1.55164700	-0.07502500

III_{bipy}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.727762 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.281619 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.380837 hartrees

C	4.60958600	-0.87195100	1.10110900
C	3.79939500	-1.75200800	0.38636500

C	2.42644400	-1.74881000	0.62892000
C	1.91833000	-0.84894100	1.57394200
C	4.01040400	-0.03687100	2.04708200
C	0.46682600	-0.79490800	1.89769200
C	0.05975900	-0.83906300	3.23447700
C	-1.29258600	-0.83320000	3.55616600
H	-1.61170700	-0.87281200	4.59245000
C	-2.22818600	-0.78660400	2.52191100
C	-1.77267100	-0.71430500	1.21522600
H	5.68052800	-0.82909900	0.93505400
H	4.22485200	-2.43169700	-0.34515400
H	4.61343300	0.65565100	2.62950300
H	-3.29466200	-0.78732100	2.71456200
H	-2.46200100	-0.63569600	0.38409500
H	0.82331000	-0.88561800	4.00131000
H	1.76724200	-2.43475200	0.10926600
N	-0.45476100	-0.70647900	0.90314000
N	2.69545500	-0.02128500	2.29324900
Pt	0.01149200	-0.31254100	-1.08799800
C	-1.13339100	2.42877000	0.11838500
C	-2.20968100	2.83520600	0.53895600
C	-3.45274700	3.27264900	1.05241100
C	-4.30002900	4.09299000	0.27557800
C	-3.85766100	2.86940200	2.34486200
C	-5.52710200	4.50153900	0.78866300
H	-3.98440100	4.39794200	-0.71688200
C	-5.08971400	3.28119200	2.84275000
H	-3.20344700	2.23463500	2.93392100
C	-5.92323200	4.09668100	2.06846400
H	-6.17723300	5.13361400	0.19160300
H	-5.40212100	2.96832500	3.83433100
H	-6.88331600	4.41653100	2.46274100
F	0.40622500	0.08112700	-2.98202100
C	2.55884600	1.59920600	-0.88499500
C	3.26873600	2.48808100	-0.05582700
C	4.63653300	2.66700000	-0.24612900
C	5.30313200	1.96704700	-1.25721300
C	4.59659400	1.08981600	-2.08584700
C	3.22881300	0.89956300	-1.90390400
H	2.74635500	3.01426300	0.73664600
H	5.18356800	3.34779400	0.39927000
H	6.37098400	2.10645100	-1.39871600
H	5.11261300	0.55195900	-2.87565200
H	2.65502600	0.24810000	-2.55306300

C	1.14186900	1.42028500	-0.67692900
C	0.01913200	1.89018700	-0.33250700
N	-0.78516500	-2.13555600	-1.63371500
C	-1.17015800	-3.18262100	-1.93522100
C	-1.65625200	-4.49721800	-2.31900500
H	-2.75025400	-4.50052500	-2.30614200
H	-1.30417500	-4.73594000	-3.32697900
H	-1.28197100	-5.24619700	-1.61487600

II_{dppe}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2655.258084 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.528505 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.665514 hartrees

P	-3.99242800	-2.05059900	0.28168500
P	0.00513800	-0.04111200	0.61093400
C	-1.28604900	-1.34209000	0.76114000
H	-0.80893200	-2.30155300	0.54325200
H	-1.60303700	-1.36383100	1.80911600
C	-2.45351100	-1.08244600	-0.20711600
H	-2.71478300	-0.01955200	-0.23965300
H	-2.16801100	-1.39242800	-1.21790700
C	-4.37878500	-1.13398900	1.84585900
C	-3.96865000	-1.71399000	3.05832200
C	-4.97845900	0.13640200	1.87342900
C	-4.13152600	-1.03138700	4.26786600
H	-3.51766600	-2.70360000	3.05869400
C	-5.16588600	0.80553100	3.08346500
H	-5.29911000	0.60479600	0.94809400
C	-4.73404000	0.22843100	4.28227700
H	-3.79834700	-1.48885300	5.19507900
H	-5.63695700	1.78467200	3.08982000
H	-4.87085100	0.75693000	5.22141300

C	-5.22552100	-1.32687900	-0.89046200
C	-6.59127800	-1.47952000	-0.58749100
C	-4.87583500	-0.69065800	-2.09306600
C	-7.57448600	-0.99016600	-1.44692600
H	-6.88843700	-1.96849700	0.33721300
C	-5.86260800	-0.20597400	-2.95770100
H	-3.83568400	-0.56737900	-2.37530100
C	-7.21331800	-0.34927000	-2.63625400
H	-8.62292300	-1.10902700	-1.18759100
H	-5.56951600	0.28433600	-3.88216400
H	-7.97868800	0.03154100	-3.30645100
C	1.34518400	-0.37308200	1.78211900
C	2.17666900	0.68493300	2.18344000
C	1.58301300	-1.67351600	2.25417200
C	3.24186400	0.43860900	3.04863800
H	1.99922700	1.69266000	1.82478300
C	2.64201700	-1.90683100	3.13113200
H	0.96039900	-2.50492200	1.94355300
C	3.47391800	-0.85501300	3.52457100
H	3.88712000	1.25831500	3.34878600
H	2.82357800	-2.91317300	3.49474800
H	4.30336300	-1.04392800	4.19948400
C	-0.74587000	1.55331300	1.06115500
C	-1.77353800	1.57198400	2.02121600
C	-0.28551500	2.76139100	0.51172300
C	-2.33276200	2.78766800	2.41499700
H	-2.15118200	0.65877800	2.46738900
C	-0.85190100	3.97106000	0.91339000
H	0.50805600	2.76382200	-0.22470000
C	-1.87725900	3.98625200	1.86249400

H	-3.13083300	2.78793100	3.14950700
H	-0.48976700	4.89879300	0.48116700
H	-2.31991600	4.92889700	2.17002000
Pt	0.68800400	-0.13590200	-1.67708900
F	1.21710500	-0.27499300	-3.62211300
C	2.06026600	1.14508700	-1.26194500
C	2.94588600	1.90099700	-0.92030500
C	3.96280200	2.78999600	-0.45906000
C	4.96524000	2.30775400	0.40650400
C	3.96421000	4.14738200	-0.83264100
C	5.94689400	3.17204000	0.88697000
H	4.95820400	1.26228300	0.69798300
C	4.95157800	5.00301700	-0.34717000
H	3.19047000	4.51855900	-1.49769700
C	5.94336400	4.51951500	0.51219700
H	6.71534300	2.79344700	1.55475800
H	4.94660000	6.04916600	-0.63919000
H	6.71036800	5.19028600	0.88845100
C	1.99088800	-1.49846500	-1.20010000
C	2.86357800	-2.29219800	-0.89697300
C	3.87225600	-3.21721300	-0.49989300
C	4.74414200	-2.88532700	0.55770600
C	4.01417500	-4.46110900	-1.14649000
C	5.73300300	-3.78203000	0.95597000
H	4.63338100	-1.92875000	1.05668500
C	5.00323100	-5.35304100	-0.73659800
H	3.34506400	-4.71728200	-1.96226100
C	5.86425000	-5.01741800	0.31346400
H	6.40056600	-3.51726300	1.77096700
H	5.10376200	-6.31126900	-1.23814900

H	6.63460200	-5.71536900	0.62865500
N	-0.81026600	1.31490900	-2.23028600
C	-1.70863500	2.02539900	-2.37605700
C	-2.84818600	2.91497800	-2.50086800
H	-3.77031900	2.32988700	-2.42089200
H	-2.81010800	3.64917600	-1.68960300
H	-2.82097400	3.42823600	-3.46599400

$TS_{II,dppe}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2655.241933 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.513568 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.649795 hartrees

P	4.02076200	1.79329300	1.13886300
P	0.05653500	-0.29628700	0.73254400
C	1.37264800	0.79295800	1.41916800
H	0.88185000	1.69648500	1.79137600
H	1.78641300	0.27167100	2.28926100
C	2.43753100	1.13756500	0.36712700
H	2.69460600	0.25857800	-0.23163600
H	2.04132400	1.90489200	-0.30612600
C	4.57921800	0.20766400	1.92071700
C	4.31323200	0.02331600	3.28791900
C	5.16706300	-0.84454200	1.19817900
C	4.60626500	-1.19200400	3.91457900
H	3.87182700	0.83139700	3.86644300
C	5.48055400	-2.04906400	1.82904900
H	5.37864200	-0.72351600	0.14001400
C	5.19314100	-2.22908900	3.18628800
H	4.38463200	-1.32252600	4.96998300

H	5.93849900	-2.85268000	1.25884800
H	5.42921800	-3.17132600	3.67256600
C	5.11209100	1.86585000	-0.35287700
C	6.49536400	2.00774400	-0.13699800
C	4.64364200	1.82804200	-1.67658600
C	7.38369800	2.08625500	-1.20911800
H	6.88288400	2.04016900	0.87871100
C	5.53456800	1.91311800	-2.75172600
H	3.58402000	1.73579000	-1.89062600
C	6.90572200	2.03769800	-2.52248600
H	8.44890200	2.18550000	-1.01928400
H	5.15068800	1.88050200	-3.76779900
H	7.59657700	2.09986600	-3.35845100
C	-1.20957700	-0.48319600	2.01784200
C	-1.70206800	-1.75464000	2.35143100
C	-1.68896700	0.65265700	2.69165600
C	-2.66463300	-1.88641200	3.35350500
H	-1.33749800	-2.63790500	1.83860600
C	-2.63698900	0.50880900	3.70411900
H	-1.33919400	1.64526000	2.42870300
C	-3.13006500	-0.75776200	4.03210300
H	-3.04273200	-2.87235300	3.60617600
H	-2.99272200	1.38762700	4.23314100
H	-3.87294800	-0.86343700	4.81693500
C	0.77256300	-1.93044900	0.39297900
C	1.94748900	-2.35307300	1.03540500
C	0.13174800	-2.78174700	-0.52526500
C	2.47709300	-3.61299400	0.75116100
H	2.46343000	-1.72081500	1.74872000
C	0.66479200	-4.04080900	-0.79530900

H	-0.77378300	-2.46175800	-1.02960200
C	1.84067200	-4.45578800	-0.16186900
H	3.39176700	-3.92442600	1.24427700
H	0.16535800	-4.69290600	-1.50518900
H	2.25921200	-5.43359500	-0.38078100
Pt	-0.66695800	0.68261300	-1.30213900
F	-1.12224400	1.57831200	-3.04515500
C	-2.37021200	-0.31531700	-1.19082700
C	-3.19334700	-1.21582200	-1.22789100
C	-4.15114200	-2.26751800	-1.23043700
C	-4.46585500	-2.93296500	-0.02662000
C	-4.78966700	-2.66148400	-2.42443100
C	-5.39559700	-3.96988500	-0.02455200
H	-3.97816200	-2.62623900	0.89309400
C	-5.71888400	-3.69929500	-2.40945600
H	-4.54835500	-2.15067000	-3.35157800
C	-6.02409700	-4.35672500	-1.21296300
H	-5.63112200	-4.47703100	0.90677200
H	-6.20564100	-3.99709600	-3.33372000
H	-6.74850700	-5.16604500	-1.20689500
C	-2.25534000	1.50859700	-0.50280000
C	-3.11193900	2.25913200	-0.04757500
C	-4.12671600	3.09723400	0.47444600
C	-4.74170700	2.79142900	1.70854000
C	-4.54199100	4.24176100	-0.24224600
C	-5.74392200	3.61631300	2.21051200
H	-4.42938700	1.90612000	2.25106900
C	-5.54182100	5.06120600	0.27261800
H	-4.07060800	4.47412900	-1.19208000
C	-6.14423600	4.75206400	1.49763300

H	-6.21499100	3.37425100	3.15860500
H	-5.85461400	5.94142400	-0.28113200
H	-6.92544200	5.39388300	1.89436400
N	0.94755100	-0.28549000	-2.32865600
C	1.87645700	-0.83579000	-2.73876200
C	3.05941200	-1.54294800	-3.19390300
H	3.94251100	-0.92582400	-2.99720000
H	3.14022500	-2.48448200	-2.64122900
H	2.98654000	-1.74880500	-4.26531700

III_{dppe}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2655.331574 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.602175 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.739520 hartrees

P	-4.01988800	-0.30569900	1.45224700
P	0.31262200	0.46302300	0.53472200
C	-1.19067700	0.02067700	1.50654500
H	-0.93582900	-0.84019300	2.13087900
H	-1.40961300	0.85430300	2.18187300
C	-2.36131100	-0.31371000	0.57291200
H	-2.42158000	0.40686500	-0.24797900
H	-2.19891000	-1.30475900	0.13892200
C	-4.13095500	1.52597000	1.72036600
C	-3.78429900	2.02487900	2.98678400
C	-4.44368000	2.43690300	0.69717500
C	-3.73122900	3.40257300	3.22093800
H	-3.54940300	1.33442500	3.79340200
C	-4.41275000	3.81101400	0.93696000
H	-4.71039400	2.07197300	-0.29024000

C	-4.04866800	4.29772700	2.19692200
H	-3.45121900	3.77297300	4.20307500
H	-4.66014400	4.50316700	0.13674500
H	-4.01587300	5.36824500	2.37868500
C	-5.15472000	-0.53466200	0.00856100
C	-6.51020600	-0.19573400	0.17552800
C	-4.75167800	-1.07913800	-1.22251200
C	-7.42700800	-0.37225900	-0.86059200
H	-6.84889500	0.22639800	1.11875800
C	-5.67290300	-1.26240300	-2.25941700
H	-3.72053000	-1.37196000	-1.39111900
C	-7.01097500	-0.90552100	-2.08450000
H	-8.46663400	-0.09336800	-0.71222900
H	-5.33832000	-1.68457800	-3.20328800
H	-7.72438100	-1.04463800	-2.89173000
C	1.66460600	0.66470000	1.73861700
C	2.53631400	1.76064400	1.66247200
C	1.87400800	-0.32374700	2.71532900
C	3.59939500	1.87003700	2.56042700
H	2.38959700	2.52749800	0.90958500
C	2.94014300	-0.21090600	3.60613700
H	1.21891800	-1.18655500	2.78139600
C	3.80505000	0.88542200	3.52958700
H	4.26873600	2.72245800	2.49618300
H	3.09478000	-0.97869500	4.35827400
H	4.63537500	0.97145300	4.22438100
C	0.01824900	2.08806300	-0.23205500
C	-0.94863500	2.98180600	0.25219800
C	0.79616400	2.44241700	-1.34916000
C	-1.13897000	4.21046800	-0.38373400

H	-1.56542600	2.73800700	1.10987400
C	0.60686300	3.67489400	-1.97218600
H	1.54373900	1.75391500	-1.73279100
C	-0.36578900	4.55812400	-1.49296800
H	-1.89911000	4.88786500	-0.00876500
H	1.21172900	3.94092800	-2.83378000
H	-0.52065100	5.51398400	-1.98480100
Pt	0.64721000	-1.13302800	-1.11235900
F	0.81191500	-2.59979300	-2.50107100
C	3.74665700	-0.95371700	-0.37435300
C	4.69953300	-0.20262200	-0.52518200
C	5.79535100	0.68320500	-0.66129800
C	6.42836400	1.20115900	0.49013000
C	6.24913200	1.06610600	-1.94203600
C	7.49428000	2.08546800	0.35483000
H	6.07157200	0.90558200	1.47068300
C	7.31266400	1.95596000	-2.06184800
H	5.76076000	0.66445400	-2.82413500
C	7.93625800	2.46540300	-0.91741800
H	7.98003100	2.48171400	1.24140800
H	7.65790100	2.25183500	-3.04784600
H	8.76684400	3.15798600	-1.01718400
C	2.64563400	-1.72248500	-0.19354100
C	1.70317300	-2.49898700	0.12010600
C	1.07717500	-3.62493500	0.75989500
C	1.47814300	-4.00085600	2.05598700
C	0.05215400	-4.32952100	0.10039200
C	0.84382100	-5.06857700	2.68787500
H	2.27342500	-3.45462800	2.55323600
C	-0.56951600	-5.39643300	0.74326400

H	-0.20693700	-4.03956200	-0.91258300
C	-0.18160200	-5.76273700	2.03719100
H	1.14898900	-5.35749600	3.68911300
H	-1.35695200	-5.94497100	0.23505600
H	-0.67478100	-6.59159500	2.53650400
N	-0.75584700	-0.22234700	-2.30630500
C	-1.58243000	0.31922200	-2.90483900
C	-2.63878600	1.02551100	-3.60710200
H	-3.60728300	0.71003800	-3.20375000
H	-2.51141400	2.10124500	-3.45065700
H	-2.59591700	0.80015300	-4.67624900

B6. XYZ Cartesian coordinates of Reactant and Products in path II

$TS_{III,bipy}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.663426 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.218451 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.319326 hartrees

C	0.73401600	-0.60965600	3.75032300
C	2.00153800	-0.11798800	4.05383700
C	2.84614600	0.28011400	3.01948500
C	2.41798500	0.18346900	1.69649700
C	0.34849900	-0.69035100	2.41808100
C	3.23914400	0.58243400	0.53496100
C	4.52699300	1.11370800	0.61176500
C	5.19012800	1.45155100	-0.56870900
H	6.19170700	1.86558000	-0.52310800
C	4.56163500	1.25608100	-1.79863400
C	3.27620500	0.72154600	-1.81130300

H	0.04520800	-0.92789500	4.52371100
H	2.33382200	-0.04199400	5.08339300
H	-0.62319800	-1.05973300	2.11700700
H	5.05104100	1.50960800	-2.73170200
H	2.71085100	0.53329700	-2.71784300
H	5.01072800	1.26470900	1.56846000
H	3.83318700	0.66422000	3.24267400
N	2.65274700	0.40295000	-0.67249600
N	1.17099100	-0.30775800	1.42587100
Pt	0.68172000	-0.42140500	-0.56793600
C	-0.70835400	0.98100500	-0.39855600
C	-1.21030400	2.09670400	-0.30416300
C	-1.84423200	3.35911900	-0.18697900
C	-2.29264400	4.04875700	-1.33562500
C	-2.03921200	3.94665000	1.08325500
C	-2.91620900	5.28753000	-1.21125400
H	-2.14565900	3.60218800	-2.31433900
C	-2.66400900	5.18603800	1.19439800
H	-1.69654100	3.42089500	1.96939400
C	-3.10483500	5.86123600	0.05090200
H	-3.25680800	5.80798700	-2.10192300
H	-2.80823100	5.62753400	2.17649000
H	-3.59187300	6.82772100	0.14272900
N	1.77136100	-2.40917900	-0.69283500
C	2.30037700	-3.43562600	-0.66220200
C	2.96337800	-4.73015900	-0.62862800
H	2.70288200	-5.25092100	0.29752200
H	2.64018200	-5.32996400	-1.48447900
H	4.04723500	-4.58966500	-0.67304000
C	-1.27763000	-0.77499000	-0.35786700

C	-2.34854200	-1.36245900	-0.22157700
C	-3.60519900	-1.99517900	-0.05915300
C	-4.38921800	-2.33194800	-1.18567400
C	-4.09331700	-2.29935000	1.23183900
C	-5.62272300	-2.95545600	-1.01962100
H	-4.01801900	-2.10000300	-2.17920700
C	-5.32806800	-2.92371300	1.38467600
H	-3.49573300	-2.04176900	2.10101100
C	-6.09645500	-3.25401500	0.26278300
H	-6.21718900	-3.21010700	-1.89233200
H	-5.69357700	-3.15365800	2.38139300
H	-7.05916100	-3.74121500	0.38731800
F	0.50097100	-0.42884900	-2.52833800

IV_{bipy}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.755909 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.308507 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.407365 hartree

C	0.30169800	-1.05622400	3.71786000
C	-0.31288500	-2.30045200	3.83651200
C	-0.90709900	-2.87300500	2.71336200
C	-0.87877800	-2.19546100	1.49660400
C	0.30228700	-0.42079800	2.48151700
C	-1.47462400	-2.70991300	0.25110600
C	-2.13672300	-3.92872500	0.11748300
C	-2.65054100	-4.29196200	-1.12772200
H	-3.17024600	-5.23730400	-1.24071000
C	-2.49083200	-3.43776500	-2.21884200
C	-1.82212400	-2.23347100	-2.03129300
H	0.77606200	-0.57229600	4.56345400

H	-0.33229300	-2.82183300	4.78724200
H	0.76135600	0.54823400	2.34131400
H	-2.87579300	-3.69134100	-3.19947900
H	-1.65892100	-1.50587000	-2.81754400
H	-2.25576100	-4.58859600	0.96741100
H	-1.38973700	-3.83919500	2.78655100
N	-1.33856800	-1.89238100	-0.82635300
N	-0.27136300	-0.97349300	1.39751300
Pt	-0.41006500	-0.10963400	-0.44478400
C	2.48495500	1.15743700	-0.16294000
C	3.66178500	0.84105500	-0.23767000
C	5.03265400	0.48499800	-0.32526200
C	5.64649800	0.33399100	-1.58707700
C	5.78800000	0.27454100	0.84822600
C	6.99028900	-0.02100000	-1.66661000
H	5.06306500	0.49678700	-2.48766400
C	7.13118600	-0.07924200	0.75408100
H	5.31316700	0.39073100	1.81724600
C	7.73394400	-0.22766700	-0.49972000
H	7.45905300	-0.13644600	-2.63923300
H	7.70930800	-0.24018300	1.65903700
H	8.78203100	-0.50419200	-0.56730100
N	-3.84304900	-0.19926400	0.86944900
C	-3.92663700	0.11641200	-0.24514600
C	-3.99851200	0.49975200	-1.65202400
H	-4.56327300	-0.24927300	-2.21537400
H	-4.49564200	1.46920400	-1.75004800
H	-2.98476600	0.57544700	-2.06030800
C	1.15786100	1.45778100	-0.07273700
C	0.03002300	1.98116900	0.08470000

C	-1.05551600	2.90116700	0.27428000
C	-1.93267700	3.15009000	-0.79870300
C	-1.25192800	3.53143500	1.51575300
C	-2.99317000	4.03480700	-0.62672800
H	-1.76293600	2.63101000	-1.73520100
C	-2.32004900	4.41297000	1.67361000
H	-0.57499500	3.32697200	2.33886500
C	-3.18987500	4.66481000	0.60761100
H	-3.66877200	4.23215300	-1.45377500
H	-2.47491300	4.90217100	2.63052100
H	-4.02144000	5.35087600	0.73890600
F	-0.77709500	0.56332700	-2.28627000

$TS_{III,dppe}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2655.292246 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.563969 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.697366 hartrees

P	2.43752600	0.76567200	0.39313900
P	-0.05053000	-0.89337600	1.59006900
C	1.07012500	0.06621900	2.70556500
H	0.62703300	1.06270900	2.79707100
H	1.05871600	-0.37923500	3.70486000
C	2.49191900	0.15522400	2.13664700
H	3.11787000	0.78639200	2.77295000
H	2.95990500	-0.83353500	2.09715700
C	2.29186200	2.57662900	0.37609800
C	1.86142000	3.16477100	-0.82677200
C	2.59441500	3.37833600	1.48559000
C	1.76430700	4.55286000	-0.91675100
H	1.59239100	2.53151500	-1.66757200

C	2.46960700	4.76617000	1.39075300
H	2.92672200	2.93821000	2.42023800
C	2.06118500	5.35357100	0.19082600
H	1.44676800	5.00956500	-1.84975100
H	2.69705900	5.38543400	2.25331000
H	1.97087700	6.43354600	0.11923400
C	4.00421000	0.29051200	-0.39720800
C	5.15832400	0.02527800	0.35569100
C	4.02889900	0.16702400	-1.79707200
C	6.33156500	-0.36849600	-0.29121200
H	5.15388900	0.11916700	1.43711400
C	5.20764200	-0.22382200	-2.43283700
H	3.11832000	0.34083600	-2.36260200
C	6.35724000	-0.49425700	-1.68284000
H	7.22224000	-0.57860000	0.29332200
H	5.22498500	-0.32848400	-3.51369900
H	7.27059100	-0.80482800	-2.18186100
C	-1.74206000	-0.60718100	2.18129700
C	-2.62219700	-1.68031600	2.39375300
C	-2.16751200	0.70675800	2.44230500
C	-3.91499600	-1.43795100	2.86087700
H	-2.30692200	-2.69999200	2.20487800
C	-3.45591200	0.93735100	2.92157100
H	-1.51247300	1.55075800	2.25873000
C	-4.33291100	-0.13193600	3.12556800
H	-4.59011900	-2.27284900	3.02184600
H	-3.77519500	1.95443600	3.12552400
H	-5.33793500	0.05332400	3.49253700
C	0.32241500	-2.66104800	1.70853500
C	1.19847100	-3.17008700	2.67775200

C	-0.25906800	-3.52341200	0.76129500
C	1.49182200	-4.53534300	2.69556800
H	1.65621200	-2.52269500	3.41781500
C	0.02792600	-4.88552200	0.79702100
H	-0.91671600	-3.12660600	-0.00699800
C	0.90866900	-5.39136500	1.75910000
H	2.17598200	-4.92563900	3.44256100
H	-0.42433200	-5.54907000	0.06649800
H	1.14142000	-6.45186200	1.77605000
Pt	0.44539800	-0.18499300	-0.58014900
F	1.03332800	0.52262600	-2.43592700
C	-1.44249600	-0.56301700	-1.24523900
C	-2.45687300	-1.15892700	-1.60016100
C	-3.66069900	-1.82027000	-1.94958800
C	-4.56616400	-2.20886000	-0.93619300
C	-3.97630300	-2.10119600	-3.29698400
C	-5.74960100	-2.86233300	-1.26783400
H	-4.32729000	-1.98933100	0.09962600
C	-5.16396900	-2.75441900	-3.61615100
H	-3.28338100	-1.80384500	-4.07824400
C	-6.05311500	-3.13784100	-2.60590200
H	-6.43849900	-3.15710700	-0.48122900
H	-5.39777100	-2.96629200	-4.65559200
H	-6.97772800	-3.64796000	-2.86027000
C	-1.03849800	1.14107200	-0.61789200
C	-1.64230000	2.20230500	-0.50224200
C	-2.42083500	3.38078200	-0.35090300
C	-3.68510400	3.32128500	0.27658200
C	-1.94839300	4.62702200	-0.81495100
C	-4.44267100	4.47822400	0.44361500

H	-4.05869400	2.36408700	0.62439200
C	-2.71658800	5.77682500	-0.64772300
H	-0.97593000	4.67900400	-1.29209100
C	-3.96326500	5.70941300	-0.01629800
H	-5.41250200	4.41829900	0.92982200
H	-2.33947600	6.73019400	-1.00739100
H	-4.55740600	6.60926100	0.11487300
N	1.70549200	-2.01015000	-1.04739500
C	2.60027100	-2.73036300	-1.17421900
C	3.74388700	-3.61537800	-1.31598400
H	3.62740900	-4.23765600	-2.20775200
H	4.65024800	-3.00839900	-1.41217500
H	3.82147300	-4.25607700	-0.43285900

IV_{dppe}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2655.385539 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.655016 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.788950 hartrees

P	0.08977700	2.02530300	0.72213500
P	0.29763500	-1.02089900	1.32976000
C	-0.25389600	0.11468900	2.69254300
H	-1.34576500	0.17549000	2.65946900
H	0.03403400	-0.30087000	3.66226700
C	0.37682500	1.49618300	2.47005600
H	-0.01262600	2.23004200	3.18031200
H	1.46241100	1.45436600	2.60553800
C	-1.61843200	2.65086800	0.56484700
C	-2.12366300	2.82803200	-0.73678200
C	-2.41683400	2.95353300	1.67676600
C	-3.41456300	3.32207200	-0.91368000

H	-1.51148700	2.54840600	-1.59003500
C	-3.71502400	3.43582600	1.48627700
H	-2.04721400	2.82218300	2.68812700
C	-4.21165900	3.62563200	0.19527200
H	-3.80515600	3.45442100	-1.91824200
H	-4.33369800	3.66239900	2.34937200
H	-5.22173000	3.99787400	0.05255600
C	1.23239200	3.38185800	0.34090900
C	1.66125600	4.25403400	1.35531800
C	1.65935100	3.56682900	-0.98352600
C	2.52512500	5.30420100	1.04241200
H	1.33388800	4.12206000	2.38179300
C	2.52240800	4.62226500	-1.28327500
H	1.31444700	2.88491100	-1.75478200
C	2.95795500	5.48676400	-0.27531500
H	2.86255300	5.97463800	1.82696600
H	2.86303000	4.76090100	-2.30494700
H	3.63538400	6.30145000	-0.51386100
C	-0.78841300	-2.47574000	1.37175900
C	-0.27117600	-3.77474200	1.24887300
C	-2.17840200	-2.27948400	1.41826600
C	-1.13974500	-4.86582000	1.19252800
H	0.80056300	-3.93548400	1.19771000
C	-3.03951500	-3.37408600	1.36715200
H	-2.59643100	-1.27881700	1.46657300
C	-2.52171000	-4.66759300	1.25489400
H	-0.73482500	-5.86910000	1.09998900
H	-4.11281000	-3.21289000	1.39780200
H	-3.19442500	-5.51902100	1.20989800
C	1.97643700	-1.55188300	1.78938600

C	2.18380400	-2.25612000	2.98862600
C	3.06836100	-1.25071500	0.96239700
C	3.47063700	-2.65317600	3.34913800
H	1.34494200	-2.50543100	3.63254100
C	4.35410600	-1.65414500	1.32750800
H	2.92057200	-0.71117500	0.03500200
C	4.55610500	-2.35374400	2.51858200
H	3.62583700	-3.19830900	4.27526300
H	5.19104700	-1.42515600	0.67489700
H	5.55645800	-2.66861900	2.80095600
Pt	0.19990500	0.17602700	-0.59879500
F	0.10387100	1.30620300	-2.31253900
C	-0.82780600	-1.64905800	-1.90548900
C	0.39487800	-1.83324500	-1.98526000
C	1.72901200	-2.32540400	-2.11294200
C	2.01556700	-3.65858300	-1.75542700
C	2.76492400	-1.46491800	-2.52169200
C	3.32986900	-4.11582900	-1.80730900
H	1.21162600	-4.30951300	-1.42723000
C	4.07421400	-1.93498300	-2.56691500
H	2.53812100	-0.43239300	-2.76209000
C	4.35903400	-3.25697800	-2.20931800
H	3.55320000	-5.14039000	-1.52541100
H	4.87017200	-1.25867000	-2.86016700
H	5.38319400	-3.61724000	-2.23765400
C	-2.16647700	-1.45391500	-1.77683600
C	-3.34243900	-1.24046200	-1.52806900
C	-4.64218300	-0.91537500	-1.06278900
C	-5.78469500	-1.62068100	-1.48995500
C	-4.77282300	0.12608000	-0.11712000

C	-7.03521800	-1.28698700	-0.97487700
H	-5.68014700	-2.42163000	-2.21474900
C	-6.02911800	0.44963400	0.38669700
H	-3.89140100	0.67111800	0.20424900
C	-7.16056100	-0.25481000	-0.03856000
H	-7.91436300	-1.83284900	-1.30396900
H	-6.12283800	1.25453800	1.10920800
H	-8.13880700	0.00014600	0.35843800
N	4.27110900	1.34214700	-1.89781100
C	4.39238500	1.65360700	-0.78596600
C	4.54530200	2.05056900	0.60955800
H	5.59777500	1.99135200	0.90243100
H	4.19086200	3.07611700	0.74360800
H	3.96365600	1.38295100	1.25133300

B7. XYZ Cartesian coordinates of Reactant and Products in path III

$TS_{diss,bipy}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.673982 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.230169 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.324631 hartrees

C	4.11205500	-2.02505900	-1.97366500
C	4.69149700	-2.40487000	-0.76324500
C	3.96976900	-2.27603400	0.42466600
C	2.67281000	-1.76848800	0.37625100
C	2.81479300	-1.52197500	-1.96261700
C	1.79277100	-1.57849600	1.54569400
C	2.15251600	-1.89402700	2.85390500
C	1.24638800	-1.68087400	3.89158900
H	1.52464000	-1.92593100	4.91074200

C	-0.01047300	-1.15221900	3.60620300
C	-0.32818900	-0.85176800	2.28757200
H	4.64763300	-2.11297000	-2.91138300
H	5.70153000	-2.79929500	-0.73769100
H	2.28458300	-1.20068700	-2.85227800
H	-0.74291100	-0.97020200	4.38346200
H	-1.28641000	-0.44148200	1.99713100
H	3.13171900	-2.30484500	3.06349400
H	4.41639600	-2.56888600	1.36620800
N	0.55191200	-1.06662100	1.29569000
N	2.13429200	-1.40821400	-0.81537700
Pt	0.16341200	-0.68694100	-0.68778500
C	-1.70381800	-0.08622500	-0.48070500
C	-2.84817500	0.29609900	-0.30379900
C	-4.19441200	0.72130500	-0.09383700
C	-4.93222000	1.30128100	-1.14589800
C	-4.80048500	0.57577500	1.17081000
C	-6.24220800	1.72550300	-0.93345500
H	-4.46822100	1.41469300	-2.12092400
C	-6.11146800	1.00189300	1.37351000
H	-4.23638500	0.12759300	1.98321900
C	-6.83538200	1.57805600	0.32455600
H	-6.80147500	2.17220200	-1.75050800
H	-6.56917700	0.88546900	2.35169100
H	-7.85673900	1.91039000	0.48663900
F	0.06297600	-0.37794400	-2.63888200
C	1.78859300	3.52180700	0.00571900
C	2.76261600	3.69569600	1.00872900
C	3.28900100	4.96103400	1.26154800
C	2.85451700	6.06542500	0.52185500

C	1.88722800	5.89995600	-0.47438000
C	1.35380600	4.63861300	-0.73386800
H	3.09760700	2.83533700	1.58032100
H	4.03973000	5.08520100	2.03675500
H	3.26743700	7.05016800	0.72103400
H	1.54680200	6.75556700	-1.05051800
H	0.60206200	4.50687200	-1.50608800
C	1.24598000	2.22376600	-0.24617600
C	0.79602900	1.11904300	-0.46303900
N	-0.53486300	-3.24746900	-0.23233400
C	-1.68009600	-3.44777400	-0.20639400
C	-3.11573600	-3.67332400	-0.17142800
H	-3.42929500	-4.22162400	-1.06428500
H	-3.38835000	-4.24233800	0.72202400
H	-3.61976600	-2.70091300	-0.14832000

3_{bipy}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.679262 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.233851 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.326435 hartrees

C	4.38640100	-1.39212500	-1.95200500
C	4.97680600	-1.69169200	-0.72433900
C	4.20494600	-1.68825000	0.43893100
C	2.84827500	-1.38158400	0.34972600
C	3.02792800	-1.09295700	-1.98184300
C	1.91401700	-1.32955700	1.49151200
C	2.27337700	-1.61870700	2.80565700
C	1.31946500	-1.53615200	3.81880900
H	1.59780600	-1.76224000	4.84232300

C	0.01593900	-1.15890600	3.50393500
C	-0.29941900	-0.87868800	2.18049000
H	4.95972900	-1.38705700	-2.87135500
H	6.03414900	-1.92634700	-0.66631100
H	2.48442500	-0.84899200	-2.88789100
H	-0.75396700	-1.07871900	4.26190900
H	-1.29149400	-0.58056500	1.86752500
H	3.28977700	-1.90802400	3.03960900
H	4.66038200	-1.91860600	1.39346200
N	0.62597600	-0.97291300	1.21032900
N	2.30195400	-1.09226300	-0.85711900
Pt	0.24076000	-0.63087800	-0.78784500
C	-1.68314800	-0.21070200	-0.62232200
C	-2.86789700	0.03302800	-0.46174600
C	-4.26099400	0.27112800	-0.26653500
C	-5.02386900	0.92681600	-1.25397300
C	-4.89348600	-0.15857700	0.91847300
C	-6.38530500	1.14767900	-1.05527700
H	-4.54007000	1.25741600	-2.16805900
C	-6.25574000	0.06377600	1.10659100
H	-4.30946400	-0.66721700	1.67963000
C	-7.00492900	0.71712300	0.12248500
H	-6.96463700	1.65493800	-1.82142500
H	-6.73400100	-0.27302600	2.02193000
H	-8.06685000	0.88924700	0.27255500
F	0.13954800	-0.41305300	-2.73136200
C	1.22852200	3.73944700	0.06476700
C	2.48352000	4.07655300	0.60838300
C	2.78164800	5.40426600	0.90986600
C	1.83862500	6.40954700	0.67331300

C	0.59119100	6.08193300	0.13249500
C	0.28327600	4.75706100	-0.17111700
H	3.21283300	3.29301800	0.79079600
H	3.75148800	5.65479900	1.33012100
H	2.07440400	7.44319700	0.90978000
H	-0.14434800	6.85978800	-0.05170700
H	-0.68509300	4.49854800	-0.58869200
C	0.91206800	2.37792200	-0.23324100
C	0.64044800	1.22728300	-0.50261600
N	0.24214000	-4.07220800	0.20195800
C	-0.91527100	-3.96912900	0.18332300
C	-2.36518300	-3.80130300	0.15668800
H	-2.79777900	-4.38782000	-0.65934000
H	-2.80010600	-4.13171600	1.10474900
H	-2.60144200	-2.74306700	0.00241300

4_{bipy} (only $[(bipy)Pt(C{\equiv}CPh)_2F]^{+1}$)

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.904027 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.509241 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.596979 hartrees

C	4.44021300	-1.56643500	-1.90117000
C	5.04283800	-1.82858100	-0.67103600
C	4.26704600	-1.87140400	0.48873700
C	2.89453000	-1.64853000	0.39342700
C	3.06610100	-1.35125600	-1.93719700
C	1.95439000	-1.65006000	1.53180400
C	2.32636900	-1.89586600	2.85137400
C	1.36283000	-1.86859800	3.85868300
H	1.65124400	-2.05768000	4.88690600

C	0.03658900	-1.59402900	3.53208200
C	-0.29123000	-1.35327500	2.20368500
H	5.01644900	-1.52449800	-2.81776700
H	6.11249200	-1.99683100	-0.60811400
H	2.51404700	-1.13558500	-2.84521600
H	-0.74112700	-1.56047500	4.28560700
H	-1.29943300	-1.12693400	1.88186000
H	3.36007000	-2.10541200	3.09445700
H	4.73167600	-2.07147800	1.44570200
N	0.64494600	-1.39009000	1.23917000
N	2.33451200	-1.39695600	-0.81634600
Pt	0.26029200	-1.02276200	-0.75731900
C	-1.67663900	-0.65775900	-0.60238000
C	-2.86692000	-0.42698100	-0.46885300
C	-4.26597500	-0.19474900	-0.31886700
C	-5.07893900	0.02662300	-1.44959500
C	-4.85638700	-0.19298400	0.96181300
C	-6.44700600	0.24231900	-1.29861900
H	-4.62767500	0.02468700	-2.43709300
C	-6.22525800	0.02417500	1.10298700
H	-4.23425200	-0.36393300	1.83520400
C	-7.02409300	0.24137600	-0.02447100
H	-7.06468500	0.41009400	-2.17620200
H	-6.67035900	0.02223100	2.09381300
H	-8.09138200	0.40818600	0.08927300
F	0.17187500	-0.76132700	-2.69516300
C	0.96580600	3.39220900	0.15159300
C	2.26283000	3.93322200	0.24085900
C	2.43843200	5.28088400	0.55098800
C	1.32987200	6.10325200	0.77526400

C	0.03897200	5.57247800	0.68822200
C	-0.14678600	4.22661500	0.37852700
H	3.12138400	3.29181500	0.06656600
H	3.44233200	5.69017100	0.61801200
H	1.47107900	7.15280000	1.01696800
H	-0.82483100	6.20771600	0.86215400
H	-1.14710900	3.80991000	0.31034400
C	0.76868800	2.01078800	-0.15768100
C	0.57402200	0.84650500	-0.43423100

$TS_{C\text{-}C,bipy}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.887636 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.494602 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.582139 hartrees

C	4.89676200	0.05536100	-1.95848100
C	5.58438900	0.00594700	-0.74597400
C	4.88757400	-0.23563500	0.43915400
C	3.50810600	-0.42559300	0.38745700
C	3.51959600	-0.13973700	-1.95184800
C	2.64138300	-0.67694100	1.55473000
C	3.10253500	-0.76165200	2.86658600
C	2.20005900	-0.98881800	3.90454400
H	2.55600300	-1.05137800	4.92703200
C	0.84518800	-1.13018800	3.61347000
C	0.43013600	-1.04083500	2.29063600
H	5.41002200	0.24247600	-2.89420200
H	6.65822700	0.15592700	-0.71653800
H	2.90268700	-0.11343300	-2.84315200
H	0.11028900	-1.30510200	4.39009300

H	-0.60800000	-1.13917300	2.00182600
H	4.15761600	-0.64750700	3.07942500
H	5.41789600	-0.27120400	1.38223200
N	1.30690800	-0.82532000	1.29372100
N	2.86190900	-0.37160000	-0.80657300
Pt	0.78505100	-0.64268100	-0.68688900
C	-1.17300400	-0.90491400	-0.47850200
C	-2.31451400	-1.33373800	-0.35564600
C	-3.63282500	-1.83426800	-0.20756300
C	-4.47344400	-1.97821200	-1.33312000
C	-4.11545700	-2.20345700	1.06746500
C	-5.76241100	-2.48126400	-1.18121400
H	-4.10245100	-1.69607000	-2.31345700
C	-5.40637000	-2.70481800	1.20678800
H	-3.47034000	-2.09403000	1.93370800
C	-6.23172800	-2.84596300	0.08561400
H	-6.40282000	-2.59130400	-2.05132600
H	-5.77040900	-2.98760500	2.19010100
H	-7.23765900	-3.23957200	0.19874600
F	0.59271700	-0.43635500	-2.62969100
C	-1.35871000	3.33123300	0.07461700
C	-1.44772400	3.86063000	1.37880500
C	-1.99469700	5.12534800	1.58440300
C	-2.45863000	5.87902900	0.50122500
C	-2.37296800	5.36095200	-0.79519300
C	-1.82810600	4.09752500	-1.01283600
H	-1.08812600	3.27281300	2.21785800
H	-2.06001500	5.52403000	2.59272600
H	-2.88522500	6.86416600	0.66641600
H	-2.73261900	5.94242200	-1.63931600

H	-1.76169500	3.69208200	-2.01782700
C	-0.81363300	2.03451600	-0.14274000
C	-0.37209600	0.91503400	-0.33734300

5_{bipy}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.978838 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.584041 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.671144 hartrees

C	2.83699700	3.49589300	-2.17143400
C	2.83229100	4.39605300	-1.10576700
C	2.24935500	4.03087800	0.10820400
C	1.67685800	2.76652400	0.23441600
C	2.24921400	2.24827200	-1.99415400
C	1.04268700	2.23384100	1.45405400
C	0.93545600	2.93953200	2.65044200
C	0.33568000	2.33777100	3.75523000
H	0.24814400	2.88159100	4.68945700
C	-0.14179900	1.03423100	3.64133100
C	-0.01225600	0.37382400	2.42494900
H	3.28439200	3.74882600	-3.12541300
H	3.28065800	5.37787200	-1.21342900
H	2.20534700	1.48409500	-2.76184700
H	-0.60984600	0.52456800	4.47524100
H	-0.36378200	-0.63985800	2.28731400
H	1.31801400	3.94974100	2.72212100
H	2.24568200	4.72423500	0.93971200
N	0.55847700	0.95767800	1.35564500
N	1.68806800	1.91066100	-0.82221600
Pt	0.80182900	0.09657900	-0.48288900

C	-0.80245200	-1.50659400	-0.14180400
C	0.36217600	-1.96754200	-0.03689000
C	1.38932600	-2.95857900	0.14715300
C	2.52352600	-2.95815000	-0.68734800
C	1.25322200	-3.92742100	1.15883700
C	3.50792100	-3.92661800	-0.50785000
H	2.59252400	-2.21124200	-1.47131000
C	2.24958500	-4.88623700	1.33030600
H	0.37674600	-3.91712800	1.79903500
C	3.37623100	-4.88718800	0.50102700
H	4.37972400	-3.93274000	-1.15534700
H	2.14700900	-5.63299200	2.11202600
H	4.14986000	-5.63665200	0.64049800
F	1.20531000	-0.53686600	-2.31586600
C	-4.66314000	-0.48605700	-0.33794500
C	-5.38734000	-0.21729000	0.84376200
C	-6.72978700	0.14265300	0.76720900
C	-7.36217000	0.24047900	-0.47709300
C	-6.64981500	-0.02310500	-1.65217700
C	-5.30740900	-0.38570400	-1.59017100
H	-4.88883000	-0.29471800	1.80469500
H	-7.28445800	0.34789400	1.67781100
H	-8.40973500	0.52194900	-0.53094500
H	-7.14233000	0.05325400	-2.61683500
H	-4.74775200	-0.59369100	-2.49645900
C	-3.29533100	-0.85272800	-0.26866800
C	-2.11863200	-1.17919600	-0.21265200

$[(bipy)PtF]^{+1}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -714.307797 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -714.131198 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -714.181702 hartrees

C	2.37903100	2.69566200	-0.00002000
C	1.28944100	3.56672300	-0.00007600
C	-0.00324100	3.04642500	-0.00008300
C	-0.18906500	1.66638800	-0.00003400
C	2.15357400	1.32510200	0.00002100
C	-1.48190900	0.97438500	-0.00002100
C	-2.73025500	1.59226300	0.00004000
C	-3.88048300	0.80445600	0.00006100
H	-4.85884700	1.27225200	0.00010800
C	-3.75754600	-0.58476800	0.00001800
C	-2.48589400	-1.14748400	-0.00003100
H	3.39843100	3.06291300	-0.00001500
H	1.44088200	4.64049300	-0.00011100
H	2.93985600	0.58122200	0.00007900
H	-4.62712900	-1.23128900	0.00001200
H	-2.32608000	-2.21966100	-0.00008500
H	-2.80627900	2.67242100	0.00007800
H	-0.86155000	3.70665200	-0.00012400
N	-1.37856800	-0.38519600	-0.00003400
N	0.89681300	0.83504100	0.00001200
F	2.43648000	-1.58273500	-0.00016000
Pt	0.53054800	-1.09005400	0.00003100

$[(bipy)Pt(NCCH_3)F]^{+1}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -847.111420 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -846.882174 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -846.944653 hartrees

C	-3.39609300	-2.18923800	0.00000700
C	-4.18195500	-1.03697700	-0.00024300
C	-3.56759800	0.21497700	-0.00037700
C	-2.17654000	0.29218800	-0.00026200
C	-2.01208900	-2.05961000	0.00012100
C	-1.39250400	1.53776900	-0.00038900
C	-1.94448700	2.81681800	-0.00066200
C	-1.10440400	3.92869500	-0.00075700
H	-1.52563200	4.92800200	-0.00096600
C	0.27585600	3.73677000	-0.00057500
C	0.77554200	2.43954900	-0.00031000
H	-3.83968900	-3.17787000	0.00011800
H	-5.26431900	-1.10743700	-0.00033400
H	-1.32564000	-2.89779500	0.00031900
H	0.96568100	4.57248800	-0.00063100
H	1.83837800	2.23754500	-0.00014900
H	-3.01946500	2.94541900	-0.00079500
H	-4.16700400	1.11655200	-0.00057100
N	-0.03564900	1.36575600	-0.00022400
N	-1.42936000	-0.84776700	-0.00001200
F	0.87472300	-2.53414000	0.00046600
Pt	0.56207600	-0.58187800	0.00015900
N	2.54314400	-0.27657400	0.00031400
C	3.69027700	-0.13288200	0.00039900
C	5.13221700	0.05124000	0.00045500
H	5.43110900	0.60802200	-0.89267600
H	5.43094400	0.60875400	0.89318400
H	5.62491900	-0.92566200	0.00090100

$TS_{C\text{-}F,bipy}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.850135 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.457511 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.544994 hartrees

C	4.50564000	-1.07648400	-1.57740000
C	5.04700200	-1.61015500	-0.40831300
C	4.21173400	-1.90207600	0.67053000
C	2.84472500	-1.65554400	0.55361800
C	3.13387200	-0.85102600	-1.63521600
C	1.84816400	-1.89714400	1.61029000
C	2.15326600	-2.40469300	2.87061400
C	1.14261900	-2.58308000	3.81287800
H	1.38125100	-2.97658100	4.79480300
C	-0.16808600	-2.24910200	3.47900400
C	-0.43536400	-1.74668300	2.21307200
H	5.12674100	-0.83408200	-2.43147400
H	6.11257800	-1.79651700	-0.33043600
H	2.64317000	-0.42743700	-2.50391100
H	-0.98453900	-2.37044500	4.18077000
H	-1.43006800	-1.46715200	1.89551000
H	3.17678300	-2.65654600	3.11694800
H	4.62571500	-2.31095000	1.58324800
N	0.54916100	-1.58053400	1.30450000
N	2.33895000	-1.14222900	-0.59606300
Pt	0.25732100	-0.81514500	-0.53721200
C	-1.69687300	-0.57379700	-0.39560800
C	-2.90349200	-0.41155800	-0.29325500
C	-4.31425800	-0.24185900	-0.16499900
C	-5.13913200	-0.19055600	-1.30761600

C	-4.90490600	-0.12548800	1.11057300
C	-6.51646000	-0.02724600	-1.17359900
H	-4.68936800	-0.28028600	-2.29182100
C	-6.28317200	0.03670300	1.23500500
H	-4.27401500	-0.16334200	1.99368000
C	-7.09299700	0.08633900	0.09564500
H	-7.14175300	0.01047900	-2.06110200
H	-6.72681600	0.12462500	2.22272100
H	-8.16717300	0.21264400	0.19633900
F	0.26387500	0.35848100	-2.29607800
C	1.07856900	3.69538600	-0.25445900
C	2.41070700	4.16193500	-0.19576300
C	2.67837400	5.47192300	0.19322100
C	1.63298400	6.33841500	0.53102500
C	0.31058600	5.88441400	0.47732600
C	0.02955700	4.57668700	0.09053400
H	3.22142900	3.48934400	-0.45921500
H	3.70704300	5.81906500	0.23295200
H	1.84710500	7.35941100	0.83332000
H	-0.50532300	6.55255200	0.73836000
H	-0.99638400	4.22370200	0.04837400
C	0.79614600	2.36576000	-0.66160100
C	0.55865600	1.18065800	-0.86031800

7_{bipy}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.935993 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.541445 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.630720 hartrees

C	4.72182300	1.14170700	-0.71960800

C	5.38773700	0.08762400	-0.09788700
C	4.65267200	-0.99983500	0.37033000
C	3.26644800	-1.01436800	0.20878900
C	3.33895500	1.07102900	-0.84954000
C	2.39942200	-2.11930500	0.66906200
C	2.87828900	-3.27468600	1.28702000
C	1.98306500	-4.26412600	1.68926900
H	2.35160800	-5.16377600	2.17042100
C	0.61954400	-4.08285300	1.46695100
C	0.19422100	-2.91487300	0.84560500
H	5.25345600	2.00622400	-1.09954200
H	6.46540900	0.10653300	0.02374600
H	2.77229600	1.86424800	-1.32162100
H	-0.10991300	-4.82630500	1.76613800
H	-0.85007000	-2.71101600	0.64507500
H	3.93903600	-3.40804400	1.45509700
H	5.15957400	-1.82311100	0.85672800
N	1.06140400	-1.96088600	0.45842900
N	2.62966900	0.02435700	-0.39794200
Pt	0.51141300	-0.18992600	-0.50914800
C	-1.42347100	-0.50942300	-0.47729800
C	-2.63265900	-0.67249200	-0.38207400
C	-4.04223100	-0.85427500	-0.24958200
C	-4.93416600	0.18011200	-0.60378900
C	-4.57075500	-2.06284100	0.25053500
C	-6.30955600	0.00833300	-0.45820600
H	-4.53570700	1.11341100	-0.99105300
C	-5.94748500	-2.22693400	0.39282400
H	-3.89167500	-2.86447200	0.52615100
C	-6.82194000	-1.19386400	0.04026400

H	-6.98361400	0.81472900	-0.73377900
H	-6.33939600	-3.16304200	0.78107500
H	-7.89443500	-1.32453200	0.15332200
F	0.12799900	1.30304400	-3.12155700
C	-0.20872200	2.97254600	0.28948100
C	0.80117200	3.81754800	0.79876900
C	0.52281600	4.64501100	1.88138300
C	-0.74790500	4.62619200	2.46872100
C	-1.74960500	3.77958800	1.97568900
C	-1.48869700	2.95302200	0.88984400
H	1.78297500	3.81910800	0.33693100
H	1.29353500	5.30223900	2.27138300
H	-0.95794100	5.27137400	3.31665100
H	-2.73004800	3.76749100	2.44130900
H	-2.24214400	2.27530900	0.50164700
C	0.04397300	2.14065500	-0.82781500
C	0.17328400	1.36420900	-1.81132700

[(bipy)Pt(C≡CPh)]$^{+1}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -922.278311 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -921.996804 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -922.063964 hartrees

C	-4.54177500	-2.22610100	0.00037900
C	-5.28075500	-1.04349500	0.00013900
C	-4.61445000	0.18123600	-0.00005600
C	-3.22041800	0.19280400	-0.00001100
C	-3.15170800	-2.14730600	0.00041500
C	-2.38999900	1.40565200	-0.00022400
C	-2.89548700	2.70425600	-0.00048800

C	-2.02635800	3.79178600	-0.00069800
H	-2.41903200	4.80255000	-0.00092000
C	-0.65290200	3.55923600	-0.00062400
C	-0.18511700	2.25241900	-0.00035300
H	-5.02537900	-3.19583200	0.00054100
H	-6.36512900	-1.06930500	0.00010400
H	-2.52264400	-3.03036800	0.00062000
H	0.06388700	4.37196400	-0.00077500
H	0.86845400	2.01429400	-0.00029500
H	-3.96631000	2.86240600	-0.00053500
H	-5.17619400	1.10682600	-0.00023900
N	-1.03406700	1.19933700	-0.00016700
N	-2.51366300	-0.96754400	0.00022000
Pt	-0.42989600	-0.68627800	0.00011600
C	1.51715900	-0.34593800	0.00001100
C	2.73744900	-0.22883600	-0.00000700
C	4.16371300	-0.15343100	-0.00000700
C	4.88292500	-0.12892900	1.21356700
C	4.88308700	-0.13246200	-1.21355300
C	6.27612100	-0.08950800	1.20947700
H	4.33772200	-0.14779800	2.15264500
C	6.27628200	-0.09302600	-1.20939200
H	4.33801000	-0.15407700	-2.15264400
C	6.97833400	-0.07314200	0.00006200
H	6.81565700	-0.07562800	2.15251200
H	6.81594300	-0.08190000	-2.15239300
H	8.06435400	-0.04729200	0.00009600

[(bipy)Pt(C≡CPh)(NCCH$_3$)]$^{+1}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1055.086400 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1054.753103 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1054.830318 hartrees

C	4.74789700	1.50739100	0.00017200
C	5.35720300	0.25398200	-0.00021000
C	4.56164000	-0.89019000	-0.00051900
C	3.17251500	-0.75885100	-0.00045600
C	3.35866200	1.57428900	0.00022000
C	2.23293300	-1.89556700	-0.00066100
C	2.63205600	-3.23155600	-0.00091500
C	1.67319400	-4.24177000	-0.00094700
H	1.97996500	-5.28214700	-0.00114000
C	0.32441900	-3.89480500	-0.00071500
C	-0.02445400	-2.55001600	-0.00050500
H	5.32937300	2.42190100	0.00044900
H	6.43806600	0.16302000	-0.00025300
H	2.83532800	2.52200500	0.00058900
H	-0.45683200	-4.64585100	-0.00069600
H	-1.05481500	-2.21992600	-0.00034300
H	3.68418200	-3.48555700	-0.00107800
H	5.02295900	-1.86930000	-0.00080500
N	0.90414700	-1.57231300	-0.00049600
N	2.59191200	0.47136700	-0.00010800
Pt	0.47790900	0.42344300	-0.00017700
N	0.20559400	2.40421800	0.00053700
C	0.03161600	3.54655800	0.00188800
C	-0.18091700	4.98443300	0.00440200
H	-0.95232100	5.24160000	-0.72752900
H	-0.50340300	5.30550600	0.99946000
H	0.75164100	5.49325700	-0.25685300

C	-1.47975100	0.19616400	-0.00026700
C	-2.69376400	0.04310200	-0.00028300
C	-4.11116500	-0.14348800	-0.00022100
C	-4.82437500	-0.24439900	1.21255900
C	-4.82664800	-0.22816500	-1.21290600
C	-6.20695600	-0.42335200	1.20866500
H	-4.28310400	-0.18044400	2.15201700
C	-6.20921800	-0.40722200	-1.20879900
H	-4.28716100	-0.15164000	-2.15245000
C	-6.90552500	-0.50507700	-0.00001800
H	-6.74075600	-0.49874100	2.15218100
H	-6.74478400	-0.47003700	-2.15223600
H	-7.98298200	-0.64390200	0.00005800

$TS_{diss,dppe}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2655.301521 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.572159 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.701418 hartrees

P	2.43508300	0.15622400	0.23765300
P	-0.46898200	-0.54036300	1.58878400
C	0.82731200	0.38301100	2.52229500
H	0.65474600	1.44455900	2.32595400
H	0.69162700	0.22308800	3.59584900
C	2.23698200	-0.03343700	2.06895800
H	2.98814900	0.54132500	2.61584600
H	2.41634500	-1.09006800	2.28907000
C	2.99502100	1.83884400	-0.16596800
C	2.80581200	2.28008700	-1.48763600

C	3.64435700	2.65995300	0.76581700
C	3.27707200	3.53546200	-1.86795000
H	2.27504800	1.64859900	-2.19375000
C	4.10481500	3.92002100	0.37534600
H	3.79947800	2.33711800	1.78965400
C	3.92618800	4.35615300	-0.93961300
H	3.12755200	3.87780000	-2.88759400
H	4.60185000	4.55691500	1.10073100
H	4.28556300	5.33635000	-1.23885900
C	3.72815800	-0.99356900	-0.31465600
C	4.69156100	-1.50741300	0.56698300
C	3.75294100	-1.34062600	-1.67640100
C	5.67287200	-2.37596600	0.08549300
H	4.68754200	-1.23903100	1.61865300
C	4.74039400	-2.20630000	-2.14605500
H	2.98069300	-0.96325100	-2.34041900
C	5.69714800	-2.72617600	-1.26769300
H	6.41466700	-2.77893300	0.76823300
H	4.75457400	-2.48535500	-3.19526400
H	6.45915300	-3.40627700	-1.63668700
C	-2.10346800	0.13529800	1.96269000
C	-3.22336300	-0.71265800	1.95317500
C	-2.26701000	1.51035800	2.20298000
C	-4.49394800	-0.18516300	2.17836000
H	-3.11306600	-1.77544500	1.77237300
C	-3.54201700	2.02728900	2.42646300
H	-1.41989600	2.18429600	2.20568200
C	-4.65599000	1.18331700	2.40962500
H	-5.35624400	-0.84396600	2.16348200
H	-3.66072700	3.09098000	2.60738700

H	-5.64803600	1.59141300	2.57798200
C	-0.39729600	-2.29764500	2.03059200
C	0.25176400	-2.72264900	3.20214800
C	-0.99104200	-3.24391700	1.17450200
C	0.30562200	-4.08319700	3.50878200
H	0.70890000	-2.01151300	3.88127900
C	-0.94137500	-4.59894800	1.49732200
H	-1.47676200	-2.92325800	0.25808300
C	-0.28949300	-5.01997400	2.65994700
H	0.81272500	-4.40727700	4.41199100
H	-1.40118500	-5.32421300	0.83357300
H	-0.24167700	-6.07717600	2.90219700
Pt	0.23956500	-0.35244700	-0.67482900
F	0.98578400	-0.04227800	-2.57262000
C	-1.62122300	-0.75302500	-1.31515500
C	-2.79268000	-0.93273400	-1.61031500
C	-4.16727500	-1.14764600	-1.92531500
C	-5.16217500	-0.36934100	-1.29754600
C	-4.55554600	-2.13397600	-2.85426200
C	-6.50778700	-0.57731100	-1.59327600
H	-4.86757600	0.38912200	-0.57991400
C	-5.90417600	-2.33696000	-3.14150800
H	-3.79326000	-2.73474500	-3.34136900
C	-6.88393300	-1.56080100	-2.51383900
H	-7.26462700	0.02886200	-1.10324800
H	-6.19162000	-3.10158600	-3.85771500
H	-7.93397900	-1.72121100	-2.74131300
C	-0.22609200	1.50828500	-0.47571300
C	-0.47933400	2.67967800	-0.28832100
C	-0.74419900	4.05660900	-0.02273700

C	-2.06851300	4.52441900	0.08665800
C	0.32590900	4.95465100	0.15973400
C	-2.31268900	5.86712900	0.37063300
H	-2.89176500	3.82936100	-0.04611500
C	0.07022000	6.29523400	0.44039400
H	1.34473600	4.59115700	0.08061100
C	-1.24656500	6.75528700	0.54599500
H	-3.33624100	6.22107400	0.45404700
H	0.90060200	6.98198900	0.57825100
H	-1.44124100	7.80120400	0.76540000
N	0.85559300	-2.83083600	-1.70703800
C	1.49172000	-3.48549100	-0.98482400
C	2.29798800	-4.27889900	-0.07051000
H	2.07471200	-3.97443000	0.95695400
H	2.06139200	-5.34043200	-0.18474900
H	3.35902800	-4.11128500	-0.27688500

3_{dppe}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2655.301609 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.571026 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.700741 hartrees

P	2.42970100	0.17515600	0.23964100
P	-0.47656600	-0.55045400	1.57731300
C	0.80735100	0.38419300	2.51760700
H	0.62347800	1.44405000	2.32262600
H	0.66926500	0.22111200	3.59039600
C	2.22437600	-0.01397000	2.07050200
H	2.96481200	0.57220200	2.61994400
H	2.41722000	-1.06744600	2.29409600

C	2.97874800	1.86108800	-0.16558000
C	2.78779300	2.29964400	-1.48787700
C	3.62542600	2.68583500	0.76483900
C	3.25405500	3.55640600	-1.86992000
H	2.26084500	1.66455200	-2.19362700
C	4.08140600	3.94695500	0.37249800
H	3.78208600	2.36479100	1.78901900
C	3.90045900	4.38073300	-0.94292600
H	3.10306600	3.89676600	-2.89000900
H	4.57655500	4.58653000	1.09680800
H	4.25615000	5.36182000	-1.24363400
C	3.73703700	-0.96219100	-0.30536400
C	4.70202200	-1.46555100	0.58071200
C	3.77196900	-1.30906700	-1.66688400
C	5.69450300	-2.32396200	0.10387400
H	4.69064300	-1.19716800	1.63233400
C	4.77019500	-2.16483400	-2.13172500
H	2.99865800	-0.94044800	-2.33450200
C	5.72814000	-2.67473700	-1.24899800
H	6.43750900	-2.71888000	0.78999200
H	4.79173000	-2.44415500	-3.18075800
H	6.49850600	-3.34736200	-1.61434300
C	-2.11762600	0.11045200	1.94873900
C	-3.22877800	-0.74898900	1.94665600
C	-2.29426400	1.48438900	2.18627000
C	-4.50363400	-0.23415000	2.17698300
H	-3.10807200	-1.81103300	1.76818100
C	-3.57347200	1.98858200	2.41484400
H	-1.45437500	2.16729800	2.18374600
C	-4.67868400	1.13304700	2.40614600

H	-5.35911100	-0.90187900	2.16802000
H	-3.70215900	3.05141900	2.59401300
H	-5.67396900	1.53121600	2.57906500
C	-0.39166600	-2.30803200	2.01556400
C	0.25562900	-2.73015400	3.18917600
C	-0.97561400	-3.25708000	1.15577600
C	0.31707700	-4.09074700	3.49439400
H	0.70554200	-2.01679300	3.87080200
C	-0.91838100	-4.61213900	1.47724100
H	-1.45943900	-2.93828500	0.23775700
C	-0.26876500	-5.03028900	2.64214000
H	0.82284800	-4.41274700	4.39908600
H	-1.37061300	-5.33960400	0.81068900
H	-0.21516700	-6.08745300	2.88335300
Pt	0.24389400	-0.35797700	-0.68160200
F	0.99708800	-0.05135700	-2.57666000
C	-1.60940300	-0.77971000	-1.32902600
C	-2.78246000	-0.95255700	-1.62286400
C	-4.16074100	-1.15200000	-1.93156600
C	-5.14196900	-0.36225000	-1.29629300
C	-4.56693400	-2.13085600	-2.86058900
C	-6.49177300	-0.55182000	-1.58480100
H	-4.83355900	0.39070000	-0.57871900
C	-5.91980400	-2.31547700	-3.14046600
H	-3.81545100	-2.74026400	-3.35366900
C	-6.88584400	-1.52817100	-2.50548900
H	-7.23773500	0.06305100	-1.08894500
H	-6.22134300	-3.07446800	-3.85684900
H	-7.93915300	-1.67433300	-2.72739200
C	-0.23835200	1.49892400	-0.49265700

C	-0.49752300	2.66742900	-0.29514500
C	-0.76486300	4.04095400	-0.01458100
C	-2.08947700	4.50630300	0.10095000
C	0.30461800	4.93706700	0.18092000
C	-2.33450000	5.84462300	0.40444100
H	-2.91229500	3.81270200	-0.04174800
C	0.04810400	6.27323300	0.48099800
H	1.32361000	4.57529900	0.09728900
C	-1.26900300	6.73079500	0.59317100
H	-3.35826900	6.19664700	0.49306600
H	0.87810300	6.95827800	0.62930600
H	-1.46439200	7.77316400	0.82827600
N	0.92191000	-2.85975300	-1.73629500
C	1.54327100	-3.48476300	-0.97606200
C	2.33484800	-4.24487700	-0.02097600
H	2.07881400	-3.92345900	0.99331500
H	2.11814400	-5.31225600	-0.11906800
H	3.39862800	-4.06508900	-0.20117700

4_{dppe} ([(dppe)Pt(C≡CPh)$_2$F]$^{+1}$)

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2522.529264 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2521.851333 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2521.974061 hartrees

P	-2.50907300	-0.26780100	-0.14679900
P	0.37917900	-0.75853300	-1.53396600
C	-0.98853500	0.03645300	-2.48366800
H	-0.88127100	1.11446600	-2.33311600
H	-0.85920700	-0.16001900	-3.55206600
C	-2.35865300	-0.45328400	-1.98498900

H	-3.15587300	0.07817000	-2.50959100
H	-2.48878300	-1.51890900	-2.19452900
C	-3.23668400	1.34369000	0.27241400
C	-3.05507000	1.80112600	1.59000000
C	-3.96757300	2.10923500	-0.64587600
C	-3.61396300	3.01708000	1.97909900
H	-2.45871800	1.21679300	2.28502100
C	-4.51641700	3.33043200	-0.24684400
H	-4.11621800	1.77353300	-1.66649700
C	-4.34322600	3.78302100	1.06327300
H	-3.47000700	3.37321700	2.99480800
H	-5.07645500	3.92522900	-0.96201800
H	-4.76975700	4.73398400	1.36867300
C	-3.59494700	-1.58672900	0.46603900
C	-4.62677500	-2.10917500	-0.33023600
C	-3.39496800	-2.06113700	1.77402700
C	-5.45235300	-3.11043400	0.18145400
H	-4.79455800	-1.74016500	-1.33772800
C	-4.23005900	-3.06185100	2.27388100
H	-2.59963600	-1.64357400	2.38512600
C	-5.25363600	-3.58740600	1.48076000
H	-6.24970300	-3.51604200	-0.43402600
H	-4.07752000	-3.43255900	3.28320800
H	-5.89790600	-4.36839300	1.87400200
C	1.96227700	-0.04183100	-2.02952500
C	3.09442100	-0.86561400	-2.13799500
C	2.07095100	1.33827900	-2.27238200
C	4.32503500	-0.30868100	-2.48539700
H	3.02243300	-1.93213400	-1.95629000
C	3.30631200	1.88472200	-2.61508300

H	1.21080400	1.99044100	-2.18852900
C	4.43393400	1.06476100	-2.71873100
H	5.19754800	-0.94914700	-2.56764000
H	3.38414900	2.95164200	-2.79971100
H	5.39488400	1.49515000	-2.98395200
C	0.37217400	-2.54272800	-1.84495400
C	-0.24678100	-3.07453200	-2.98876700
C	0.99384500	-3.39999700	-0.91750900
C	-0.24547400	-4.45350800	-3.19657100
H	-0.72141300	-2.43006900	-3.72071400
C	0.99344200	-4.77651400	-1.13961100
H	1.47685500	-2.99393600	-0.03354100
C	0.37104600	-5.30361200	-2.27420300
H	-0.72614700	-4.86157900	-4.08010700
H	1.47584400	-5.43475200	-0.42391500
H	0.36607500	-6.37658400	-2.44028900
Pt	-0.24637900	-0.49948500	0.70526600
F	-0.94206500	-0.31293600	2.63577800
C	1.66110700	-0.66983000	1.33222900
C	2.83970100	-0.70009200	1.65479800
C	4.21841500	-0.75402800	2.01333600
C	5.20012600	-0.28366300	1.11604100
C	4.62295800	-1.27424200	3.25993400
C	6.54891900	-0.33604400	1.46073000
H	4.89203600	0.11786200	0.15635500
C	5.97459100	-1.32542300	3.59453800
H	3.87043300	-1.63585500	3.95427300
C	6.94106000	-0.85753500	2.69803500
H	7.29607100	0.02926800	0.76170100
H	6.27513600	-1.73001900	4.55687700

H	7.99379900	-0.89853600	2.96282800
C	0.02092800	1.38938600	0.44952000
C	0.15460900	2.56836900	0.19644600
C	0.29915100	3.94782900	-0.13984400
C	1.57596900	4.48747900	-0.39263900
C	-0.83699200	4.77329800	-0.25238200
C	1.70946000	5.82765300	-0.75169000
H	2.44979100	3.84860500	-0.30959200
C	-0.69152700	6.11250500	-0.60923800
H	-1.82001900	4.35577000	-0.06052600
C	0.57834700	6.64304400	-0.85998500
H	2.69696800	6.23593600	-0.94675100
H	-1.57176500	6.74348900	-0.69391400
H	0.68587800	7.68714100	-1.13971800

$TS_{C\text{-}C,dppe}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2522.511883 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2521.835606 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2521.958326 hartrees

P	2.62728000	0.21484200	0.20826800
P	-0.01107700	-1.02612000	1.49993400
C	1.20519000	-0.13820400	2.56854300
H	0.89392000	0.91082200	2.59216700
H	1.14699000	-0.51604500	3.59341800
C	2.62151500	-0.27733100	1.99064800
H	3.33251700	0.30955800	2.57706700
H	2.95808900	-1.31815800	2.02304000
C	2.75509900	2.02874500	0.08955700
C	2.42317300	2.61227900	-1.14657400

C	3.15693200	2.83589900	1.16329700
C	2.51262300	3.99480700	-1.30262100
H	2.07570700	1.98386100	-1.96159400
C	3.22725300	4.22134300	1.00027700
H	3.41691600	2.40602200	2.12477700
C	2.90974300	4.80073400	-0.23031600
H	2.25742300	4.44465100	-2.25764100
H	3.53206500	4.84422600	1.83583900
H	2.96630300	5.87843500	-0.35293100
C	4.07618200	-0.53778300	-0.58116700
C	5.26422900	-0.74720600	0.13738300
C	3.99450800	-0.88599700	-1.93956100
C	6.36695800	-1.31130800	-0.50448100
H	5.33641300	-0.47465700	1.18616900
C	5.10695300	-1.44534700	-2.57071000
H	3.07186700	-0.70549300	-2.48361500
C	6.28884400	-1.65994200	-1.85637700
H	7.28530500	-1.47744500	0.05075000
H	5.04803200	-1.71618400	-3.62086700
H	7.15016500	-2.09866700	-2.35185600
C	-1.68012600	-0.69050000	2.11058600
C	-2.61019000	-1.73555400	2.22865400
C	-2.05537300	0.62481700	2.43293000
C	-3.90636900	-1.46282900	2.66806200
H	-2.33015900	-2.75412700	1.98289700
C	-3.35221300	0.88624100	2.87158900
H	-1.35556600	1.44589200	2.32916600
C	-4.27915500	-0.15426500	2.98548200
H	-4.62208900	-2.27399600	2.76031300
H	-3.63767100	1.90463500	3.11545200

H	-5.28965100	0.05480100	3.32349900
C	0.32426600	-2.80659700	1.57897600
C	1.00463700	-3.37120800	2.67042400
C	-0.10601600	-3.62580400	0.51843700
C	1.25682800	-4.74292600	2.69395500
H	1.33562100	-2.75821900	3.50196300
C	0.14543600	-4.99688300	0.55617700
H	-0.63805900	-3.19783300	-0.32610800
C	0.83023600	-5.55453400	1.63926100
H	1.78629600	-5.17542100	3.53714500
H	-0.18982100	-5.62623200	-0.26230400
H	1.03174500	-6.62127300	1.66168500
Pt	0.47721900	-0.37777600	-0.68174300
F	1.13715100	0.10855800	-2.57284700
C	-1.43357000	-0.56438600	-1.32024400
C	-2.55822900	-0.90313100	-1.67656700
C	-3.86788300	-1.29910800	-2.04522100
C	-4.83068600	-1.55354400	-1.04286800
C	-4.22791100	-1.44360300	-3.40286400
C	-6.11876300	-1.94411600	-1.39645300
H	-4.55288600	-1.43973500	-0.00009700
C	-5.51899700	-1.83675900	-3.74383400
H	-3.48825400	-1.24785000	-4.17301500
C	-6.46603000	-2.08824900	-2.74450500
H	-6.85384800	-2.13794700	-0.62070300
H	-5.78922700	-1.94793400	-4.78982200
H	-7.47193900	-2.39531000	-3.01590600
C	-0.75806400	1.16327900	-0.59768400
C	-1.21415800	2.26281900	-0.33210400
C	-1.79241300	3.51392600	0.02933700

C	-3.12724700	3.56479000	0.48316200
C	-1.03969700	4.70389000	-0.03073200
C	-3.68929900	4.77902000	0.87219700
H	-3.70632500	2.64810600	0.53000800
C	-1.61366400	5.91369600	0.35527800
H	-0.01011600	4.66450900	-0.37149900
C	-2.93622000	5.95610100	0.80886900
H	-4.71707200	4.80706500	1.22308600
H	-1.02542800	6.82579700	0.30693200
H	-3.37774000	6.90119300	1.11197300

5_{dppe}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2522.611041 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2521.933321 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2522.057683 hartrees

P	0.57069200	-2.08848200	-0.76841000
P	0.32763500	0.95601600	-1.36476800
C	0.01131900	-0.24371600	-2.74984100
H	-1.05706400	-0.47623400	-2.76820400
H	0.27388200	0.22342600	-3.70313200
C	0.83745400	-1.51311600	-2.50423000
H	0.59320600	-2.29442000	-3.22925900
H	1.90936700	-1.30508600	-2.59037300
C	-1.05959200	-2.89899800	-0.65557100
C	-1.59458900	-3.09352200	0.63156500
C	-1.79192000	-3.28210600	-1.78764500
C	-2.85309300	-3.67593300	0.77431400
H	-1.03234400	-2.76381200	1.50155700
C	-3.05824500	-3.85241200	-1.63280800
H	-1.39559500	-3.14019900	-2.78764300

C	-3.58865300	-4.05001200	-0.35623700
H	-3.26698200	-3.82325600	1.76747800
H	-3.62738900	-4.13945000	-2.51183400
H	-4.57443600	-4.49101000	-0.24070300
C	1.88292400	-3.27474700	-0.36205700
C	2.42495600	-4.09552200	-1.36529600
C	2.33917900	-3.37572300	0.96252700
C	3.42684700	-5.01067500	-1.04130200
H	2.07618500	-4.02906900	-2.39126500
C	3.34006200	-4.29799800	1.27260200
H	1.90134200	-2.74036100	1.72678200
C	3.88537900	-5.11133100	0.27546100
H	3.84899500	-5.64198000	-1.81748000
H	3.69646500	-4.37758100	2.29558500
H	4.66734000	-5.82361800	0.52265900
C	-1.01648200	2.17759300	-1.38959900
C	-0.76427900	3.53033700	-1.11117200
C	-2.33931800	1.73658300	-1.55779100
C	-1.82503400	4.43323100	-1.02913100
H	0.25253900	3.87841400	-0.96086900
C	-3.39307900	2.64598400	-1.48431600
H	-2.56056300	0.68577500	-1.71616600
C	-3.13787400	3.99415500	-1.22014300
H	-1.62383000	5.47874000	-0.81558900
H	-4.41297600	2.29613000	-1.60836700
H	-3.96138600	4.69912500	-1.15409100
C	1.88172400	1.79829500	-1.79979800
C	1.91433300	2.69651600	-2.88193800
C	3.05947900	1.52277200	-1.08857400
C	3.11128100	3.31650900	-3.23623100

H	1.00808900	2.92214400	-3.43699100
C	4.25471900	2.14791000	-1.44944800
H	3.04699500	0.83075100	-0.25434300
C	4.28128400	3.04502800	-2.51845200
H	3.13046900	4.01307700	-4.06902400
H	5.15828700	1.93817800	-0.88545600
H	5.21092600	3.53448400	-2.79406700
Pt	0.43789700	-0.24811900	0.55678300
F	0.54526600	-1.35483800	2.28978300
C	-0.55301600	1.55903300	1.94557400
C	0.67694400	1.67831800	2.02511200
C	2.05421700	2.00015300	2.22371300
C	2.52460900	3.29571900	1.93782100
C	2.95046200	0.99554700	2.64358700
C	3.88216500	3.57784200	2.07008200
H	1.82825600	4.05786500	1.60348800
C	4.30457100	1.29204700	2.76775100
H	2.56121300	0.00167700	2.84319500
C	4.77258500	2.57953500	2.47881300
H	4.24780400	4.57499100	1.84451200
H	4.99731400	0.51875500	3.08583600
H	5.83110200	2.80399900	2.57133600
C	-1.89985600	1.40957400	1.84625800
C	-3.08782000	1.21043400	1.64861000
C	-4.41884600	0.88423200	1.28537800
C	-5.45988200	1.82941000	1.37481800
C	-4.68078500	-0.40047500	0.76128400
C	-6.74072100	1.48937200	0.94576400
H	-5.25166600	2.81943100	1.76735300
C	-5.96470300	-0.72565300	0.33398800

H	-3.87452500	-1.12314200	0.68716700
C	-6.99593200	0.21594900	0.42478200
H	-7.54118300	2.22007600	1.01323900
H	-6.15848700	-1.71398800	-0.07266200
H	-7.99622700	-0.04087200	0.08855000

[(dppe)PtF]$^{+1}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1906.941243 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1906.481853 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1906.572393 hartrees

P	1.45586600	0.05979900	-0.53368000
P	-1.64233800	-0.06885400	-0.41774600
C	-0.82983000	-0.36978400	-2.05786200
H	-0.65708400	-1.44734000	-2.14417400
H	-1.48036900	-0.06235700	-2.88088800
C	0.48781300	0.41531000	-2.07120100
H	1.08957700	0.20213000	-2.95843600
H	0.29848800	1.49376100	-2.06130100
C	2.45192200	-1.44021300	-0.75891600
C	2.97959000	-2.05682200	0.39090300
C	2.72028200	-1.96825900	-2.03116300
C	3.77584400	-3.19276600	0.25585200
H	2.74651200	-1.64696100	1.37013900
C	3.51430100	-3.11025400	-2.15136200
H	2.32467000	-1.50555500	-2.92851800
C	4.04213800	-3.72098800	-1.01172700
H	4.18381400	-3.67024700	1.14174100
H	3.71787600	-3.51968200	-3.13615200
H	4.65841600	-4.60983100	-1.11065900

C	2.56086100	1.46623400	-0.24634900
C	3.94188600	1.36432800	-0.46589100
C	1.99627600	2.68335600	0.17277400
C	4.75387600	2.48395900	-0.27347000
H	4.38013300	0.42389700	-0.78374700
C	2.81484800	3.79500600	0.36023900
H	0.92787600	2.75270200	0.35870100
C	4.19304000	3.69521200	0.13798400
H	5.82347700	2.40681900	-0.44349400
H	2.38050300	4.73569300	0.68481300
H	4.82916700	4.56236900	0.28921600
C	-2.90505100	-1.35219200	-0.17526100
C	-4.27759000	-1.07360800	-0.11423600
C	-2.44627800	-2.67040400	0.00100000
C	-5.18530500	-2.11180900	0.10633000
H	-4.63816100	-0.05747800	-0.23501000
C	-3.35924100	-3.70138500	0.21494400
H	-1.37984000	-2.88185700	-0.02071200
C	-4.72922000	-3.42221900	0.26801400
H	-6.24814600	-1.89414000	0.15354100
H	-3.00308400	-4.71862600	0.34738000
H	-5.43918700	-4.22571600	0.44109100
C	-2.44348800	1.55962200	-0.54414900
C	-3.27710700	1.86869300	-1.63314600
C	-2.21348200	2.52507200	0.44948300
C	-3.87179200	3.12726700	-1.72204500
H	-3.47051200	1.13315300	-2.40863800
C	-2.80976600	3.78365400	0.35294600
H	-1.56824600	2.29857300	1.29286900
C	-3.63769800	4.08518200	-0.73072800

H	-4.51502700	3.35970200	-2.56532200
H	-2.62440200	4.52654900	1.12289700
H	-4.09935700	5.06543200	-0.80497400
Pt	0.01965200	-0.19762000	1.13673600
F	1.50513000	-0.34932400	2.50531500

[(dppe)Pt(NCCH$_3$)F]$^{+1}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2039.732011 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2039.220347 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2039.321424 hartrees

P	1.75709200	0.04249100	-0.52238800
P	-1.35729700	0.15546600	-0.83918200
C	-0.33377400	-0.08508800	-2.36572000
H	-0.22474400	-1.16521800	-2.50860600
H	-0.83788300	0.32216300	-3.24636600
C	1.02782800	0.58922700	-2.14297000
H	1.71281900	0.38938100	-2.97019400
H	0.91426600	1.67621600	-2.07195900
C	2.76751100	-1.44525900	-0.79083400
C	2.94163000	-2.33303700	0.28639900
C	3.39529300	-1.70040800	-2.02037300
C	3.73257500	-3.47009700	0.12051200
H	2.46663400	-2.11421800	1.23882300
C	4.18311700	-2.84246700	-2.17422300
H	3.28546200	-1.02023000	-2.85830800
C	4.34985500	-3.72834200	-1.10691300
H	3.86568500	-4.15602000	0.95209100
H	4.66431400	-3.03758000	-3.12793200
H	4.96159900	-4.61722600	-1.23157200

C	2.84077800	1.38582000	0.04628600
C	4.23557500	1.31011700	-0.07019400
C	2.24028500	2.53230600	0.59470800
C	5.02437900	2.38206300	0.35330400
H	4.70372700	0.42333100	-0.48579500
C	3.03477600	3.59907200	1.01153700
H	1.15973700	2.58415200	0.69921900
C	4.42660000	3.52404000	0.89184400
H	6.10496000	2.32215200	0.26375600
H	2.56944100	4.48413400	1.43515300
H	5.04399100	4.35430600	1.22233000
C	-2.77223300	-0.98303100	-0.91247300
C	-4.10060200	-0.53856300	-0.94337300
C	-2.49271200	-2.35835100	-0.83158800
C	-5.14327200	-1.46868200	-0.90306100
H	-4.32445900	0.52206700	-0.99060000
C	-3.53677300	-3.28009300	-0.79901900
H	-1.46241500	-2.69995500	-0.77086700
C	-4.86345700	-2.83539900	-0.83175900
H	-6.17223600	-1.12238800	-0.92455700
H	-3.31763600	-4.34177000	-0.73684400
H	-5.67665400	-3.55439500	-0.79652500
C	-1.96889500	1.86618500	-0.88321300
C	-2.52356800	2.40272600	-2.05784600
C	-1.88408400	2.66100900	0.27161800
C	-2.98276800	3.71976700	-2.07355400
H	-2.60434900	1.80137500	-2.95847600
C	-2.34506400	3.97824600	0.24850800
H	-1.45884900	2.25353800	1.18338800
C	-2.89237000	4.50805200	-0.92240500

H	-3.40870800	4.12963800	-2.98435200
H	-2.27373000	4.58847800	1.14377800
H	-3.24791600	5.53411200	-0.93961200
F	1.33977500	-0.80127400	2.38399400
Pt	0.02569100	-0.31706600	0.89734200
N	-1.64308400	-0.69393100	2.15689500
C	-2.68329300	-0.97256100	2.57819600
C	-4.00679000	-1.32878300	3.06139500
H	-4.43677400	-0.49219100	3.61962200
H	-4.64369600	-1.55808500	2.20062600
H	-3.94310300	-2.20579500	3.71171700

$TS_{C\text{-}F,dppe}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2522.485679 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2521.809763 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2521.932909 hartrees

P	2.39942000	-0.75122300	0.17967100
P	-0.57108000	-0.68019800	1.44871900
C	0.89902400	-0.22727000	2.46550500
H	1.04070700	0.85081100	2.33960800
H	0.67590100	-0.40221000	3.52228100
C	2.13037800	-1.01373100	1.99761300
H	3.01377600	-0.73499400	2.57611800
H	1.98703400	-2.08998400	2.13541500
C	3.52444500	0.65262600	-0.06541500
C	3.61087800	1.19537000	-1.35994200
C	4.31217000	1.18367200	0.96655500
C	4.48764800	2.24790300	-1.61528100
H	2.96586000	0.82111500	-2.14644100

C	5.18128300	2.24497000	0.70375000
H	4.26377600	0.78458300	1.97333800
C	5.27344900	2.77421700	-0.58541200
H	4.54673500	2.66602100	-2.61557700
H	5.78533800	2.65369000	1.50797900
H	5.95044000	3.59940300	-0.78582600
C	3.20383900	-2.24706700	-0.46905100
C	4.57710500	-2.27834100	-0.75366800
C	2.41501100	-3.39220100	-0.68277300
C	5.15777500	-3.45068800	-1.24046600
H	5.18820800	-1.39485400	-0.59884700
C	3.00511600	-4.55995900	-1.16506200
H	1.34792200	-3.38153800	-0.47527000
C	4.37484700	-4.58964700	-1.44529300
H	6.22113900	-3.47227100	-1.45941300
H	2.39455700	-5.44311700	-1.32745300
H	4.83008200	-5.49932300	-1.82584100
C	-1.92002000	0.45163100	1.83283600
C	-3.18744000	-0.03974500	2.18106700
C	-1.68973900	1.83525300	1.75016800
C	-4.21966500	0.85842900	2.45211600
H	-3.36960700	-1.10763100	2.23624300
C	-2.73052800	2.72219000	2.01609500
H	-0.72076100	2.22046100	1.45709900
C	-3.99426100	2.23539200	2.36700300
H	-5.20122100	0.48095300	2.72090400
H	-2.55051400	3.79028800	1.94345200
H	-4.80386100	2.92950900	2.57171500
C	-1.02990500	-2.39602600	1.79672800
C	-0.63619200	-3.00978700	2.99872100

C	-1.77362100	-3.12073400	0.84663800
C	-0.98511300	-4.33765700	3.24307200
H	-0.06883100	-2.46832200	3.74767200
C	-2.11974300	-4.44601900	1.10549000
H	-2.08145000	-2.64868000	-0.08056200
C	-1.72314100	-5.05593100	2.29880500
H	-0.67828600	-4.80858900	4.17162600
H	-2.69523600	-5.00177400	0.37179500
H	-1.98825100	-6.09084400	2.49284800
Pt	0.15733100	-0.51560800	-0.72037400
F	0.81168900	0.60531500	-2.55792100
C	-1.75050700	-0.44560100	-1.34521600
C	-2.94106900	-0.34081600	-1.60862500
C	-4.33720200	-0.19680800	-1.85837700
C	-4.99293800	-0.97323500	-2.83498400
C	-5.08555500	0.73459300	-1.10721600
C	-6.36164700	-0.82156900	-3.04989200
H	-4.42137400	-1.69089600	-3.41587400
C	-6.45295900	0.87964800	-1.33000600
H	-4.58414500	1.33162900	-0.35264200
C	-7.09566300	0.10342800	-2.30012700
H	-6.85714500	-1.42608700	-3.80436100
H	-7.01857700	1.59910700	-0.74449100
H	-8.16222800	0.21850600	-2.47111500
C	0.42634200	1.43839600	-1.04813800
C	0.52146300	2.62911800	-0.78091400
C	0.61632000	3.93833100	-0.23717900
C	1.84014100	4.38967700	0.30624400
C	-0.50536400	4.79529500	-0.19402600
C	1.93186600	5.66016700	0.86949100

H	2.70494400	3.73420200	0.28119100
C	-0.40040600	6.06394000	0.37386100
H	-1.45082900	4.45326900	-0.60447300
C	0.81578900	6.50359800	0.90724500
H	2.88001900	5.99340500	1.28314200
H	-1.27235000	6.71190400	0.40005400
H	0.89287100	7.49310100	1.34863300

7_{dppe}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2522.550597 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2521.873838 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2522.000160 hartrees

P	2.52800000	0.12135900	-0.42863600
P	-0.24075100	1.50796400	-1.21545000
C	1.06869100	1.30093900	-2.51864400
H	0.83009100	0.35743300	-3.01969400
H	0.98974700	2.09607900	-3.26590500
C	2.46946000	1.26926100	-1.89352600
H	3.23135500	0.99224700	-2.62850900
H	2.73548600	2.25618900	-1.50024400
C	3.02341000	-1.53282200	-1.00673000
C	3.48496500	-2.46528000	-0.06091200
C	2.82778100	-1.93657900	-2.33549600
C	3.75371900	-3.77862300	-0.44513900
H	3.63838000	-2.16729600	0.97214900
C	3.09275800	-3.25499200	-2.71336600
H	2.46944900	-1.23717200	-3.08335600
C	3.55404700	-4.17688800	-1.77068900
H	4.11311900	-4.49073200	0.29152400

H	2.93802300	-3.55825500	-3.74442100
H	3.75644000	-5.20190100	-2.06654000
C	3.85885200	0.72660500	0.65368700
C	5.20612300	0.41870500	0.40527500
C	3.51858600	1.55025300	1.73911200
C	6.20148100	0.93204800	1.23695800
H	5.47551400	-0.22592000	-0.42609900
C	4.51989000	2.06327600	2.56497200
H	2.47727400	1.79091200	1.93568800
C	5.85951700	1.75310400	2.31594100
H	7.24239100	0.68991600	1.04380400
H	4.25282700	2.69846800	3.40437900
H	6.63700800	2.14853900	2.96321200
C	-1.79197200	0.94662300	-1.98870300
C	-2.81446400	1.83026200	-2.35448000
C	-1.95766700	-0.43639300	-2.17887800
C	-3.99566500	1.33126000	-2.91218800
H	-2.70078100	2.89842800	-2.20039100
C	-3.13673200	-0.92640500	-2.73483000
H	-1.17888000	-1.12881100	-1.86980600
C	-4.15894200	-0.04281800	-3.09991800
H	-4.78856900	2.01874700	-3.19144200
H	-3.26238600	-1.99698300	-2.86756000
H	-5.08241400	-0.42671500	-3.52352200
C	-0.35683500	3.27189600	-0.80784300
C	-0.32913100	4.25625900	-1.81106200
C	-0.47394600	3.65204700	0.53917000
C	-0.41708000	5.60482800	-1.46526600
H	-0.24447900	3.98228100	-2.85849100
C	-0.56019100	5.00336400	0.87676000

H	-0.50149500	2.89295800	1.31439500
C	-0.53056800	5.97888400	-0.12301000
H	-0.39468500	6.36154600	-2.24362100
H	-0.64800300	5.29231100	1.91982600
H	-0.59481100	7.03015300	0.14218700
Pt	0.36834200	0.12097100	0.52915900
F	1.98261700	-1.11582900	2.91513800
C	-1.51654900	0.17397800	1.21107500
C	-2.70604100	0.08786800	1.48914000
C	-4.10540200	-0.06506200	1.71899100
C	-4.59810400	-0.58330700	2.93450900
C	-5.02553900	0.26817300	0.70124700
C	-5.96812200	-0.76043700	3.12433000
H	-3.89683600	-0.84487500	3.72177500
C	-6.39283600	0.08571000	0.89855400
H	-4.65300900	0.66080300	-0.23996000
C	-6.87064400	-0.42772900	2.10916900
H	-6.33244200	-1.16106500	4.06649200
H	-7.08820300	0.34331800	0.10402300
H	-7.93734200	-0.56863900	2.25962700
C	1.05736500	-1.32111100	2.00280000
C	0.37134400	-2.23258200	1.47286300
C	-0.50914300	-3.05792000	0.74372700
C	-0.08139800	-3.62817700	-0.47913100
C	-1.84213500	-3.23478300	1.18181000
C	-0.98123000	-4.35404500	-1.24943700
H	0.93934100	-3.47743000	-0.80953500
C	-2.73054100	-3.96178800	0.39941400
H	-2.16381000	-2.76845300	2.10545100
C	-2.30353000	-4.51698000	-0.81412600

H	-0.65946400	-4.78689700	-2.19131400
H	-3.75826300	-4.08836500	0.72462000
H	-3.00504000	-5.07769600	-1.42485200

[(dppe)Pt(C≡CPh)]$^{+1}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2114.910842 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2114.346445 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2114.451637 hartrees

P	-0.40471800	-0.16540400	1.26738700
P	2.50744400	0.13308300	0.09788500
C	2.30649200	-0.32997700	1.88801600
H	2.28562300	-1.42302700	1.94245000
H	3.15638200	0.02122300	2.47918000
C	0.99374000	0.27817300	2.39723100
H	0.75936400	-0.02791200	3.42120600
H	1.03736700	1.37274900	2.39034400
C	-0.84781600	-1.90495100	1.55008000
C	-1.70611400	-2.54167400	0.63580900
C	-0.35993200	-2.61399600	2.65982300
C	-2.07394100	-3.87036700	0.83861600
H	-2.07728500	-1.99714400	-0.22630900
C	-0.72748200	-3.94756200	2.84885100
H	0.29918000	-2.14561300	3.38201600
C	-1.58280800	-4.57592200	1.94157900
H	-2.73940200	-4.35636500	0.13147100
H	-0.34346800	-4.49150100	3.70637600
H	-1.86479400	-5.61387200	2.09180200
C	-1.80320800	0.89022000	1.73147900
C	-2.90634200	0.37498100	2.42484300

C	-1.74728300	2.25390600	1.40054300
C	-3.94987400	1.22836900	2.79151400
H	-2.95737100	-0.68032000	2.67202700
C	-2.79092000	3.09813200	1.77285600
H	-0.90105700	2.64279700	0.84050600
C	-3.89305000	2.58571200	2.46771100
H	-4.80741400	0.82888200	3.32425000
H	-2.75036600	4.15190900	1.51445400
H	-4.70884600	3.24472600	2.74977400
C	3.57336600	-1.13644900	-0.65762800
C	4.88181000	-0.89130300	-1.09617400
C	3.00480000	-2.41160500	-0.83230000
C	5.61934700	-1.91844200	-1.69024300
H	5.32488800	0.09228500	-0.98038000
C	3.74965400	-3.43371400	-1.41833900
H	1.98074800	-2.59851200	-0.51745100
C	5.05782800	-3.18757900	-1.84843700
H	6.63269700	-1.72412600	-2.02920500
H	3.30744000	-4.41720400	-1.54735000
H	5.63508500	-3.98273200	-2.31129900
C	3.36938700	1.73455900	0.08519900
C	4.54620600	1.93997900	0.82666300
C	2.83229000	2.78929800	-0.66932200
C	5.17729400	3.18345900	0.80472800
H	4.97562500	1.13479900	1.41613900
C	3.46724600	4.03273100	-0.68586600
H	1.91741000	2.64023000	-1.23508600
C	4.63851800	4.22976800	0.04906600
H	6.08670200	3.33573300	1.37826200
H	3.04489300	4.84535500	-1.26940100

H	5.13086200	5.19783300	0.03653700
Pt	0.31903800	0.15433600	-0.81050100
C	-1.56825600	0.19073300	-1.47645000
C	-2.77531500	0.21715000	-1.70083500
C	-4.18892400	0.28845100	-1.87641200
C	-4.97434900	0.95739300	-0.91196400
C	-4.83069100	-0.30835500	-2.98079400
C	-6.35892300	1.02136400	-1.05228700
H	-4.48601400	1.41712500	-0.05879400
C	-6.21644700	-0.23537500	-3.11498700
H	-4.23375100	-0.82579600	-3.72606900
C	-6.98566600	0.42735800	-2.15305800
H	-6.95056900	1.53675600	-0.30044100
H	-6.69812600	-0.69862100	-3.97173600
H	-8.06545600	0.48016900	-2.26032100

[(dppe)Pt(C≡CPh)(NCCH$_3$)]$^{+1}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2247.703313 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2247.086672 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2247.203407 hartrees

P	0.65089800	-0.92627100	1.16208300
P	-2.35847300	-0.31100400	0.41139500
C	-1.98556100	-1.01775800	2.08682800
H	-1.81641300	-0.17933600	2.77072800
H	-2.83173400	-1.59940900	2.46377400
C	-0.72995900	-1.89255100	1.95712200
H	-0.40589400	-2.27040800	2.93067100
H	-0.92508200	-2.75785000	1.31456300
C	1.47262200	-0.02294000	2.51140900

C	1.73871400	1.35064400	2.40024100
C	1.83611300	-0.70841000	3.68472000
C	2.35645500	2.02813300	3.45315200
H	1.47692300	1.88269100	1.49307200
C	2.45699600	-0.02572300	4.73003000
H	1.64973500	-1.77356900	3.78535600
C	2.71489400	1.34366500	4.61644500
H	2.55736200	3.09138200	3.36127500
H	2.73719100	-0.56279400	5.63113300
H	3.19521200	1.87419900	5.43345600
C	1.80607100	-2.14888300	0.47015900
C	3.12507300	-2.28151700	0.92156200
C	1.34646100	-2.93831300	-0.59754000
C	3.97737200	-3.20588000	0.31140500
H	3.49316700	-1.66568000	1.73514400
C	2.20045300	-3.86138800	-1.19807800
H	0.33126700	-2.81970700	-0.96782900
C	3.51779600	-3.99443500	-0.74554000
H	5.00047500	-3.30401100	0.66207800
H	1.84180600	-4.47006800	-2.02277100
H	4.18432400	-4.70917400	-1.21925800
C	-3.55786000	1.04527400	0.59255100
C	-4.82110900	1.03460600	-0.01345700
C	-3.11448100	2.19881300	1.26396700
C	-5.63886300	2.16591900	0.06227400
H	-5.16529500	0.15701000	-0.55048600
C	-3.93770300	3.32031500	1.34316000
H	-2.11871600	2.22527000	1.70024500
C	-5.20034500	3.30622800	0.73909600
H	-6.61588200	2.15387500	-0.41160900

H	-3.59092400	4.20833700	1.86312300
H	-5.83674400	4.18466400	0.79228600
C	-3.12616400	-1.67466500	-0.51694900
C	-4.24581400	-2.35012700	-0.00019900
C	-2.57255900	-2.08585200	-1.74031100
C	-4.80426200	-3.41827900	-0.70138800
H	-4.68727500	-2.04213400	0.94346900
C	-3.13388500	-3.15932200	-2.43571700
H	-1.70428900	-1.57604900	-2.14714300
C	-4.24789200	-3.82414100	-1.91856400
H	-5.67013500	-3.93395200	-0.29707000
H	-2.69839100	-3.47500900	-3.37905200
H	-4.68216500	-4.65900100	-2.46082600
Pt	-0.28284900	0.41925700	-0.40985900
N	-1.26645500	1.74463400	-1.71805800
C	-2.00692000	2.49007900	-2.20090500
C	-2.96904000	3.42103300	-2.76758000
H	-3.28162200	3.07633700	-3.75754100
H	-3.84140000	3.47010300	-2.10717300
H	-2.52045100	4.41475100	-2.85398000
C	1.57224200	0.93272200	-1.00281800
C	2.74300400	1.14333000	-1.29635800
C	4.12467700	1.32882200	-1.60530600
C	5.04819100	0.29059100	-1.35465600
C	4.60003500	2.53730300	-2.15516100
C	6.40028700	0.46084300	-1.64573400
H	4.69045600	-0.64364200	-0.93147500
C	5.95476900	2.70043500	-2.44191200
H	3.89766600	3.34214000	-2.35214300
C	6.86019500	1.66490400	-2.18964900

H	7.09789800	-0.34847800	-1.44701100
H	6.30497200	3.63840700	-2.86441900
H	7.91498500	1.79493100	-2.41512100

Acetonitrile

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -132.763680 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -132.713574 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -132.742092 hartrees

N	1.44018200	0.00000000	-0.00002900
C	0.27908700	0.00000000	0.00007400
C	-1.18096300	0.00000100	-0.00002400
H	-1.55662700	0.90126100	-0.49320900
H	-1.55661900	-0.87776900	-0.53390300
H	-1.55677200	-0.02349800	1.02701300

1,4-diphenyl-1,3-butadiyne

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -615.641711 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -615.425257 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -615.482149 hartrees

C	-5.43186300	0.85630200	-0.85572900
C	-4.03915500	0.86071100	-0.86011600
C	-3.32516300	0.00003400	-0.00005700
C	-4.03899700	-0.86071700	0.86006000
C	-5.43170500	-0.85645200	0.85578400
C	-6.13160100	-0.00011100	0.00005600
H	-5.97280500	1.52257800	-1.52153100
H	-3.49274000	1.52422700	-1.52314500
H	-3.49245900	-1.52417700	1.52304500
H	-5.97252500	-1.52278400	1.52163000

H	-7.21778000	-0.00016800	0.00010000
C	-1.90213300	0.00010800	-0.00011500
C	-0.68034600	0.00015700	-0.00014400
C	0.68034600	0.00013600	-0.00008300
C	1.90213300	0.00010300	-0.00004500
C	3.32516300	0.00003400	0.00000600
C	4.03906600	-0.86091700	-0.85985300
C	4.03908700	0.86092200	0.85991200
C	5.43177400	-0.85664100	-0.85547700
H	3.49258100	-1.52453900	-1.52271900
C	5.43179400	0.85652000	0.85562800
H	3.49261800	1.52459500	1.52274000
C	6.13160100	-0.00009300	0.00009900
H	5.97264700	-1.52313000	-1.52112300
H	5.97268400	1.52296000	1.52130900
H	7.21778000	-0.00014100	0.00013600

(fluoroethynyl)benzene

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -407.612040 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -407.501042 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -407.541681 hartrees

C	-2.64510600	0.00029100	-0.00001200
C	-1.43983500	0.00076200	-0.00002500
C	-0.00776600	0.00036700	-0.00001500
C	0.70552600	-1.21384600	-0.00001400
C	0.70626100	1.21416400	-0.00002300
C	2.09936000	-1.20957100	0.00000000
H	0.15948800	-2.15233800	-0.00001800
C	2.10008200	1.20904900	0.00000800

H	0.16078500	2.15297500	-0.00002400
C	2.80097200	-0.00047600	0.00002800
H	2.63879600	-2.15255800	0.00001000
H	2.64010100	2.15170300	0.00002000
H	3.88726300	-0.00079400	0.00005300
F	-3.93371200	-0.00038100	0.00003100

B8. XYZ Cartesian coordinates of Reactant and Products in path IV

$TS_{IV,bipy}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.642429 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.197345 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.296657 hartrees

C	2.58674900	3.93233500	-0.05528600
C	3.91800200	3.52223000	-0.07144900
C	4.21568400	2.16333400	-0.16122200
C	3.17621600	1.23538600	-0.23585500
C	1.59095300	2.96441700	-0.12921400
C	3.38577400	-0.22721400	-0.32250800
C	4.64423900	-0.83085100	-0.34849100
C	4.73836600	-2.22020600	-0.40892000
H	5.71346900	-2.69486100	-0.42658400
C	3.57454600	-2.98620500	-0.44599500
C	2.34711200	-2.33309100	-0.42386400
H	2.31365400	4.97869100	0.01361900
H	4.72152300	4.24865500	-0.01488400
H	0.53713700	3.21498800	-0.11884600
H	3.60605300	-4.06830600	-0.49212600
H	1.40488300	-2.86710300	-0.45372200
H	5.54385500	-0.23022100	-0.31938200

H	5.24757100	1.83729800	-0.17106900
N	2.26371600	-0.99478100	-0.36052600
N	1.88469300	1.65884300	-0.21603500
Pt	0.42825100	0.10749400	-0.36000600
F	0.70860800	0.25434500	-2.28574900
C	-1.14754500	1.24398400	-0.18994200
C	-2.11862100	1.98554000	-0.11316000
C	-3.24820200	2.83257400	0.02208400
C	-4.55275300	2.29878200	-0.08567200
C	-3.08627200	4.21578700	0.26238700
C	-5.66064000	3.13059700	0.04070200
H	-4.67708300	1.23590400	-0.26804200
C	-4.20138100	5.03844900	0.38575400
H	-2.08518400	4.62692200	0.34684300
C	-5.48910300	4.50000900	0.27586600
H	-6.65984200	2.71386700	-0.04374600
H	-4.06981300	6.10086600	0.56783000
H	-6.35673800	5.14591800	0.37356700
C	-0.78070700	-1.43176600	-0.33168700
C	-1.49291500	-2.42463100	-0.25272600
C	-2.31723100	-3.56832400	-0.09340400
C	-3.72412000	-3.44692400	-0.15124900
C	-1.74302000	-4.83760200	0.14439800
C	-4.52949700	-4.56790300	0.02363700
H	-4.16526000	-2.47143700	-0.33068000
C	-2.55803500	-5.95153000	0.31850000
H	-0.66258600	-4.93139500	0.19238700
C	-3.95068900	-5.82060200	0.25945300
H	-5.60982800	-4.46757200	-0.02093200
H	-2.11017100	-6.92356700	0.50232300

H	-4.58321700	-6.69249200	0.39829800
N	0.80853700	0.67759400	2.63288200
C	1.68261800	-0.03647100	2.91478000
C	2.77981800	-0.93423800	3.25584500
H	3.73757700	-0.46518400	3.01257900
H	2.75630600	-1.16592800	4.32467600
H	2.68199400	-1.86545400	2.68923600

V_{bipy}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.648353 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.201976 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1462.302140 hartrees

C	-2.90187200	-3.89839800	0.20180400
C	-4.20724700	-3.41200500	0.23291400
C	-4.43135200	-2.04085300	0.12058900
C	-3.34608200	-1.17475000	-0.01974900
C	-1.85765500	-2.99156500	0.05971700
C	-3.47853400	0.29322000	-0.15095800
C	-4.69811600	0.96919500	-0.09321100
C	-4.72049500	2.35687900	-0.22260100
H	-5.66508100	2.88812900	-0.17587100
C	-3.52505900	3.04764700	-0.40973900
C	-2.33910700	2.32335900	-0.45696500
H	-2.68591400	-4.95702700	0.28437700
H	-5.04748400	-4.08942500	0.34095900
H	-0.82019200	-3.30222300	0.02722700
H	-3.50032100	4.12599400	-0.51321000
H	-1.37462000	2.79828500	-0.58951200
H	-5.62285300	0.42727200	0.05641000

H	-5.44276400	-1.65655600	0.13971300
N	-2.32559500	0.98874500	-0.33081900
N	-2.08054700	-1.67224700	-0.04520500
Pt	-0.54917300	-0.20933200	-0.30633200
F	-0.83356400	-0.45975600	-2.20751200
C	0.98050200	-1.41766800	-0.12294900
C	1.91077700	-2.21028600	-0.06217100
C	2.99733600	-3.11875400	0.03824400
C	4.31986300	-2.67020100	-0.17674000
C	2.77145100	-4.47955600	0.34253200
C	5.38329700	-3.56380600	-0.09352700
H	4.49396400	-1.62419000	-0.40925000
C	3.84228300	-5.36462400	0.42290500
H	1.75611600	-4.82560500	0.50950000
C	5.14856200	-4.91096300	0.20536300
H	6.39683100	-3.21223200	-0.26224300
H	3.66090800	-6.41000000	0.65440100
H	5.98123500	-5.60542600	0.26859600
C	0.72169700	1.27304900	-0.40820800
C	1.46935400	2.24095400	-0.42435400
C	2.32451900	3.37288500	-0.36166400
C	3.72111500	3.22385100	-0.50784700
C	1.78764600	4.65905400	-0.13096300
C	4.55411800	4.33592700	-0.42758200
H	4.13394700	2.23506400	-0.68167800
C	2.63018400	5.76384100	-0.04960400
H	0.71391200	4.77483400	-0.01888000
C	4.01299000	5.60620200	-0.19793700
H	5.62715900	4.21432500	-0.54179800
H	2.21041500	6.74930700	0.12894200

H	4.66712800	6.47079200	-0.13382600
N	-1.60706100	1.06773300	2.81332200
C	-0.55679000	1.56231200	2.87313500
C	0.76184700	2.18349400	2.94415500
H	0.75508300	3.13664300	2.40776100
H	1.04020300	2.35830900	3.98748200
H	1.50091400	1.52915100	2.47377900

VI_{bipy}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.874434 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.480341 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.568902 hartrees

C	-3.27847900	3.49991800	-0.02951500
C	-4.53529900	2.90090400	0.02633400
C	-4.63387600	1.51048800	0.02194900
C	-3.47299500	0.73821000	-0.04062400
C	-2.15469400	2.68278400	-0.08558100
C	-3.47307900	-0.74218400	-0.05864500
C	-4.63489900	-1.51539200	-0.03900900
C	-4.53604800	-2.90564500	-0.05888000
H	-5.43594500	-3.51106500	-0.04415500
C	-3.27812100	-3.50369300	-0.09790700
C	-2.15377800	-2.68572800	-0.11954900
H	-3.16008000	4.57698300	-0.02817800
H	-5.43451400	3.50564600	0.07400000
H	-1.14813100	3.08163100	-0.12484400
H	-3.15943700	-4.58061300	-0.11360600
H	-1.14663500	-3.08383200	-0.15069600
H	-5.60948900	-1.04589200	-0.01218100

H	-5.60736800	1.04018800	0.06852100
N	-2.25663300	-1.34808100	-0.10256700
N	-2.25730500	1.34508400	-0.09180400
Pt	-0.58464600	-0.00153900	-0.09722200
F	-0.80592800	-0.00524700	1.82526300
C	0.82338000	-1.37103100	-0.13050900
C	1.67108200	-2.25086400	-0.07825500
C	2.66238600	-3.26820400	-0.04944600
C	2.29558400	-4.63096900	-0.10195500
C	4.02975700	-2.92542100	0.04123000
C	3.27345100	-5.62044700	-0.05909400
H	1.24532500	-4.89665000	-0.17248900
C	4.99958200	-3.92283700	0.08165300
H	4.31275400	-1.87802100	0.08036300
C	4.62560000	-5.27065600	0.03233500
H	2.98334000	-6.66630500	-0.09699700
H	6.04870400	-3.65130600	0.15250000
H	5.38546300	-6.04602700	0.06494500
C	0.82247000	1.36891800	-0.13035500
C	1.66811100	2.25113100	-0.08438400
C	2.65575900	3.27218600	-0.06497200
C	2.28312600	4.63326200	-0.12100600
C	4.02505000	2.93523400	0.01811100
C	3.25724300	5.62681500	-0.08937800
H	1.23134900	4.89440100	-0.18563600
C	4.99108900	3.93670300	0.04733600
H	4.31252100	1.88916200	0.05992000
C	4.61137900	5.28278000	-0.00569900
H	2.96268500	6.67131900	-0.13017300
H	6.04176000	3.66971800	0.11217400

H	5.36834800	6.06129800	0.01796600

$TS_{V,bipy}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.869484 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.476791 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.564807 hartrees

C	4.39235900	1.81768200	-0.76158100
C	5.29495800	0.84023900	-0.34741300
C	4.81477000	-0.39314400	0.08889600
C	3.43929700	-0.62806500	0.10218600
C	3.03283800	1.52665300	-0.72700900
C	2.82899900	-1.89558400	0.55568600
C	3.55498800	-2.98446400	1.04238600
C	2.88032900	-4.13228000	1.45381100
H	3.43997000	-4.98093800	1.83209900
C	1.48978400	-4.17794500	1.37388600
C	0.81291100	-3.06652900	0.88250500
H	4.72446800	2.79013900	-1.10564300
H	6.36260300	1.03126300	-0.36024400
H	2.28344800	2.24736500	-1.02937600
H	0.92881900	-5.05238200	1.68215100
H	-0.26538900	-3.03383400	0.78604100
H	4.63480800	-2.94116900	1.10215500
H	5.50789700	-1.15806800	0.41404300
N	1.47587200	-1.96801300	0.49572000
N	2.57475200	0.33657800	-0.30810100
Pt	0.52039000	-0.24665100	-0.30895000
F	0.98607300	-1.37768200	-1.91289400
C	-1.33268900	-0.89070800	-0.23893000

C	-2.47118900	-1.33121000	-0.19870200
C	-3.79423400	-1.85596100	-0.15585600
C	-4.01202100	-3.24971700	-0.10370200
C	-4.90879800	-0.98985900	-0.17071100
C	-5.30814800	-3.75786800	-0.06877400
H	-3.15740200	-3.91957300	-0.09326700
C	-6.20134100	-1.50734500	-0.13668800
H	-4.74603800	0.08296300	-0.21076000
C	-6.40602100	-2.89055000	-0.08581600
H	-5.46376600	-4.83219600	-0.02959200
H	-7.05170700	-0.83158600	-0.15031800
H	-7.41558900	-3.29047400	-0.06019400
C	-0.17474400	1.51322100	-0.06092800
C	-0.57873900	2.67783600	0.10993600
C	-1.02906900	3.97900000	0.32060600
C	-0.10396100	5.06038300	0.35632600
C	-2.41908200	4.23235800	0.49482100
C	-0.56344800	6.35142600	0.55836800
H	0.95290600	4.85492400	0.22309800
C	-2.86136100	5.52968000	0.69559300
H	-3.11429700	3.40012100	0.46523300
C	-1.93736000	6.58608100	0.72728700
H	0.13581900	7.18048900	0.58598500
H	-3.91939600	5.73030900	0.82749600
H	-2.29075100	7.60065300	0.88482100

VII_{bipy}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.878764 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.484593 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.573356 hartrees

C	4.42275700	-0.85774100	-2.10966200
C	5.12059900	-1.25965100	-0.97166100
C	4.42777600	-1.50197200	0.21517600
C	3.04477700	-1.33482600	0.22951500
C	3.03988900	-0.70751600	-2.02961900
C	2.17643500	-1.54557900	1.39488200
C	2.61699900	-1.91691800	2.66354300
C	1.70195500	-2.07393600	3.70126900
H	2.04790200	-2.35960300	4.68839300
C	0.34657100	-1.85764800	3.46002500
C	-0.06435700	-1.48981900	2.18637500
H	4.93076500	-0.66161600	-3.04632100
H	6.19731200	-1.38561800	-1.00228400
H	2.43626300	-0.39804300	-2.87500300
H	-0.39892800	-1.96614400	4.23852700
H	-1.09872000	-1.30800100	1.93602900
H	3.67372900	-2.07693400	2.83583900
H	4.95948900	-1.81595500	1.10445300
N	0.83917500	-1.34739500	1.19538200
N	2.38682100	-0.94423600	-0.88766400
Pt	0.27776400	-0.82360400	-0.64800800
F	0.21698000	-2.77989100	-1.10099200
C	-1.67516900	-0.73374400	-0.55418000
C	-2.89055500	-0.67459100	-0.42432900
C	-4.30200500	-0.58207300	-0.29802200
C	-5.12142400	-1.71233400	-0.51118100
C	-4.90143100	0.64757300	0.05535300
C	-6.50234500	-1.61134700	-0.36891800
H	-4.66179700	-2.65740500	-0.78312100

C	-6.28322900	0.73800700	0.19368100
H	-4.27162200	1.51685900	0.21770900
C	-7.08622600	-0.38883600	-0.01740000
H	-7.12617000	-2.48521500	-0.53180600
H	-6.73674800	1.68645000	0.46600500
H	-8.16430700	-0.31445500	0.09178000
C	0.36359800	1.11578200	-0.28557600
C	0.46630100	2.31411900	-0.07035200
C	0.58078700	3.71968700	0.11972800
C	1.80833500	4.37389100	-0.12127800
C	-0.53269500	4.48111400	0.53503000
C	1.91436800	5.75177900	0.04877000
H	2.66543100	3.79021400	-0.44321500
C	-0.41686400	5.85876300	0.70232400
H	-1.47870700	3.98068600	0.71818800
C	0.80403200	6.49785300	0.45939400
H	2.86263700	6.24625100	-0.14119200
H	-1.27974500	6.43684200	1.02009700
H	0.88959700	7.57299300	0.58812400

$TS_{VII,bipy}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.870070 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.476944 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.564621 hartrees

C	4.53712700	1.76017100	-1.47386000
C	5.43397300	0.89476200	-0.84862800
C	4.95658600	-0.23205300	-0.17791900
C	3.58271800	-0.46177400	-0.14611000
C	3.17506500	1.47825800	-1.40407100

C	2.93007200	-1.60971700	0.49890700
C	3.60120100	-2.64725300	1.14260800
C	2.88372400	-3.69501400	1.71382200
H	3.40928200	-4.49997900	2.21514800
C	1.49225800	-3.69549800	1.63756400
C	0.84856100	-2.64864900	0.99288900
H	4.87668100	2.64017900	-2.00697400
H	6.50023000	1.08993700	-0.88203100
H	2.42342000	2.10627200	-1.86744600
H	0.89439600	-4.48787400	2.07139400
H	-0.22641300	-2.58169700	0.91079200
H	4.68233200	-2.63375300	1.19180500
H	5.64652100	-0.91122100	0.30626900
N	1.56494900	-1.65267100	0.43458600
N	2.72939300	0.40067500	-0.74868700
Pt	0.67914900	-0.12355900	-0.54900400
F	0.46867200	-0.00438000	-2.52743200
C	-1.21115400	-0.63471000	-0.40585100
C	-2.35435300	-1.04489800	-0.28028700
C	-3.68302200	-1.52584000	-0.11141700
C	-4.11699300	-1.96002300	1.15993100
C	-4.57472800	-1.59228900	-1.20259900
C	-5.40817900	-2.45272900	1.32894500
H	-3.43174000	-1.90768600	2.00059200
C	-5.86519200	-2.08396700	-1.02242900
H	-4.24335400	-1.25893300	-2.18116000
C	-6.28501600	-2.51612100	0.24041000
H	-5.73235000	-2.78776300	2.30993500
H	-6.54518000	-2.13280100	-1.86789500
H	-7.29171700	-2.90085700	0.37575100

C	0.60484300	0.56011100	1.29790700
C	0.62778700	0.88667700	2.47020700
C	0.61904400	1.29928200	3.83587700
C	1.62109600	2.15585300	4.33499700
C	-0.39024600	0.84065600	4.70728800
C	1.61146200	2.53951900	5.67448000
H	2.39913000	2.51087500	3.66600700
C	-0.39045200	1.22845000	6.04539800
H	-1.16324900	0.18104700	4.32462300
C	0.60818900	2.07790100	6.53290700
H	2.38827500	3.19940700	6.04998700
H	-1.17092400	0.86784900	6.70929300
H	0.60453900	2.37875300	7.57662600

$TS_{VI,bipy}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.842665 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.450766 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1329.538689 hartrees

C	4.87638600	0.37488800	-1.89730800
C	5.48441800	0.41213200	-0.64353000
C	4.74411900	0.08081000	0.49133200
C	3.40475000	-0.28197600	0.33704000
C	3.53373300	0.00622200	-1.97527200
C	2.51722200	-0.66447200	1.45158200
C	2.93311600	-0.75635000	2.78052600
C	2.04146100	-1.15037200	3.77352500
H	2.37353500	-1.21919900	4.80348800

C	0.72767200	-1.45856200	3.42795400
C	0.34047900	-1.35648800	2.10010500
H	5.42231200	0.62573900	-2.79938500
H	6.52635800	0.69660400	-0.54342800
H	3.00017700	-0.04006600	-2.91830600
H	-0.00162200	-1.77523100	4.16383100
H	-0.66441100	-1.57831700	1.76988800
H	3.95940600	-0.52613800	3.03472400
H	5.20954900	0.10953100	1.46826000
N	1.21733600	-0.96260000	1.15390700
N	2.83136500	-0.30929100	-0.88437500
Pt	0.66074700	-0.86568000	-0.75859100
F	1.36451300	-2.75389300	-0.95078100
C	-1.33249400	-0.73293400	-0.46085000
C	-2.51678900	-1.04027900	-0.34050700
C	-3.89694300	-1.34376300	-0.22679200
C	-4.44849600	-1.74923500	1.00853000
C	-4.74329500	-1.23605600	-1.35312600
C	-5.80833100	-2.03244300	1.10883100
H	-3.80272200	-1.83586400	1.87714500
C	-6.10006100	-1.52743400	-1.24091700
H	-4.32393200	-0.92421400	-2.30484900
C	-6.63847200	-1.92476900	-0.01218800
H	-6.22236100	-2.34101300	2.06453900
H	-6.74051400	-1.44207400	-2.11422000
H	-7.69783100	-2.14952100	0.07080700
C	-0.36578900	0.82818700	-0.49566700
C	-0.60635800	2.01959100	-0.27620900
C	-0.95837100	3.35751000	-0.00292000
C	-1.05735300	4.30699000	-1.04754800

C	-1.21143900	3.76723300	1.32832900
C	-1.40119300	5.62412000	-0.76262500
H	-0.86210200	3.99451100	-2.06854800
C	-1.54956200	5.08867000	1.59940300
H	-1.13677400	3.03885300	2.12975400
C	-1.64657500	6.01953700	0.55797300
H	-1.47661000	6.34710400	-1.56945200
H	-1.74077500	5.39607100	2.62329700
H	-1.91243900	7.04997200	0.77484700

$TS_{IV,dppe}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2655.259665 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.531472 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.663421 hartrees

P	1.63068200	-1.47126300	0.77606600
P	-1.65274700	-1.38656300	0.80986400
C	-0.74332700	-2.42390200	2.03911000
H	-0.64596800	-1.77821700	2.91607400
H	-1.34087800	-3.29159000	2.33396600
C	0.63220900	-2.86496700	1.50993600
H	1.21310300	-3.33920600	2.30606200
H	0.50486500	-3.59891200	0.70940700
C	2.80562500	-0.88022900	2.02560200
C	4.10603000	-0.50468700	1.65033300
C	2.39561800	-0.73440800	3.36266700
C	4.98490700	0.00872100	2.60377900
H	4.43849400	-0.62090800	0.62450400
C	3.28293300	-0.22417400	4.30958600
H	1.39471200	-1.01248700	3.66903600
C	4.57498700	0.15179000	3.93229800

H	5.99110100	0.29049800	2.30808900
H	2.96307800	-0.12050900	5.34198800
H	5.26246100	0.55012600	4.67258100
C	2.59302600	-2.14472800	-0.60920400
C	2.91383600	-3.51150500	-0.67061200
C	3.05703700	-1.27270600	-1.60886800
C	3.68069400	-3.99858500	-1.72948600
H	2.58165000	-4.19949800	0.09966500
C	3.83105500	-1.76748700	-2.65862300
H	2.80326300	-0.21920900	-1.57124700
C	4.13887600	-3.12952300	-2.72385800
H	3.92028800	-5.05641600	-1.77489200
H	4.18295200	-1.08940700	-3.42997100
H	4.73347100	-3.51319500	-3.54748500
C	-3.11994500	-0.68644300	1.61832200
C	-4.40018400	-1.19564400	1.35036500
C	-2.96294600	0.39732600	2.49996000
C	-5.51623700	-0.62385700	1.96452100
H	-4.53047900	-2.02532300	0.66367200
C	-4.08436000	0.96196200	3.10521100
H	-1.97384600	0.79357500	2.69902700
C	-5.36011300	0.45587500	2.83724000
H	-6.50541300	-1.01909900	1.75417600
H	-3.96201600	1.80343500	3.78051000
H	-6.23118200	0.90463100	3.30551700
C	-2.22470800	-2.40794000	-0.56974400
C	-2.20003200	-3.81086700	-0.53406000
C	-2.73519100	-1.74211900	-1.69843500
C	-2.67997800	-4.54033500	-1.62431300
H	-1.82118200	-4.34143200	0.33312200

C	-3.22086200	-2.47833600	-2.77714900
H	-2.73793700	-0.65648500	-1.73132700
C	-3.19031200	-3.87655900	-2.74244100
H	-2.65578600	-5.62518000	-1.59574300
H	-3.61351200	-1.96166300	-3.64740300
H	-3.56168700	-4.44744100	-3.58809400
Pt	0.01345100	0.23880400	0.19589800
C	-1.44025900	1.48756400	-0.36563200
C	-2.43477900	2.16797200	-0.60206300
C	-3.64066600	2.87177700	-0.84106800
C	-4.87131200	2.28187600	-0.46597500
C	-3.64235600	4.15788400	-1.42621200
C	-6.06467500	2.96653500	-0.66835700
H	-4.86808000	1.29600900	-0.01306100
C	-4.84298900	4.83155900	-1.62808300
H	-2.69878600	4.61165800	-1.71308800
C	-6.05487900	4.24041200	-1.24992900
H	-7.00443600	2.50966700	-0.37208900
H	-4.83794900	5.81990200	-2.07813900
H	-6.98891400	4.77199900	-1.40736300
N	0.08213800	-0.24378800	-2.70708100
C	0.17325300	-1.37988600	-2.94143300
C	0.29214800	-2.80191100	-3.22259900
H	-0.29860800	-3.05980200	-4.10576900
H	1.34171600	-3.05916100	-3.39040000
H	-0.08728000	-3.37017100	-2.36829300
C	1.47361100	1.53322800	-0.29011200
C	2.39800300	2.30295700	-0.51936900
F	0.11001100	0.53476400	2.16403000
C	3.50905000	3.14606400	-0.79986600

C	3.35596500	4.31704400	-1.57334700
C	4.79077700	2.81477000	-0.30715600
C	4.45481000	5.12809800	-1.84547900
H	2.37249200	4.57614500	-1.95368400
C	5.88299600	3.63279300	-0.58212500
H	4.90856300	1.91948200	0.29482800
C	5.72004000	4.78987500	-1.35242400
H	4.32605900	6.02631900	-2.44257900
H	6.86359100	3.36915900	-0.19610300
H	6.57456100	5.42533800	-1.56664600

V_{dppe}

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2655.264253 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.534831 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2654.666890 hartrees

P	1.62321800	-1.47414600	0.81470600
P	-1.65000000	-1.39299800	0.83876800
C	-0.74874100	-2.41144300	2.08971800
H	-0.66249000	-1.75105500	2.95714600
H	-1.34712200	-3.27572700	2.39291900
C	0.63530200	-2.85675300	1.58551000
H	1.21484300	-3.29441300	2.40332100
H	0.52291500	-3.62253100	0.81290800
C	2.80726200	-0.85665500	2.04321700
C	4.11028300	-0.50462100	1.65493200
C	2.39887200	-0.66146900	3.37434800
C	4.99379900	0.03418600	2.59017600
H	4.44024100	-0.65608800	0.63278000
C	3.29047200	-0.12541400	4.30285300

H	1.39476800	-0.91803700	3.68938400
C	4.58559500	0.22655900	3.91286900
H	6.00193500	0.29809600	2.28467000
H	2.97148700	0.01758200	5.33085000
H	5.27627600	0.64527500	4.63879000
C	2.57312100	-2.15765400	-0.57228500
C	2.92962400	-3.51647000	-0.60688000
C	2.99893800	-1.29620300	-1.59777700
C	3.69721200	-4.00610800	-1.66362900
H	2.62452800	-4.19488000	0.18309100
C	3.77651400	-1.79315400	-2.64431300
H	2.71971500	-0.24880400	-1.57943900
C	4.12198000	-3.14677500	-2.68176800
H	3.96591400	-5.05763700	-1.68839800
H	4.10056400	-1.12354800	-3.43501500
H	4.71960500	-3.53254600	-3.50222400
C	-3.13056900	-0.69598300	1.62357000
C	-4.40483900	-1.21096600	1.33896000
C	-2.98958400	0.39097800	2.50395700
C	-5.53131400	-0.64264100	1.93709700
H	-4.52198900	-2.04270100	0.65226200
C	-4.12129600	0.95221000	3.09291900
H	-2.00483200	0.79300800	2.71284300
C	-5.39113100	0.43946400	2.80968200
H	-6.51601700	-1.04231900	1.71453700
H	-4.01175500	1.79623700	3.76721400
H	-6.27020600	0.88538100	3.26553700
C	-2.19111100	-2.42010300	-0.54675200
C	-2.18476300	-3.82285100	-0.49611100
C	-2.65708300	-1.75807300	-1.69710500

C	-2.64084900	-4.55672300	-1.59289500
H	-1.83741900	-4.34802600	0.38755600
C	-3.12125300	-2.49956600	-2.78176200
H	-2.64529800	-0.67303700	-1.74092000
C	-3.11052700	-3.89738900	-2.73168500
H	-2.63125100	-5.64147800	-1.55383200
H	-3.48000400	-1.98723600	-3.66901700
H	-3.46482800	-4.47225800	-3.58199700
Pt	0.00965600	0.22460500	0.21322700
C	-1.44322500	1.49057400	-0.34273200
C	-2.43534900	2.17387000	-0.58083600
C	-3.64071000	2.87691600	-0.82740700
C	-4.87289900	2.28423200	-0.46275600
C	-3.64054100	4.16198100	-1.41427000
C	-6.06641600	2.96510700	-0.67736100
H	-4.87127200	1.29867700	-0.00920100
C	-4.84127200	4.83194200	-1.62852800
H	-2.69573800	4.61776700	-1.69384100
C	-6.05492300	4.23793600	-1.26099000
H	-7.00756600	2.50567700	-0.38952400
H	-4.83480200	5.81936400	-2.08060700
H	-6.98902800	4.76629300	-1.42863300
N	0.07931200	-0.20974200	-3.35324200
C	0.18504800	-1.36305900	-3.26476900
C	0.31434300	-2.81199400	-3.16836500
H	-0.29968500	-3.29306700	-3.93426600
H	1.35965500	-3.10301900	-3.29992900
H	-0.02848100	-3.14567700	-2.18634400
C	1.47398500	1.52473500	-0.27724400
C	2.39449100	2.29923400	-0.50869600

F	0.08564900	0.56556600	2.16983100
C	3.49984300	3.14785100	-0.79268600
C	3.33299100	4.33138900	-1.54415000
C	4.78969900	2.80912900	-0.32676600
C	4.42676400	5.14731900	-1.82151800
H	2.34317900	4.59563100	-1.90391700
C	5.87662900	3.63254700	-0.60622800
H	4.91753100	1.90394900	0.25819400
C	5.70010800	4.80181900	-1.35493800
H	4.28791900	6.05485200	-2.40201000
H	6.86369800	3.36367800	-0.24094400
H	6.55066600	5.44121200	-1.57317200

VII$_{dppe}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2522.535173 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2521.857446 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2521.979171 hartrees

Pt	0.29073600	-0.56443200	-0.87846400
F	0.53196900	-2.51104400	-1.44010100
C	-1.58283100	-0.68128400	-1.56155300
C	-2.77926600	-0.76372400	-1.79950700
C	-4.18316700	-0.82577300	-2.02585000
C	-4.99774100	0.27443400	-1.68033600
C	-4.78737700	-1.98583600	-2.55350400
C	-6.37790600	0.20932300	-1.85473500
H	-4.53591700	1.16442700	-1.26529700
C	-6.16860600	-2.04124500	-2.72629700
H	-4.16477700	-2.83503100	-2.81845700
C	-6.96735300	-0.94677600	-2.37740500

H	-6.99526600	1.06007500	-1.58076400
H	-6.62453600	-2.94025000	-3.13101600
H	-8.04425800	-0.99518100	-2.51112400
C	0.07110800	1.37677400	-0.60170800
C	-0.07099600	2.56252300	-0.35964900
C	-0.22867600	3.94199600	-0.04453200
C	0.89757500	4.73793900	0.24965500
C	-1.51411400	4.52032300	0.00614300
C	0.73661800	6.08087300	0.58292100
H	1.88576700	4.29225100	0.21398700
C	-1.66451100	5.86357100	0.34450400
H	-2.38124600	3.90540500	-0.21319700
C	-0.54178600	6.64724100	0.63177400
H	1.60996600	6.68699600	0.80668900
H	-2.65829000	6.30039000	0.38371900
H	-0.66283200	7.69458800	0.89338800
P	2.55366700	-0.40594900	0.06941900
C	2.25398000	-0.64856000	1.87844600
C	3.27049400	1.24416700	-0.18928600
C	3.82227900	-1.60961100	-0.42408600
C	0.94324200	0.02970700	2.29152400
H	3.08812500	-0.26953400	2.47435100
H	2.20698600	-1.73053400	2.03974400
C	3.89649800	1.97502700	0.82943400
C	3.21783700	1.76719700	-1.49266100
C	3.43365100	-2.86614700	-0.91583900
C	5.18447600	-1.29965500	-0.26836800
P	-0.46873700	-0.65214800	1.31738200
H	0.98511900	1.10759300	2.11653000
H	0.71664500	-0.14909500	3.34767500

C	4.47215500	3.21607500	0.54259300
H	3.94776500	1.59323700	1.84352700
C	3.79824300	3.00168300	-1.77372000
H	2.71333800	1.21401700	-2.28002500
C	4.41105700	-3.81007400	-1.23687200
H	2.38101100	-3.07425000	-1.07129500
C	6.15025900	-2.25229700	-0.59068300
H	5.49026800	-0.32440700	0.09769400
C	-1.96490000	0.28677200	1.66053400
C	-0.74237100	-2.35113900	1.88393000
C	4.42726700	3.72722000	-0.75608800
H	4.95413200	3.77921700	1.33583800
H	3.75331200	3.40148000	-2.78212200
C	5.76495200	-3.50745200	-1.07257200
H	4.11217500	-4.78063500	-1.62231000
H	7.20251200	-2.01274300	-0.46932900
C	-1.90417500	1.60904400	2.13190100
C	-3.20966700	-0.33192300	1.44592900
C	-1.31265500	-2.47453400	3.16844600
C	-0.33915400	-3.48903400	1.17209900
H	4.87476800	4.69213400	-0.97506700
H	6.52111900	-4.24511900	-1.32570800
C	-3.08493100	2.29966000	2.39603200
H	-0.95576300	2.10862300	2.28330700
C	-4.38296800	0.37000800	1.70827200
H	-3.26108400	-1.34726300	1.06941800
C	-1.46381400	-3.73857200	3.73274200
H	-1.64031800	-1.60022400	3.72203700
C	-0.50518300	-4.74883700	1.75177500
H	0.07361600	-3.38803900	0.17436100

C	-4.32172200	1.68443900	2.18140000
H	-3.03500000	3.32125700	2.75842600
H	-5.34186900	-0.10523300	1.53075300
C	-1.06056100	-4.87594000	3.02594900
H	-1.90235000	-3.83263500	4.72128300
H	-0.19974200	-5.63198000	1.19902200
H	-5.23872900	2.23104600	2.37962700
H	-1.18532900	-5.85956600	3.46892500

$TS_{VII,dppe}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2522.518214 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2521.840554 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2521.961175 hartrees

Pt	0.32358400	-0.45474200	-0.75545600
F	1.10157900	-1.20157700	-2.48019800
C	-1.50587900	-0.88829400	-1.43913100
C	-2.64351300	-1.15850300	-1.79343900
C	-3.97877400	-1.49119500	-2.16482400
C	-5.06722600	-0.82858200	-1.55870200
C	-4.23573000	-2.49534500	-3.12090900
C	-6.37480100	-1.16870900	-1.89885000
H	-4.87372700	-0.05598600	-0.82181900
C	-5.54671200	-2.82963800	-3.45388900
H	-3.40119000	-3.00726900	-3.59055200
C	-6.61922700	-2.16969700	-2.84476000
H	-7.20475000	-0.65277900	-1.42437000
H	-5.73293400	-3.60696500	-4.18951800
H	-7.63986700	-2.43403200	-3.10634800
C	-0.32411600	1.33912500	-0.34732100

C	-0.70714300	2.45858600	-0.07110000
C	-1.14922200	3.76797200	0.28392500
C	-0.25174600	4.85386200	0.26666700
C	-2.48520000	3.98017300	0.67982900
C	-0.68674800	6.12385700	0.64059500
H	0.77693700	4.68854700	-0.03796300
C	-2.90860100	5.25387300	1.05445900
H	-3.17394000	3.14168200	0.69934300
C	-2.01301800	6.32799300	1.03562900
H	0.01103900	6.95629100	0.62511400
H	-3.93903200	5.40825900	1.36175600
H	-2.34709600	7.31943300	1.32790500
P	2.54342800	0.14791900	0.06207600
C	2.42284500	0.19276000	1.91347900
C	2.91142900	1.79395000	-0.61110000
C	3.92038100	-0.97411000	-0.31808800
C	0.99189800	0.47236300	2.39034900
H	3.11083600	0.92651400	2.34070900
H	2.75571500	-0.79190100	2.25487700
C	3.27297000	2.89353500	0.17589300
C	2.76169600	1.93628100	-2.00253000
C	3.78575900	-1.94513600	-1.32255600
C	5.12021200	-0.86067600	0.40613000
P	-0.21027200	-0.62373500	1.51614800
H	0.70292600	1.50460100	2.18195100
H	0.89841800	0.28696600	3.46483000
C	3.48840200	4.13419400	-0.43045600
H	3.38178500	2.80361200	1.25135500
C	2.98197200	3.17599700	-2.59807200
H	2.45509800	1.08354300	-2.60434900

C	4.85341000	-2.80575500	-1.58963100
H	2.86290700	-2.00769200	-1.88929400
C	6.17777900	-1.72464000	0.12795200
H	5.23356800	-0.10647700	1.17973200
C	-1.89996600	-0.20932200	1.97083700
C	0.13479900	-2.34451500	1.98907900
C	3.34215400	4.27640100	-1.81238300
H	3.76519300	4.98802300	0.18059900
H	2.86318100	3.28652100	-3.67161900
C	6.04372800	-2.69863700	-0.86758300
H	4.75156500	-3.55966800	-2.36463600
H	7.10406800	-1.63873600	0.68795400
C	-2.18842200	0.96974100	2.67620500
C	-2.93930400	-1.06763400	1.57019600
C	-0.64627600	-2.94122400	2.99692000
C	1.21478900	-3.05769700	1.43317700
H	3.50468800	5.24427900	-2.27720000
H	6.86962000	-3.37147000	-1.07936900
C	-3.51220200	1.27987500	2.98615000
H	-1.40162700	1.64875000	2.98268600
C	-4.25740700	-0.74822300	1.88715800
H	-2.72244700	-1.96993300	1.01008300
C	-0.34585200	-4.22953700	3.43748500
H	-1.47758800	-2.40700200	3.44190100
C	1.50212900	-4.34588700	1.88009800
H	1.83964700	-2.63831900	0.65377900
C	-4.54479000	0.42527800	2.59152400
H	-3.73302600	2.19216800	3.53090700
H	-5.05806500	-1.40972800	1.57304500
C	0.72334600	-4.93421000	2.87953700

H	-0.95159000	-4.68044000	4.21718500
H	2.33578700	-4.88619400	1.44287100
H	-5.57421900	0.67355900	2.83135700
H	0.95013200	-5.93878500	3.22334200

$TS_{VI,dppe}$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2522.498056 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2521.822433 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2521.946404 hartrees

Pt	0.29709400	-0.17064200	-0.77406900
F	1.18382700	-1.47824400	-2.15746000
C	-1.67611700	-0.40187500	-1.22529400
C	-2.73737800	-0.85554400	-1.65647300
C	-3.98254000	-1.33849500	-2.12038800
C	-4.33092500	-1.23127500	-3.48649900
C	-4.89920500	-1.93034600	-1.22106300
C	-5.56195000	-1.70120300	-3.93360600
H	-3.62847200	-0.77800500	-4.17921300
C	-6.12529800	-2.40037000	-1.68216000
H	-4.63373400	-2.01348700	-0.17253800
C	-6.46187100	-2.28744100	-3.03596000
H	-5.82142400	-1.61245700	-4.98461100
H	-6.82267500	-2.85468200	-0.98421800
H	-7.42065900	-2.65465500	-3.39035400
C	-1.19344700	1.03675800	-0.16897600
C	-1.75236500	2.00624200	0.34030500
C	-2.42629300	3.11806000	0.90590100
C	-3.33451200	2.94657500	1.97386400
C	-2.19133100	4.42106900	0.41234000

C	-3.97387900	4.04886100	2.53597900
H	-3.53672100	1.94710000	2.34545600
C	-2.83778500	5.51505500	0.98176500
H	-1.49619100	4.55789500	-0.40955700
C	-3.72793300	5.33611000	2.04647500
H	-4.66930600	3.90253300	3.35768300
H	-2.64567100	6.51158800	0.59393600
H	-4.22822300	6.19259200	2.48891600
P	2.35900600	0.78176800	0.03057600
C	2.32273600	0.65111400	1.89380600
C	2.29738000	2.54283600	-0.40167700
C	3.96223900	0.12877500	-0.50230500
C	0.93668900	0.23447100	2.40660100
H	2.62469200	1.60405500	2.33604100
H	3.07106900	-0.09856400	2.16475700
C	1.45055200	3.40845400	0.31194200
C	3.03772500	3.02659200	-1.49267300
C	4.02915000	-0.80387000	-1.54807900
C	5.13347100	0.55675300	0.14876200
P	0.27127100	-1.09243300	1.31894200
H	0.22387000	1.06219000	2.36044200
H	0.98173800	-0.12576900	3.43881700
C	1.37025000	4.75240700	-0.04904900
H	0.85159200	3.04455900	1.13978800
C	2.94355000	4.37125600	-1.85229600
H	3.69122100	2.36101300	-2.04808100
C	5.27372100	-1.30823100	-1.93456500
H	3.11327600	-1.13280700	-2.03010400
C	6.36725300	0.04263800	-0.24502500
H	5.08744400	1.28441100	0.95432600

C	-1.36736400	-1.60463600	1.84665900
C	1.38617900	-2.51594800	1.39802300
C	2.11382300	5.23430900	-1.13110400
H	0.72419300	5.41950700	0.51297800
H	3.52295400	4.74426400	-2.69136300
C	6.43724400	-0.89056700	-1.28561700
H	5.33014300	-2.03383200	-2.74075700
H	7.27205100	0.36846700	0.25927200
C	-2.20348100	-0.73174900	2.56243400
C	-1.81637900	-2.88658000	1.48500200
C	1.65537800	-3.03651000	2.67904200
C	1.97511400	-3.07910800	0.25664900
H	2.04689200	6.28160300	-1.41031100
H	7.40095600	-1.29086700	-1.58724500
C	-3.48196100	-1.14990300	2.92410500
H	-1.86666300	0.26076000	2.83758200
C	-3.09898000	-3.29166100	1.84669500
H	-1.17070900	-3.55845700	0.92846000
C	2.52591900	-4.11583400	2.80915700
H	1.19209200	-2.61412100	3.56609900
C	2.84402000	-4.16226000	0.40704400
H	1.75519600	-2.67954500	-0.72983100
C	-3.93101300	-2.42481400	2.56334200
H	-4.12730200	-0.48228700	3.48634300
H	-3.44980800	-4.28020100	1.56826400
C	3.12184300	-4.67684600	1.67439600
H	2.73737200	-4.51757400	3.79519300
H	3.30517900	-4.59979300	-0.47309200
H	-4.93093300	-2.74363800	2.84177200
H	3.80125900	-5.51716300	1.78203900

B9. XYZ Cartesian coordinates of Reactant and Products in the present of difference functional group on path III

$2_{bipy}(NMe_2)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1730.645949 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1730.042989 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1730.165568 hartrees

C	4.12024000	-3.44274000	-1.53083900
C	4.62477400	-3.72433300	-0.26122800
C	3.88703300	-3.38077500	0.87262100
C	2.64990400	-2.75790600	0.71119300
C	2.87968200	-2.82003300	-1.63115800
C	1.76405900	-2.33304400	1.81405600
C	2.05995800	-2.51086400	3.16396500
C	1.16194700	-2.06858100	4.13380000
H	1.39198000	-2.20439600	5.18490800
C	-0.02378600	-1.45249400	3.73986300
C	-0.28066700	-1.29666500	2.38325800
H	4.67078000	-3.69611500	-2.42902500
H	5.58889900	-4.20834100	-0.14839500
H	2.40735100	-2.56156200	-2.57255000
H	-0.74659500	-1.09198600	4.46196500
H	-1.17945400	-0.82533700	2.00686300
H	2.98498900	-2.98919500	3.45886000
H	4.27595700	-3.59649100	1.85946800
N	0.59050900	-1.73195500	1.45733800
N	2.18437300	-2.49937900	-0.53471700
Pt	0.29690400	-1.54167400	-0.57212500
C	-1.46094400	-0.64027500	-0.48811600

C	-2.53478600	-0.07452800	-0.38268200
C	-3.79269300	0.58288900	-0.24563000
C	-4.77119400	0.52238700	-1.25773800
C	-4.10766900	1.31634000	0.91607500
C	-5.99576600	1.16166900	-1.12429600
H	-4.56379300	-0.04090900	-2.16338000
C	-5.32855600	1.95951400	1.06175300
H	-3.37759600	1.37773400	1.71864900
C	-6.31151000	1.91041300	0.03922900
H	-6.71170200	1.07542700	-1.93241500
H	-5.51756500	2.50378100	1.97881100
F	0.26561800	-1.51647700	-2.54429400
C	2.38964800	2.53637400	-0.32129300
C	3.78783400	2.62253700	-0.16872200
C	4.43320800	3.84655300	-0.06496200
C	3.70677700	5.06549500	-0.10263000
C	2.29970200	4.97510000	-0.26677500
C	1.66631100	3.74493800	-0.36888100
H	4.37493900	1.70885000	-0.13437800
H	5.51056800	3.85358500	0.04579700
H	1.69453600	5.87195400	-0.31595700
H	0.58723700	3.71263600	-0.49179900
C	1.73017200	1.27629600	-0.42375700
C	1.16043600	0.20671100	-0.52838500
N	-0.64570400	-3.49336000	-0.62590800
C	-1.16336400	-4.52445500	-0.61068700
C	-1.81993500	-5.82091300	-0.59773700
H	-1.06622400	-6.61325400	-0.57392400
H	-2.45760800	-5.89784700	0.28777300
H	-2.43266000	-5.92816700	-1.49759700

N	4.33922600	6.28374100	0.01999200
N	-7.51754300	2.56681500	0.16794200
C	5.79380700	6.34505800	0.05040800
H	6.24630900	5.93669800	-0.86531800
H	6.10704000	7.38478000	0.15126800
H	6.19679900	5.78936200	0.90629200
C	3.58073100	7.51456200	-0.15351800
H	2.77561200	7.59278500	0.58767100
H	4.24511400	8.36795700	-0.01360800
H	3.13129200	7.58848500	-1.15481500
C	-8.55819100	2.36876400	-0.83124300
H	-8.87425300	1.31720800	-0.90166100
H	-9.42843500	2.97054300	-0.56669800
H	-8.21982300	2.68980700	-1.82401300
C	-7.86704300	3.19485700	1.43450100
H	-7.14269900	3.97338400	1.70350700
H	-8.84475000	3.66919700	1.34173300
H	-7.91206600	2.47014100	2.26118600

2_{bipy}(t-Bu)

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1777.228625 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1776.543678 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1776.667352 hartrees

C	3.95529800	-3.86958900	-1.55791000
C	4.43764600	-4.20438500	-0.29272800
C	3.71555900	-3.84262800	0.84557600
C	2.51649500	-3.14786800	0.69315800
C	2.75235000	-3.17585000	-1.64987100
C	1.65151900	-2.69664800	1.80163800

C	1.92884300	-2.92221800	3.14823900
C	1.05181400	-2.45180100	4.12409200
H	1.26727600	-2.62487000	5.17279300
C	-0.09456900	-1.76002000	3.73942600
C	-0.33361000	-1.55762800	2.38577400
H	4.49436800	-4.13566300	-2.45933000
H	5.37243100	-4.74419100	-0.18653400
H	2.30006000	-2.87204600	-2.58748300
H	-0.80021100	-1.37602700	4.46633800
H	-1.20152100	-1.02627400	2.01771400
H	2.82312800	-3.45992600	3.43551700
H	4.08754300	-4.09964800	1.82907000
N	0.51703000	-2.01998700	1.45409800
N	2.07201600	-2.83814500	-0.54897400
Pt	0.24828000	-1.76802300	-0.57329100
C	-1.45048800	-0.75865200	-0.48717300
C	-2.48797900	-0.13001500	-0.38966900
C	-3.70827600	0.60337800	-0.27465100
C	-4.33716000	1.14698400	-1.40798000
C	-4.31429300	0.80686300	0.98129000
C	-5.52513300	1.86776400	-1.28753600
H	-3.88910200	1.00291800	-2.38683900
C	-5.49803200	1.52771200	1.08595600
H	-3.84819400	0.39584400	1.87219600
C	-6.13560900	2.07837300	-0.04200200
H	-5.97132700	2.26770500	-2.19071300
H	-5.93219600	1.66407400	2.07203800
F	0.23375100	-1.69598000	-2.54301200
C	2.63568100	2.14439900	-0.28755000
C	4.02430200	2.14169100	-0.50313500

C	4.76374100	3.31956400	-0.39835900
C	4.15699400	4.54289000	-0.07596200
C	2.76558300	4.53293100	0.13838400
C	2.01543300	3.36718100	0.03700700
H	4.52317000	1.21004900	-0.75404600
H	5.83192100	3.26718500	-0.57410500
H	2.25227000	5.45599200	0.39085200
H	0.94321200	3.39269200	0.20807700
C	1.87379700	0.94044300	-0.39051200
C	1.22326200	-0.08057500	-0.49147100
N	-0.80872500	-3.64807000	-0.66990900
C	-1.37337600	-4.65412100	-0.68046700
C	-2.08610200	-5.92014100	-0.69904700
H	-1.36756800	-6.74437400	-0.66926500
H	-2.74573500	-5.97966700	0.17158600
H	-2.68279200	-5.98929900	-1.61328300
C	4.94105900	5.85911100	0.04862600
C	-7.44008200	2.87364200	0.12770700
C	-7.99238500	3.38812800	-1.21447100
H	-8.22533400	2.56526200	-1.89988000
H	-8.91807000	3.94740300	-1.03937800
H	-7.28623400	4.06223900	-1.71244900
C	-7.17714000	4.09365900	1.04225200
H	-6.82323800	3.79088800	2.03327500
H	-6.42274400	4.75530500	0.60093300
H	-8.10004300	4.67037500	1.17782800
C	-8.51292600	1.96764100	0.77716600
H	-9.44756100	2.52561000	0.91013200
H	-8.72164500	1.09653900	0.14534300
H	-8.19837500	1.60409900	1.76096700

C	4.39036400	6.88174400	-0.97362400
H	3.32833200	7.09132500	-0.80879100
H	4.93540300	7.82961500	-0.88959000
H	4.50729600	6.50977500	-1.99810100
C	4.76987800	6.42208200	1.47967100
H	5.15653500	5.71688800	2.22448100
H	5.32097700	7.36451500	1.58258900
H	3.71940500	6.62133800	1.71592000
C	6.44595500	5.67300800	-0.21917600
H	6.90304100	4.97856400	0.49495700
H	6.63529300	5.30003700	-1.23219500
H	6.95790000	6.63649600	-0.11937900

$2_{bipy}(NO_2)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1871.701742 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1871.244363 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1871.358054 hartrees

C	4.14575500	-3.22337800	-1.58369100
C	4.66477200	-3.52445100	-0.32465200
C	3.92679900	-3.22734500	0.82226800
C	2.67457000	-2.63037800	0.68485900
C	2.89040400	-2.62810600	-1.66193400
C	1.78622800	-2.25355500	1.80224200
C	2.09247600	-2.45595000	3.14599500
C	1.18820000	-2.05894200	4.12975900
H	1.42647700	-2.21406100	5.17627900
C	-0.01433000	-1.46325000	3.75614000
C	-0.28139400	-1.28084900	2.40494600
H	4.69603800	-3.44106700	-2.49125200

H	5.64081700	-3.98786300	-0.22995100
H	2.40652200	-2.35840400	-2.59408400
H	-0.74253100	-1.13841500	4.48954800
H	-1.19366000	-0.82222400	2.04676300
H	3.02994700	-2.91879900	3.42562900
H	4.32747400	-3.45817200	1.80095900
N	0.59650000	-1.67218700	1.46584500
N	2.19579200	-2.35205200	-0.55257100
Pt	0.28970400	-1.44802500	-0.56067200
C	-1.48972900	-0.58970200	-0.46419500
C	-2.57837300	-0.05767600	-0.35688300
C	-3.85221400	0.56433600	-0.21866200
C	-4.80227700	0.49520200	-1.25978100
C	-4.17724900	1.25890400	0.96640800
C	-6.04350600	1.10225300	-1.12325500
H	-4.55711600	-0.03727000	-2.17230000
C	-5.41637300	1.86781600	1.11018200
H	-3.44974000	1.31600000	1.76895300
C	-6.33528100	1.78144100	0.06179200
H	-6.78018300	1.05565500	-1.91515100
H	-5.67635600	2.40289100	2.01462600
F	0.25088300	-1.37904400	-2.52917200
C	2.30695300	2.66497100	-0.31041100
C	3.70924700	2.74357400	-0.17602800
C	4.33998700	3.97687700	-0.08160800
C	3.56183300	5.13594000	-0.12152300
C	2.17223400	5.09070500	-0.25399500
C	1.54830500	3.85392200	-0.34803600
H	4.29512000	1.83124400	-0.14663600
H	5.41510800	4.05016700	0.02151600

H	1.60118600	6.00993500	-0.28139300
H	0.47010400	3.79688100	-0.45090800
C	1.66349600	1.39705500	-0.40217100
C	1.11211800	0.31871000	-0.48907100
N	-0.58900100	-3.40277200	-0.64809800
C	-1.04139600	-4.46389600	-0.65749600
C	-1.60953200	-5.80060300	-0.67481600
H	-0.80214700	-6.53851900	-0.69791800
H	-2.21587400	-5.95041400	0.22329200
H	-2.23752200	-5.91837100	-1.56274300
N	4.22252800	6.43796200	-0.02076200
N	-7.64249600	2.42081200	0.21039900
O	5.45084500	6.45988800	0.09357700
O	3.51953500	7.45133900	-0.05467000
O	-8.44368900	2.33265300	-0.72394800
O	-7.88196000	3.01787200	1.26350800

$2_{bipy}(CF_3)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2136.770509 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2136.306839 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2136.426524 hartrees

C	3.78363500	-3.95836100	-1.59565100
C	4.27051700	-4.30549800	-0.33557200
C	3.57680200	-3.91453400	0.81074000
C	2.40092400	-3.17902700	0.67143600
C	2.60530500	-3.22217800	-1.67502400
C	1.56546900	-2.69703800	1.78907100
C	1.85002800	-2.93132900	3.13255800
C	1.00013300	-2.43114900	4.11761000

H	1.22110700	-2.61088800	5.16401700
C	-0.12687000	-1.70182600	3.74513500
C	-0.37423100	-1.49184300	2.39415500
H	4.30087900	-4.24661100	-2.50298700
H	5.18696200	-4.87762400	-0.23953300
H	2.15248100	-2.90501300	-2.60791000
H	-0.81134800	-1.29448300	4.47950200
H	-1.22849300	-0.93205300	2.03660600
H	2.72840900	-3.49972300	3.40972100
H	3.95234700	-4.18066700	1.79045800
N	0.45086800	-1.98220000	1.45373000
N	1.95202600	-2.85728200	-0.56626100
Pt	0.16994500	-1.72327000	-0.57220500
C	-1.49068500	-0.65383800	-0.47079200
C	-2.51057500	-0.00004400	-0.36281800
C	-3.71105500	0.76056800	-0.22992600
C	-4.63572000	0.83310900	-1.29119000
C	-3.98790700	1.45198700	0.96633900
C	-5.80441600	1.57463800	-1.15680400
H	-4.42788900	0.30711800	-2.21724500
C	-5.15873600	2.19180100	1.09807100
H	-3.27868500	1.40581200	1.78643800
C	-6.06667700	2.25468400	0.03698900
H	-6.50936400	1.63224700	-1.97947200
H	-5.36374300	2.72527600	2.01994400
F	0.13655400	-1.65087500	-2.54079300
C	2.72617000	2.08088300	-0.32090600
C	4.01903100	1.99514900	0.23347400
C	4.82210300	3.12688600	0.32244400
C	4.34669300	4.35786400	-0.14150400

C	3.06576000	4.45742000	-0.69244500
C	2.25966300	3.32700600	-0.78306600
H	4.38522800	1.03696600	0.58765300
H	5.81951400	3.05397000	0.74307000
H	2.70408300	5.41343600	-1.05527100
H	1.26642100	3.39926600	-1.21391400
C	1.90486800	0.91694900	-0.41367600
C	1.21080300	-0.07526000	-0.50252600
N	-0.95317100	-3.55528100	-0.65641700
C	-1.54974800	-4.54266800	-0.66103400
C	-2.30165700	-5.78562100	-0.67240900
H	-1.60797400	-6.63141400	-0.67374500
H	-2.93643900	-5.83551300	0.21711100
H	-2.92706400	-5.82506100	-1.56903700
C	5.19947800	5.58541100	0.00797400
C	-7.35858300	3.00460700	0.19301000
F	-7.26683500	3.99748800	1.10667800
F	-7.76388700	3.56240300	-0.97184900
F	-8.36509000	2.19105500	0.60188800
F	4.89295000	6.53471900	-0.90510900
F	5.04784300	6.15656400	1.22962100
F	6.51698300	5.30540800	-0.12518100

$2_{dppe}(NMe_2)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2923.278431 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2922.393272 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2922.546363 hartrees

P	2.50721200	-1.67973900	0.09914800
P	-0.20273300	-0.62896100	1.61197600

C	1.46426800	-0.49898800	2.39888700
H	1.87422300	0.46568300	2.08750400
H	1.36130800	-0.47503800	3.48741500
C	2.38315400	-1.64512700	1.94449900
H	3.36469100	-1.54853900	2.41502600
H	1.97418200	-2.61447300	2.24582800
C	3.81546000	-0.55358900	-0.46717700
C	3.76218400	-0.13927700	-1.80960100
C	4.86570800	-0.13539500	0.36066100
C	4.76836400	0.68117500	-2.31604700
H	2.92429000	-0.44427200	-2.42965100
C	5.86348300	0.69589000	-0.15504000
H	4.92000500	-0.44547200	1.39896500
C	5.81811900	1.09993500	-1.49145700
H	4.72656500	1.00502600	-3.35178200
H	6.67326100	1.02495700	0.48917000
H	6.59535800	1.74658800	-1.88820300
C	2.95704000	-3.36611000	-0.40814800
C	3.58651900	-4.26046600	0.47003700
C	2.64993400	-3.75956300	-1.72227200
C	3.89855800	-5.55068700	0.03618000
H	3.83523000	-3.96605400	1.48487000
C	2.96894100	-5.04993500	-2.14496200
H	2.13106300	-3.06854800	-2.38095500
C	3.58955700	-5.94608800	-1.26783200
H	4.38037800	-6.24445400	0.71849100
H	2.72335700	-5.35915900	-3.15667600
H	3.82983900	-6.95180300	-1.60022500
C	-1.14331800	0.87741600	1.97630500
C	-2.54500200	0.82238300	2.04658500

C	-0.48512200	2.10805100	2.13865700
C	-3.27667700	1.98744300	2.27151600
H	-3.07069200	-0.11624200	1.92082700
C	-1.22519400	3.26719600	2.36705800
H	0.59244200	2.18242900	2.07111200
C	-2.62000400	3.21047200	2.42881500
H	-4.36005900	1.93735800	2.30892900
H	-0.70695400	4.21397600	2.48262500
H	-3.19346500	4.11706800	2.59791300
C	-1.07831400	-2.05957000	2.30367400
C	-0.64367500	-2.65794500	3.49718200
C	-2.20171500	-2.57327400	1.63102000
C	-1.32503800	-3.76412400	4.00755200
H	0.21584800	-2.27701000	4.03741100
C	-2.88066700	-3.67207300	2.15465100
H	-2.53151700	-2.12659900	0.69809900
C	-2.44059400	-4.27196300	3.33887800
H	-0.97993200	-4.22623500	4.92720600
H	-3.74785500	-4.06388000	1.63210100
H	-2.96612500	-5.13426000	3.73803800
Pt	0.29879200	-1.01951300	-0.64725300
F	0.92152000	-1.30650900	-2.62022400
C	-1.57540300	-0.45235600	-1.14238700
C	-2.74158000	-0.09893500	-1.22883400
C	-4.09816700	0.33133500	-1.28261200
C	-4.44921800	1.65818500	-0.95829900
C	-5.14481200	-0.54944600	-1.62195100
C	-5.76921900	2.08458000	-0.96457100
H	-3.66698600	2.35928700	-0.68394100
C	-6.46933500	-0.13589000	-1.63379600

H	-4.90894200	-1.57901500	-1.87733200
C	-6.82549100	1.19762000	-1.30084900
H	-5.97936700	3.11474400	-0.70403000
H	-7.23257600	-0.85663300	-1.90093100
C	0.86822900	0.85245100	-0.67836300
C	1.27154700	1.99580900	-0.57191400
C	1.77273900	3.31673100	-0.40339600
C	0.91055500	4.42835900	-0.31996500
C	3.15639800	3.55182800	-0.26947300
C	1.39975300	5.71101800	-0.11812600
H	-0.16137200	4.27469600	-0.40284200
C	3.65668700	4.82984800	-0.06970300
H	3.84296600	2.71254500	-0.31814900
C	2.79317400	5.95468600	0.00426900
H	0.69195400	6.52823400	-0.05418500
H	4.72806000	4.95291600	0.03182100
N	-0.25850900	-3.07139700	-0.67021100
C	-0.41555300	-4.21330200	-0.64694500
C	-0.58908000	-5.65287700	-0.59271400
H	-1.05804100	-5.92275000	0.35848400
H	-1.22315300	-5.98350200	-1.42013300
H	0.39302500	-6.13023600	-0.67075000
N	-8.13818600	1.61180000	-1.30103200
N	3.28648600	7.22869300	0.18400300
C	2.36755400	8.33901900	0.39231400
H	1.75090600	8.20549500	1.29349800
H	2.93903200	9.26128400	0.50284700
H	1.69497000	8.46310200	-0.46534100
C	4.70504800	7.42568700	0.44847500
H	5.03045800	6.91803000	1.36849600

H	5.31889200	7.05376100	-0.38117500
H	4.90439800	8.49228000	0.55765600
C	-9.19464000	0.68951100	-1.68965600
H	-10.15642100	1.20035000	-1.63424700
H	-9.06081300	0.32558700	-2.71802900
H	-9.23596200	-0.18273300	-1.02319500
C	-8.46790800	2.99172400	-0.97674200
H	-9.54968600	3.12226200	-1.01887600
H	-8.13423000	3.25940800	0.03491300
H	-8.01119800	3.69904900	-1.68335000

2_{dppe}(t-Bu)

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2969.861317 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2968.893194 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2969.049483 hartrees

P	2.71377300	-1.70157000	0.09824500
P	-0.07575600	-0.91685700	1.63005200
C	1.57119200	-0.68345500	2.43224700
H	1.90131100	0.32318300	2.16132200
H	1.46070900	-0.70866600	3.52001400
C	2.58565500	-1.73058900	1.94364200
H	3.55556000	-1.56077500	2.41761000
H	2.26524100	-2.74073500	2.21658300
C	3.93988500	-0.47179900	-0.43531400
C	3.87149300	-0.04183400	-1.77234500
C	4.94849400	0.00768700	0.41080900
C	4.82275700	0.85462100	-2.25552900
H	3.06346900	-0.39331700	-2.40715700
C	5.88957100	0.91570700	-0.08121800

H	5.01371200	-0.31300700	1.44512500
C	5.83121100	1.33432400	-1.41257100
H	4.76939600	1.18977600	-3.28707200
H	6.66646600	1.29207100	0.57736600
H	6.56556800	2.03925900	-1.79129500
C	3.27768000	-3.33579100	-0.46087600
C	3.97106400	-4.20938600	0.38950400
C	2.99742700	-3.70858400	-1.78684300
C	4.37131800	-5.46079200	-0.08362600
H	4.20267400	-3.92740900	1.41189600
C	3.40420700	-4.96021800	-2.24869800
H	2.43309200	-3.03497400	-2.42564300
C	4.08675000	-5.83735100	-1.39872600
H	4.90275200	-6.13929100	0.57679500
H	3.17932600	-5.25438300	-3.26962100
H	4.39546600	-6.81346500	-1.76138000
C	-1.13350800	0.49784900	2.03662900
C	-2.52376600	0.32287800	2.13541500
C	-0.57798100	1.77736300	2.20633300
C	-3.34624200	1.41819500	2.39372100
H	-2.96998300	-0.65579800	2.00819000
C	-1.40846300	2.86553000	2.47049600
H	0.48786400	1.94338000	2.11906600
C	-2.79186700	2.68971500	2.55883500
H	-4.42039800	1.27630000	2.45382100
H	-0.96971400	3.85049000	2.59512400
H	-3.43598200	3.54165400	2.75518000
C	-0.84086800	-2.43898000	2.24920700
C	-0.35483800	-3.06502700	3.40789900
C	-1.92537000	-2.99985900	1.55061500

C	-0.94599900	-4.24683700	3.85766900
H	0.47448000	-2.64732600	3.96776500
C	-2.51464300	-4.17455300	2.01426300
H	-2.29312900	-2.53115500	0.64289100
C	-2.02236000	-4.80226600	3.16317300
H	-0.56170100	-4.73005200	4.75047000
H	-3.35185400	-4.60330700	1.47230200
H	-2.47743400	-5.72321400	3.51499700
Pt	0.46732900	-1.17568600	-0.64350600
F	1.10647500	-1.34406400	-2.61709500
C	-1.43884100	-0.70964500	-1.12473100
C	-2.61376200	-0.39279500	-1.21073800
C	-3.98060800	0.01493500	-1.24028800
C	-4.33271000	1.33408600	-0.88808400
C	-5.01367200	-0.87887100	-1.56922300
C	-5.66489900	1.72723700	-0.86196100
H	-3.55160200	2.03798100	-0.61861700
C	-6.34727100	-0.47002500	-1.53871100
H	-4.76743500	-1.90094400	-1.84262900
C	-6.70847100	0.83812100	-1.18244800
H	-5.89386100	2.75043000	-0.57887900
H	-7.10897100	-1.19724400	-1.79542300
C	0.90515700	0.73043600	-0.61553100
C	1.21485700	1.90131500	-0.51394900
C	1.59982600	3.26389200	-0.34510300
C	0.63768100	4.27332900	-0.16985600
C	2.96146500	3.62537900	-0.31676700
C	1.02589100	5.59850600	0.02707000
H	-0.41609600	4.01201500	-0.17970400
C	3.33154100	4.95088700	-0.12442500

H	3.71867100	2.85884500	-0.44478800
C	2.37826400	5.97207200	0.05353100
H	0.24884000	6.34212800	0.16094300
H	4.39018300	5.19288600	-0.11004900
N	0.04741400	-3.25520100	-0.74775600
C	-0.03324400	-4.40475300	-0.77821800
C	-0.11070400	-5.85335000	-0.79064100
H	-0.55287000	-6.19743700	0.14939300
H	-0.72801800	-6.18659700	-1.62959900
H	0.90068900	-6.25910800	-0.89582600
C	2.84272800	7.42124500	0.26673300
C	-8.16674000	1.31930200	-1.12396800
C	-9.16677000	0.21148800	-1.50357100
H	-9.10123800	-0.64553700	-0.82353100
H	-10.18807600	0.60390500	-1.44609400
H	-9.00608100	-0.14754300	-2.52657900
C	-8.49009700	1.79122800	0.31388200
H	-8.36469400	0.97073800	1.02994700
H	-7.84168800	2.61592700	0.62785500
H	-9.52788500	2.14094800	0.37235600
C	-8.35697400	2.49969700	-2.10577400
H	-7.70274400	3.34280800	-1.86079400
H	-8.13867300	2.18943900	-3.13420700
H	-9.39277500	2.85808600	-2.06923600
C	3.73358600	7.49203100	1.52974500
H	4.62204500	6.85860600	1.43731200
H	4.07243800	8.52173700	1.69502000
H	3.17761600	7.16822800	2.41724000
C	1.66343300	8.39420400	0.45380600
H	1.00832400	8.41334000	-0.42467700

H	1.05752500	8.13500100	1.32964800
H	2.04620600	9.40979800	0.60398300
C	3.66012700	7.88110800	-0.96375700
H	4.54292700	7.25305200	-1.12277800
H	3.04910600	7.84332000	-1.87302700
H	4.00358300	8.91322900	-0.82482200

$2_{dppe}(NO_2)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -3064.334895 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -3063.594288 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -3063.740579 hartrees

P	2.85068500	-0.97924500	0.08399200
P	0.00534600	-0.75518400	1.70272800
C	1.60732100	-0.24503400	2.46616400
H	1.75002600	0.80832000	2.20924900
H	1.53638400	-0.30699100	3.55579400
C	2.77110500	-1.09290000	1.92682500
H	3.70984300	-0.78217000	2.39227700
H	2.62518200	-2.15181600	2.16300000
C	3.77993200	0.49326000	-0.42790800
C	3.62235900	0.91699200	-1.75980400
C	4.64703300	1.17654100	0.43463900
C	4.35075300	2.01103400	-2.22251100
H	2.91372100	0.40754700	-2.40662400
C	5.36379300	2.27914200	-0.03766300
H	4.77333600	0.86655600	1.46651900
C	5.22214800	2.69160100	-1.36470200
H	4.22862300	2.34144900	-3.24960500
H	6.03130400	2.81153200	0.63295000

H	5.78203900	3.54826700	-1.72811000
C	3.70758700	-2.45173600	-0.54206100
C	4.58666700	-3.18671700	0.26758600
C	3.46908600	-2.84396400	-1.87063100
C	5.21662200	-4.32001300	-0.25029700
H	4.78594600	-2.88964700	1.29244600
C	4.10598800	-3.97702500	-2.37663900
H	2.76308900	-2.28477900	-2.47767200
C	4.97604400	-4.71643100	-1.56827900
H	5.89242700	-4.89195300	0.37820100
H	3.91527500	-4.28723000	-3.39968900
H	5.46469800	-5.60137000	-1.96525800
C	-1.27730900	0.44789100	2.13419100
C	-2.61823100	0.03656700	2.21478700
C	-0.94927000	1.80096700	2.32495100
C	-3.61760600	0.97326400	2.47398700
H	-2.88949500	-1.00337100	2.07818400
C	-1.95551100	2.72927800	2.58700400
H	0.07519400	2.14514800	2.26030900
C	-3.28978100	2.31954200	2.65455300
H	-4.65192800	0.64890300	2.52729600
H	-1.69306900	3.77278100	2.72961100
H	-4.07165100	3.04706800	2.85045100
C	-0.46733900	-2.39545400	2.30761500
C	0.12228600	-2.93161600	3.46352000
C	-1.43967900	-3.13217900	1.60781400
C	-0.25677300	-4.19881900	3.90920100
H	0.86861700	-2.37880400	4.02310800
C	-1.81794300	-4.39181100	2.06757500
H	-1.88544100	-2.73137100	0.70301700

C	-1.22347900	-4.92835000	3.21416000
H	0.20609700	-4.61212000	4.79974700
H	-2.56951600	-4.95630800	1.52468400
H	-1.51335000	-5.91457200	3.56380700
Pt	0.52557000	-0.87243800	-0.59595700
F	1.13260200	-0.89292700	-2.58114400
C	-1.44136700	-0.77244100	-1.05295500
C	-2.64995200	-0.68519400	-1.18802000
C	-4.06352400	-0.56092500	-1.28970700
C	-4.69940400	0.61765500	-0.84048400
C	-4.84944100	-1.61111000	-1.81010400
C	-6.07999700	0.74364700	-0.90491200
H	-4.09985700	1.42307700	-0.43171700
C	-6.23080100	-1.49167600	-1.87942900
H	-4.36605700	-2.51882800	-2.15502000
C	-6.82995800	-0.31434100	-1.42479800
H	-6.57734100	1.64105400	-0.55950000
H	-6.84346300	-2.29159500	-2.27528100
C	0.58203200	1.08066600	-0.55906600
C	0.64067200	2.29118800	-0.47547200
C	0.72763100	3.70241900	-0.32088800
C	-0.44251300	4.48013400	-0.18930400
C	1.98949500	4.33118900	-0.26258200
C	-0.35670300	5.85362900	-0.00463100
H	-1.41213300	3.99596500	-0.22465800
C	2.08178800	5.70428600	-0.08035500
H	2.88852800	3.73357900	-0.35861000
C	0.90624900	6.44841600	0.04645300
H	-1.24603800	6.46189100	0.09986600
H	3.04341200	6.19936900	-0.03333600

N	0.51113600	-2.98333400	-0.72268800
C	0.64896800	-4.12587400	-0.78901100
C	0.84522700	-5.56158700	-0.85098500
H	0.53711100	-6.00819100	0.09933900
H	0.24859000	-5.98302800	-1.66488500
H	1.90597900	-5.76474400	-1.03007100
N	-8.28463900	-0.18667400	-1.49321700
N	1.00041300	7.89547300	0.24203400
O	2.12329300	8.40536300	0.28380000
O	-0.04741800	8.53703300	0.35619500
O	-8.79819800	0.85688400	-1.07989700
O	-8.93118200	-1.12847900	-1.96079700

$2_{dppe}(CF_3)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -3329.403131 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -3328.656357 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -3328.809170 hartrees

P	2.74897200	-1.65457500	0.06399500
P	-0.00200300	-0.91879000	1.68250800
C	1.66468400	-0.67557000	2.43863000
H	1.98116400	0.33540500	2.16720800
H	1.58578300	-0.71047500	3.52883300
C	2.66886000	-1.71300300	1.91050200
H	3.65055800	-1.54840100	2.36123000
H	2.35702200	-2.72785400	2.17563100
C	3.93597000	-0.39174400	-0.47882900
C	3.83060700	0.05660000	-1.80755100
C	4.94821400	0.10066900	0.35559500
C	4.74912900	0.98462100	-2.29444600

H	3.01936700	-0.30466800	-2.43268300
C	5.85636300	1.03972300	-0.14004400
H	5.04238500	-0.23419200	1.38308500
C	5.76141000	1.47695000	-1.46332800
H	4.66718000	1.33408400	-3.31927900
H	6.63626100	1.42551300	0.50938900
H	6.47014300	2.20610900	-1.84487200
C	3.31855300	-3.27168200	-0.53461100
C	4.04628200	-4.14443400	0.28768600
C	3.00893000	-3.63324900	-1.85711100
C	4.45218300	-5.38412600	-0.21033300
H	4.29992600	-3.87062200	1.30699700
C	3.42162400	-4.87351200	-2.34372700
H	2.41872900	-2.96101300	-2.47327300
C	4.13886200	-5.74980500	-1.52196800
H	5.01042200	-6.06212400	0.42807200
H	3.17456300	-5.15939900	-3.36182700
H	4.45218200	-6.71705300	-1.90385200
C	-1.06210300	0.48444500	2.11687400
C	-2.45068500	0.30090300	2.22403700
C	-0.51170000	1.76557800	2.29151800
C	-3.27697700	1.39047900	2.49434200
H	-2.89205600	-0.68021200	2.09778200
C	-1.34605300	2.84796700	2.56657200
H	0.55349000	1.93649700	2.20342900
C	-2.72807700	2.66432800	2.66155800
H	-4.34961500	1.24191800	2.56540900
H	-0.91211900	3.83427900	2.69679500
H	-3.37523500	3.51164500	2.86732700
C	-0.73314200	-2.45355000	2.30817300

C	-0.21194700	-3.08095700	3.45078600
C	-1.82938800	-3.02093100	1.63350400
C	-0.78100400	-4.27029800	3.90873900
H	0.62754900	-2.65893300	3.99191500
C	-2.39639500	-4.20310700	2.10572800
H	-2.22470900	-2.55193100	0.73761000
C	-1.86974900	-4.83168500	3.23880500
H	-0.36997200	-4.75454400	4.78894800
H	-3.24297400	-4.63682700	1.58269900
H	-2.30774100	-5.75827400	3.59733300
Pt	0.47768200	-1.14685300	-0.61197100
F	1.07157500	-1.28593600	-2.59932000
C	-1.44384500	-0.70130400	-1.05298600
C	-2.62133900	-0.40170900	-1.15308400
C	-3.99490900	-0.02284600	-1.20715100
C	-4.38471100	1.26573800	-0.78614000
C	-4.98365400	-0.92498500	-1.64657400
C	-5.72467800	1.63589700	-0.79798800
H	-3.62935800	1.96326700	-0.44106000
C	-6.32395100	-0.55157300	-1.65793500
H	-4.69222200	-1.91738500	-1.97510300
C	-6.69552900	0.72780300	-1.23366000
H	-6.01675100	2.62917300	-0.47350400
H	-7.08009600	-1.25012000	-1.99989800
C	0.88475200	0.76484000	-0.58386700
C	1.16761100	1.94307400	-0.49886700
C	1.51926200	3.31609800	-0.34961200
C	0.52068400	4.29761900	-0.19227900
C	2.87448800	3.70231000	-0.33078400
C	0.87035800	5.63309900	-0.02011700

H	-0.52329800	4.00284600	-0.20085400
C	3.21927900	5.03886700	-0.16172900
H	3.64530900	2.94910600	-0.45038800
C	2.21849400	6.00414400	-0.00755000
H	0.09913400	6.38669300	0.09727700
H	4.26347900	5.33356100	-0.15463700
N	0.08064900	-3.22622100	-0.72713100
C	0.01151200	-4.37568200	-0.77951500
C	-0.04972800	-5.82430000	-0.82188300
H	-0.46692400	-6.19439500	0.11965700
H	-0.68151100	-6.14605900	-1.65454000
H	0.96381400	-6.21525100	-0.95820900
C	2.59780700	7.43652500	0.23842700
C	-8.14634900	1.11093700	-1.18050000
F	1.64057900	8.29676100	-0.17834400
F	3.74733800	7.77323300	-0.39111800
F	2.79359300	7.68315100	1.55862600
F	-8.33159000	2.43116800	-1.41466600
F	-8.88908800	0.43151000	-2.08419800
F	-8.68820600	0.85602600	0.03787000

$4_{bipy}(NMe_2)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1597.860937 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1597.310299 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1597.417872 hartrees

C	5.13611400	-1.31812100	-1.51626400
C	5.68406300	-1.02436600	-0.26730800
C	4.85199900	-0.90655900	0.84686300
C	3.47806800	-1.08569100	0.68790000

C	3.75854700	-1.48540100	-1.61560000
C	2.47829600	-0.98402100	1.76983800
C	2.79497800	-0.70545500	3.09801800
C	1.78063200	-0.62192700	4.05002800
H	2.02597900	-0.40386000	5.08370000
C	0.45769900	-0.81764700	3.65925300
C	0.18592000	-1.09198500	2.32524400
H	5.75663800	-1.41465700	-2.39929300
H	6.75397400	-0.88517300	-0.15605000
H	3.24288000	-1.70969400	-2.54291900
H	-0.36068500	-0.75826400	4.36677100
H	-0.81882300	-1.24477300	1.95380400
H	3.82584800	-0.55226500	3.39008400
H	5.27439700	-0.67783500	1.81682800
N	1.17223400	-1.17985800	1.41491900
N	2.97340200	-1.37113800	-0.53738600
Pt	0.85796400	-1.52723500	-0.58939000
C	-1.10418700	-1.64860400	-0.52169900
C	-2.32428300	-1.55139200	-0.46699800
C	-3.73633200	-1.46736600	-0.40073500
C	-4.53361000	-1.56502600	-1.56356000
C	-4.40206700	-1.26709900	0.82960500
C	-5.91265600	-1.46183800	-1.50744400
H	-4.05091700	-1.72060800	-2.52412800
C	-5.78037800	-1.16387700	0.89943600
H	-3.81736500	-1.18951500	1.74189000
C	-6.58428100	-1.25550000	-0.27056600
H	-6.47510700	-1.54027100	-2.42953200
H	-6.23873900	-1.00788500	1.86799700
F	0.85976300	-1.92734700	-2.51234000

C	0.84745400	2.97841800	-0.25209200
C	2.08479800	3.65210100	-0.16560800
C	2.15520400	4.99812800	0.15296400
C	0.97871700	5.75620300	0.40240500
C	-0.26584200	5.07616100	0.30507900
C	-0.32343300	3.72944500	-0.01464200
H	3.00256400	3.09833500	-0.34257600
H	3.13095500	5.46340800	0.21621600
H	-1.19387100	5.60405000	0.48596800
H	-1.29028400	3.23790800	-0.07479400
C	0.79316700	1.58597100	-0.52232600
C	0.76074600	0.39882000	-0.80427200
N	-7.94938500	-1.14821000	-0.20845500
N	1.04217100	7.08900600	0.72543400
C	-8.61057300	-0.93196600	1.07233600
H	-9.68809100	-0.88199900	0.91556300
H	-8.40634000	-1.75137600	1.77373600
H	-8.28894100	0.00835800	1.53955100
C	-8.74753300	-1.22404200	-1.42572600
H	-9.80078800	-1.10429800	-1.17182000
H	-8.47540300	-0.43224400	-2.13612400
H	-8.62573700	-2.19266100	-1.92805400
C	-0.17402200	7.81967900	1.05774400
H	0.08263100	8.85068400	1.30206400
H	-0.87534700	7.83642400	0.21368100
H	-0.68930000	7.38047700	1.92315800
C	2.33502500	7.74426500	0.87464200
H	2.17828600	8.79590300	1.11544000
H	2.93231900	7.29321000	1.67942700
H	2.91792100	7.69399100	-0.05365800

$TS_{C\text{-}C,bipy}(NMe_2)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1597.846080 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1597.297210 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1597.404295 hartrees

C	5.40158500	-1.28905800	-1.80257200
C	6.03090700	-1.35941600	-0.55916200
C	5.26696600	-1.52426100	0.59676800
C	3.88010100	-1.61850000	0.48465100
C	4.01507100	-1.38706400	-1.85428400
C	2.94754300	-1.78829100	1.61548000
C	3.34814500	-1.89601400	2.94607700
C	2.39214000	-2.04703100	3.94844700
H	2.70207600	-2.13038400	4.98441700
C	1.04262700	-2.08675500	3.60398400
C	0.68851600	-1.97658600	2.26544800
H	5.96790500	-1.16188500	-2.71765700
H	7.11057000	-1.28652900	-0.48453500
H	3.44043800	-1.34231100	-2.77288500
H	0.26651900	-2.19959900	4.35163000
H	-0.34215600	-1.99348400	1.93607400
H	4.39981300	-1.86209100	3.20024600
H	5.75010600	-1.57733900	1.56411500
N	1.61694000	-1.83874300	1.30081300
N	3.29245300	-1.54495300	-0.73688900
Pt	1.18356600	-1.64649400	-0.69718800
C	-0.78017500	-1.49970300	-0.54275900
C	-2.00809300	-1.46689900	-0.42509900
C	-3.39862000	-1.36550700	-0.28297300

C	-4.24470300	-1.21166000	-1.41076500
C	-4.00691800	-1.36277300	0.99833900
C	-5.60803700	-1.05017500	-1.27151000
H	-3.80555900	-1.21328100	-2.40386500
C	-5.36899600	-1.20049400	1.14850400
H	-3.38311300	-1.48089000	1.87941600
C	-6.21918000	-1.03085600	0.01656200
H	-6.20909400	-0.93002600	-2.16386300
H	-5.78322400	-1.19768300	2.14866400
F	1.09077200	-1.54454500	-2.66340000
C	0.34951500	2.78355000	-0.16459600
C	0.46496500	3.38622300	1.10529200
C	0.51530300	4.76480700	1.25149400
C	0.44767900	5.62755700	0.12633900
C	0.32902300	5.01701800	-1.14951400
C	0.27843100	3.63755000	-1.28484100
H	0.52687100	2.75601200	1.98817700
H	0.61460500	5.17261900	2.24994000
H	0.28246200	5.62324900	-2.04580100
H	0.19398600	3.20466500	-2.27768200
C	0.34692700	1.36982800	-0.31388200
C	0.36741000	0.15642100	-0.45001300
N	-7.56489700	-0.85305500	0.16062200
N	0.49286600	6.99902900	0.26664500
C	-8.16316600	-0.79845400	1.49124400
H	-9.23704200	-0.64138600	1.39418100
H	-8.00315500	-1.73462900	2.04015600
H	-7.74829500	0.02671000	2.08403700
C	-8.41197400	-0.65384900	-1.01145200
H	-9.44634300	-0.53726900	-0.68935700

H	-8.12263400	0.24663900	-1.56839400
H	-8.36132300	-1.51335200	-1.69099500
C	0.59414300	7.84108500	-0.91766700
H	0.61878200	8.88771200	-0.61200600
H	1.50176300	7.63050900	-1.50310300
H	-0.27381500	7.70579300	-1.57406300
C	0.79305700	7.58023500	1.56809700
H	0.79273100	8.66754400	1.48337900
H	0.03393300	7.30322500	2.30946400
H	1.77538700	7.26340100	1.94942700

$5_{bipy}(NMe_2)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1597.940028 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1597.388855 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1597.497358 hartrees

C	2.17341100	-3.06788000	-2.87229900
C	2.98594300	-3.64371300	-1.89515800
C	2.82894600	-3.27554600	-0.55864500
C	1.85948100	-2.33198300	-0.22240000
C	1.22161800	-2.13194900	-2.48286700
C	1.57282300	-1.85136800	1.14181100
C	2.24331500	-2.28771200	2.28263900
C	1.88571800	-1.77885000	3.52983400
H	2.40363300	-2.11355700	4.42200200
C	0.85805900	-0.84162400	3.61106500
C	0.22251000	-0.43660100	2.44285500
H	2.26874200	-3.33469200	-3.91827500
H	3.73791100	-4.37673400	-2.16703400
H	0.54351400	-1.63611800	-3.16820500

H	0.54484800	-0.42184900	4.55979600
H	-0.58262300	0.28625700	2.44965200
H	3.03764800	-3.01892800	2.20106700
H	3.45391300	-3.72046200	0.20532900
N	0.57139200	-0.92412200	1.23810900
N	1.08185500	-1.78394200	-1.19385100
Pt	-0.28735400	-0.40495900	-0.53925800
C	-1.40434400	1.32082500	0.17958500
C	-2.29052600	0.42529100	0.20463900
C	-3.37796200	-0.47610000	0.22086000
C	-3.75394300	-1.15168400	-0.96560100
C	-4.09128800	-0.75168400	1.40841400
C	-4.80423600	-2.04708500	-0.96835200
H	-3.17594800	-0.96522700	-1.86578800
C	-5.15108700	-1.63887600	1.40944800
H	-3.80529800	-0.25484900	2.33055200
C	-5.54581100	-2.31620300	0.21955400
H	-5.05524900	-2.54716800	-1.89516900
H	-5.67590900	-1.81548700	2.33956500
F	-1.00685400	-0.09873700	-2.36046000
C	0.23010200	4.96662000	0.46483400
C	-0.55148200	6.10799200	0.75450100
C	0.01714800	7.36621200	0.84648200
C	1.41280400	7.55934500	0.65028300
C	2.19534400	6.40780400	0.35806300
C	1.61757500	5.15339300	0.27083000
H	-1.62065400	5.99429600	0.90754200
H	-0.62587500	8.20805800	1.07078400
H	3.26278900	6.49635700	0.19936700
H	2.24248600	4.29364700	0.04692600

C	-0.35296800	3.68344500	0.36761300
C	-0.86401000	2.57564500	0.28238400
N	-6.59240800	-3.19428800	0.21849100
N	1.97988200	8.80370500	0.73956100
C	-7.32062200	-3.47311700	1.45185200
H	-8.12354200	-4.17923000	1.24130900
H	-6.66723800	-3.91490300	2.21541600
H	-7.76897600	-2.56121600	1.86544600
C	-6.96386500	-3.89633900	-1.00579600
H	-7.81797700	-4.54183700	-0.80236800
H	-7.24855600	-3.19353300	-1.79871000
H	-6.14219900	-4.52254100	-1.37684200
C	3.41104800	8.97470100	0.52328900
H	3.66651700	10.02895200	0.63064200
H	4.00038100	8.40535200	1.25409100
H	3.70855200	8.65294800	-0.48350400
C	1.15346800	9.96691900	1.03736600
H	1.78390300	10.85558400	1.06976400
H	0.38323200	10.12258400	0.27033200
H	0.65415600	9.86772800	2.01013100

$4_{dppe}(NMe_2)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2790.485109 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2789.651472 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2789.794966 hartrees

P	2.64041000	0.64932500	0.12741700
P	0.30847700	-1.05412200	1.56735000
C	1.24385600	0.20458500	2.54151800
H	0.65292900	1.12280500	2.46804700

H	1.27973300	-0.08692800	3.59563100
C	2.66006300	0.40717800	1.97213700
H	3.13594200	1.25373600	2.47129500
H	3.27520300	-0.47436600	2.16723600
C	2.87547100	2.40570300	-0.28158900
C	2.39705300	2.85215200	-1.52589700
C	3.55252900	3.28927700	0.57136500
C	2.59500300	4.18010800	-1.90234300
H	1.86499900	2.16307000	-2.17468600
C	3.74107400	4.61835600	0.18496500
H	3.93962500	2.96041200	1.53009500
C	3.26241700	5.06429100	-1.04936000
H	2.21818800	4.52703300	-2.86001100
H	4.25967800	5.30161000	0.85070600
H	3.40607900	6.09974300	-1.34401100
C	4.02228900	-0.29628200	-0.58586800
C	5.18432000	-0.59325200	0.14298800
C	3.89574900	-0.72060600	-1.92098200
C	6.20945300	-1.32422500	-0.45880800
H	5.30228900	-0.25699300	1.16849400
C	4.92910500	-1.44895100	-2.51176200
H	2.99516000	-0.48128200	-2.48071900
C	6.08161400	-1.75481600	-1.78254900
H	7.10685800	-1.55586300	0.10712900
H	4.83046200	-1.78156100	-3.54090900
H	6.88053600	-2.32735400	-2.24474300
C	-1.36884400	-1.22026600	2.22130700
C	-1.72431600	-2.38202700	2.92541500
C	-2.30302500	-0.18546800	2.04525200
C	-3.00884300	-2.49990200	3.45976000

H	-1.01036300	-3.18813200	3.05612900
C	-3.58248400	-0.31657200	2.58072100
H	-2.03773900	0.70324700	1.48389600
C	-3.93682000	-1.47018700	3.28810700
H	-3.28229700	-3.39899400	4.00317300
H	-4.30575500	0.48063200	2.43906400
H	-4.93751000	-1.56858000	3.69818600
C	1.16613300	-2.64534200	1.66778400
C	2.04296300	-2.93535700	2.72648000
C	0.94228200	-3.59788800	0.65654900
C	2.69679000	-4.16687300	2.76464400
H	2.21426300	-2.22013400	3.52421500
C	1.60012100	-4.82598300	0.70655800
H	0.25718200	-3.37924300	-0.15705300
C	2.48000600	-5.10877500	1.75525700
H	3.37418700	-4.38812300	3.58344100
H	1.42649300	-5.55970500	-0.07442700
H	2.99529100	-6.06400400	1.78755500
Pt	0.54835400	-0.31943800	-0.63451600
F	0.95308000	0.29441800	-2.57434600
C	-1.12076400	-1.28475400	-1.15364300
C	-2.23319900	-1.78661300	-1.29849500
C	-3.50492200	-2.39566900	-1.38094400
C	-4.14225500	-2.85915100	-0.20544200
C	-4.19574300	-2.55293400	-2.60365800
C	-5.39699400	-3.43822200	-0.24288900
H	-3.63283300	-2.75283400	0.74642200
C	-5.45087400	-3.13323900	-2.65426500
H	-3.73141600	-2.20740000	-3.52285300
C	-6.09666600	-3.59417100	-1.47247500

H	-5.84018400	-3.77108000	0.68752900
H	-5.93871700	-3.22816200	-3.61628900
C	-0.27432700	1.37994700	-0.18866700
C	-0.68296400	2.50254900	0.04071800
C	-1.07543800	3.84865800	0.29028100
C	-2.41949300	4.26345100	0.22746300
C	-0.09967900	4.82656700	0.57174900
C	-2.77581200	5.58969400	0.42745200
H	-3.19290400	3.53277900	0.00736600
C	-0.44450400	6.15434200	0.77188900
H	0.94415700	4.53462800	0.62063600
C	-1.79744900	6.57997600	0.70737400
H	-3.82293200	5.85756300	0.35858600
H	0.34712400	6.86582800	0.97213300
N	-7.34144700	-4.16418600	-1.51651400
N	-2.14561700	7.89797800	0.91059000
C	-3.51786200	8.32715000	0.67720400
H	-4.21524500	7.80152900	1.34064400
H	-3.60009700	9.39411800	0.88735800
H	-3.83699600	8.15394000	-0.36131000
C	-1.10358200	8.90862700	1.03403300
H	-0.45658000	8.70633400	1.89615300
H	-0.46963400	8.96462000	0.13660500
H	-1.56664100	9.88400700	1.18764000
C	-8.03595000	-4.31603800	-2.78935500
H	-7.46256900	-4.93913400	-3.48784500
H	-8.99832000	-4.79801300	-2.61739400
H	-8.22061100	-3.34470600	-3.26692200
C	-7.98726900	-4.61186300	-0.28852400
H	-8.12558800	-3.78338300	0.41835600

H	-8.96903900	-5.02015500	-0.52800100
H	-7.40412200	-5.39655500	0.21093500

$TS_{C\text{-}C,dppe}(NMe_2)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2790.471610 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2789.639605 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2789.782701 hartrees

P	3.21891900	0.25162200	-0.07014300
P	0.87045600	-1.10250400	1.61454500
C	1.99041600	0.12141900	2.42705100
H	1.51242400	1.09853000	2.30359100
H	2.04967000	-0.07720900	3.50117800
C	3.37817000	0.10310300	1.76888800
H	4.00926800	0.89051000	2.18791300
H	3.88344700	-0.84959800	1.95508700
C	3.16069200	2.01229500	-0.53825000
C	2.69207200	2.30689900	-1.83116100
C	3.56527400	3.04713100	0.31597900
C	2.65337200	3.63091300	-2.26591600
H	2.34309900	1.50047900	-2.47000900
C	3.50681200	4.37190900	-0.12395300
H	3.92458700	2.84053500	1.31866400
C	3.05829200	4.66430900	-1.41404100
H	2.29243700	3.85769600	-3.26486700
H	3.81447200	5.17217300	0.54245600
H	3.01646000	5.69545400	-1.75282300
C	4.70127500	-0.49283900	-0.81079300
C	5.94143300	-0.46081400	-0.15372900
C	4.58264000	-1.09410100	-2.07498600

C	7.05801600	-1.03981100	-0.75806900
H	6.04287200	0.00900700	0.82021000
C	5.70827900	-1.66552500	-2.67111900
H	3.61891400	-1.09787400	-2.57658500
C	6.94184100	-1.64226700	-2.01448400
H	8.01654900	-1.02025700	-0.24794300
H	5.61956100	-2.13263100	-3.64775500
H	7.81343900	-2.09281400	-2.48065800
C	-0.78032100	-0.91171800	2.33693000
C	-1.49755300	-2.03509000	2.77702000
C	-1.34923500	0.36916300	2.44271100
C	-2.77452800	-1.87491500	3.31801000
H	-1.06752400	-3.02796900	2.70180000
C	-2.62692800	0.51816000	2.97884400
H	-0.81523300	1.24565500	2.09641800
C	-3.34186100	-0.60181100	3.41468300
H	-3.32495800	-2.74674800	3.65807000
H	-3.06198700	1.51023500	3.05033600
H	-4.33811900	-0.48177600	3.82974100
C	1.47909800	-2.77789100	1.94857300
C	2.31236300	-3.04945900	3.04559400
C	1.09509300	-3.81845800	1.08291300
C	2.76056900	-4.35179300	3.26830600
H	2.61209600	-2.26175600	3.72882800
C	1.54160500	-5.11796600	1.31934500
H	0.44980900	-3.60892600	0.23429300
C	2.37709700	-5.38412600	2.40802000
H	3.40815400	-4.55790300	4.11487800
H	1.24084900	-5.91919100	0.65142100
H	2.73000900	-6.39558700	2.58557800

Pt	1.12030600	-0.74163300	-0.66519200
F	1.59281400	-0.52723600	-2.66288900
C	-0.77658000	-1.24792000	-1.08009900
C	-1.94747100	-1.60458900	-1.24099400
C	-3.29167400	-1.98437300	-1.35684500
C	-4.09922700	-2.11030600	-0.19734900
C	-3.90207300	-2.23016300	-2.61183900
C	-5.43291600	-2.45321500	-0.28246200
H	-3.65543100	-1.92603000	0.77536100
C	-5.23497200	-2.57682600	-2.70752700
H	-3.30655700	-2.14203100	-3.51570300
C	-6.05004600	-2.69793700	-1.54378500
H	-6.00641600	-2.53027400	0.63270500
H	-5.65495000	-2.75430400	-3.68948100
C	-0.27993700	0.68530100	-0.70540400
C	-0.78098800	1.78117700	-0.50677800
C	-1.36808700	3.04284900	-0.21451300
C	-2.67366500	3.13168400	0.31223300
C	-0.65389400	4.24531700	-0.39259700
C	-3.23933600	4.35381700	0.64582800
H	-3.24427800	2.22070500	0.46879500
C	-1.21256400	5.47289500	-0.06995100
H	0.35833700	4.20704600	-0.78295300
C	-2.52807400	5.56816500	0.45638000
H	-4.24262900	4.36290300	1.05396300
H	-0.61617900	6.36448600	-0.22106900
N	-7.37069700	-3.03332500	-1.63407300
N	-3.09102600	6.78632700	0.76706700
C	-4.38440900	6.83866300	1.43401200
H	-4.37001200	6.32448400	2.40620500

H	-4.65892300	7.88041800	1.60299500
H	-5.16878400	6.38096500	0.81820700
C	-2.29355500	8.00058600	0.66795800
H	-1.42258000	7.98204300	1.33964100
H	-1.93045200	8.15405400	-0.35586600
H	-2.91204700	8.85852500	0.93388000
C	-7.98430800	-3.26872200	-2.93715300
H	-7.50982000	-4.10993200	-3.45808400
H	-9.03869200	-3.50613100	-2.79843700
H	-7.91540900	-2.38084200	-3.57809000
C	-8.18417800	-3.15416400	-0.42822600
H	-8.22812100	-2.20604400	0.12268100
H	-9.20002000	-3.43199300	-0.70820900
H	-7.79124700	-3.92715700	0.24412300

$5_{dppe}(NMe_2)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2790.573610 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2789.741313 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2789.885741 hartrees

P	0.04730200	2.22695700	0.75951800
P	0.46734100	-0.78517900	1.39490500
C	-0.29119400	0.28738300	2.71142000
H	-1.37873900	0.24898200	2.60211500
H	-0.03391100	-0.10552100	3.69918700
C	0.22218900	1.72359700	2.53166300
H	-0.29349200	2.41848100	3.20014200
H	1.29227000	1.78595400	2.75657500
C	-1.68516400	2.70432700	0.44082600
C	-2.06665800	2.86613100	-0.90443600

C	-2.63002800	2.86208200	1.46364800
C	-3.38391800	3.20003300	-1.21237300
H	-1.33832000	2.68877100	-1.69169300
C	-3.95205900	3.18326400	1.14200500
H	-2.35629600	2.73516000	2.50572000
C	-4.32828000	3.35629500	-0.19149800
H	-3.67910500	3.31921100	-2.25061800
H	-4.68434200	3.29620500	1.93585600
H	-5.35770300	3.60049900	-0.43668700
C	1.13474100	3.65223800	0.47318900
C	1.38562600	4.57352700	1.50333900
C	1.71653400	3.82590900	-0.79345800
C	2.22391400	5.66314400	1.26526900
H	0.93668000	4.45024600	2.48429600
C	2.55007700	4.92281100	-1.01876800
H	1.49985600	3.10913200	-1.58067200
C	2.80701400	5.83718100	0.00659000
H	2.42204300	6.37312600	2.06275000
H	3.00256400	5.05997000	-1.99671400
H	3.46087100	6.68572300	-0.17356600
C	-0.47743000	-2.33476300	1.33719400
C	0.16586300	-3.56719500	1.14152500
C	-1.88007900	-2.27613800	1.34897500
C	-0.59055300	-4.72924400	0.98547500
H	1.24926600	-3.62107100	1.11179300
C	-2.62982800	-3.44154200	1.19864200
H	-2.39671900	-1.32650900	1.44223400
C	-1.98663300	-4.66883800	1.01811800
H	-0.08787500	-5.68035800	0.83724000
H	-3.71393200	-3.38412300	1.19957000

H	-2.57189100	-5.57537500	0.89423000
C	2.14870500	-1.15294400	1.99530300
C	2.32722000	-1.99930600	3.10507300
C	3.26663500	-0.56332600	1.38601800
C	3.60972200	-2.25917900	3.58520300
H	1.47084100	-2.46548400	3.58420400
C	4.54814200	-0.82534200	1.87501800
H	3.14650800	0.08450700	0.52557600
C	4.72165600	-1.67402500	2.96924500
H	3.74148500	-2.91887600	4.43764400
H	5.40778300	-0.37483500	1.38836800
H	5.72019400	-1.88249900	3.34257600
Pt	0.42874000	0.40423500	-0.53406900
F	0.46491800	1.50921900	-2.27819200
C	-0.01384000	-1.50781000	-1.94092900
C	1.22865300	-1.49514300	-1.94872600
C	2.64261300	-1.53158500	-1.91000100
C	3.32878700	-2.65632200	-1.40405700
C	3.39387100	-0.38263500	-2.24946100
C	4.69876900	-2.63073800	-1.22140200
H	2.76744400	-3.54528900	-1.13234700
C	4.76189000	-0.34536600	-2.05708500
H	2.86402700	0.49139300	-2.61748100
C	5.45773200	-1.46348400	-1.51481600
H	5.18219300	-3.51121000	-0.81812000
H	5.29447100	0.56374900	-2.30585600
C	-1.37189600	-1.59580300	-1.98034100
C	-2.58150700	-1.56185600	-1.79407300
C	-3.93319700	-1.40383500	-1.42259900
C	-4.94213000	-2.33248700	-1.75279500

C	-4.29146800	-0.29141700	-0.62456700
C	-6.24377200	-2.16335800	-1.31049500
H	-4.69243500	-3.19878200	-2.35811300
C	-5.58904600	-0.11305900	-0.18158200
H	-3.53099600	0.43435300	-0.35307800
C	-6.61145400	-1.04587700	-0.51030700
H	-6.98299600	-2.90427500	-1.58823900
H	-5.80771900	0.75721200	0.42406400
N	6.80373100	-1.41298800	-1.26917100
N	-7.89857800	-0.87284300	-0.07228700
C	-8.92517200	-1.85247900	-0.40389600
H	-8.67467100	-2.84768800	-0.01316600
H	-9.87205600	-1.54337100	0.03896600
H	-9.06788300	-1.93589800	-1.48939300
C	-8.24344000	0.28368900	0.74465900
H	-7.68352000	0.29363700	1.68939200
H	-8.04012400	1.22447000	0.21632200
H	-9.30706100	0.25162700	0.98099400
C	7.54863800	-0.18426900	-1.51962200
H	7.18397200	0.64730700	-0.90073200
H	8.60029000	-0.34971300	-1.28584400
H	7.47960100	0.11365100	-2.57263400
C	7.46212700	-2.52063700	-0.58528700
H	7.41054600	-3.44342600	-1.17621600
H	8.51329500	-2.27475800	-0.43560700
H	7.00964700	-2.71307900	0.39698400

4_{bipy}(t-Bu)

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1644.440540 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1643.808099 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1643.917992 hartrees

C	5.26913500	0.44476600	-1.52286400
C	5.83288800	0.58285200	-0.25456500
C	5.11226600	0.18857200	0.87412800
C	3.83339800	-0.34069600	0.70906900
C	3.98817000	-0.08859700	-1.62765000
C	2.95638600	-0.79514200	1.80680900
C	3.31333700	-0.76021800	3.15283800
C	2.41516600	-1.20859100	4.12008300
H	2.69133800	-1.17985600	5.16843300
C	1.16761600	-1.68772300	3.72670900
C	0.85132500	-1.70457200	2.37423400
H	5.80409000	0.74245300	-2.41682000
H	6.82873900	0.99661900	-0.13832300
H	3.46970800	-0.23031700	-2.56948300
H	0.43988400	-2.04291200	4.44646600
H	-0.10225400	-2.05621400	2.00255200
H	4.28503900	-0.38525900	3.44709900
H	5.54621900	0.29522000	1.85997800
N	1.72764200	-1.27550900	1.44808100
N	3.31105700	-0.46428700	-0.53597700
Pt	1.33714100	-1.23976200	-0.57623200
C	-0.51602200	-1.90620700	-0.49643200
C	-1.69734400	-2.20152500	-0.40864400
C	-3.07336900	-2.55368600	-0.30231500
C	-3.84430600	-2.82205200	-1.44781500
C	-3.70474300	-2.62173200	0.95706500
C	-5.19676700	-3.14004800	-1.33596300
H	-3.37763500	-2.77639300	-2.42729600

C	-5.05383600	-2.93797300	1.05177000
H	-3.12871100	-2.41834300	1.85500300
C	-5.83710500	-3.20321200	-0.08850200
H	-5.75033700	-3.33756300	-2.24634900
H	-5.50643000	-2.97643500	2.03793200
F	1.25326700	-1.14172600	-2.53113700
C	0.01072300	3.10286100	-0.16286900
C	0.33685400	3.83393100	0.99602300
C	0.00043100	5.17876200	1.09527400
C	-0.66891800	5.85646700	0.05844800
C	-0.99211500	5.11495400	-1.08796200
C	-0.66218400	3.76497500	-1.20306600
H	0.85709600	3.33981500	1.81128600
H	0.27009900	5.71148000	2.00215900
H	-1.50844800	5.58446900	-1.91697900
H	-0.92267800	3.21839800	-2.10454800
C	0.37294900	1.72647100	-0.28257600
C	0.68647000	0.56127000	-0.40016200
C	-7.32780200	-3.53974500	0.07082900
C	-7.47399500	-4.81318900	0.93728800
C	-8.04416800	-2.35830600	0.76784900
C	-8.02058700	-3.79375400	-1.28092000
H	-6.97650700	-5.66640300	0.46190800
H	-7.04045200	-4.68032700	1.93395400
H	-8.53410400	-5.06298000	1.06438900
H	-7.95656000	-1.44334000	0.17066100
H	-9.10976500	-2.58477900	0.89256600
H	-7.62709300	-2.15618500	1.75990900
H	-9.07732700	-4.02800500	-1.11197200
H	-7.97580200	-2.91359000	-1.93243300

H	-7.57391000	-4.64100800	-1.81360200
C	-1.00830700	7.34708000	0.21372400
C	-1.73845300	7.91429800	-1.01808100
C	-1.92084500	7.53842300	1.44823700
C	0.29969900	8.14946100	0.41221400
H	-1.12749800	7.83618000	-1.92465900
H	-2.69049700	7.40220100	-1.19866300
H	-1.95787200	8.97541300	-0.85650400
H	-1.43617800	7.19971400	2.36982200
H	-2.17038100	8.59903500	1.57197300
H	-2.85603000	6.97865900	1.33146800
H	0.07321000	9.21615200	0.52731100
H	0.84575600	7.82535800	1.30439900
H	0.96326700	8.03205300	-0.45236100

$TS_{C\text{-}C,bipy}$(t-Bu)

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1644.425095 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1643.794342 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1643.904180 hartrees

C	6.02645700	-0.83488200	-1.73967100
C	6.64278600	-0.81868800	-0.48837600
C	5.87147300	-0.94445100	0.66823200
C	4.49026900	-1.08679200	0.54872200
C	4.64430200	-0.97941200	-1.79991800
C	3.54914300	-1.21887400	1.67695700
C	3.93113300	-1.21655400	3.01660100
C	2.96436100	-1.33960000	4.01321700
H	3.25952600	-1.33661500	5.05678400
C	1.62428900	-1.46262000	3.65364400

C	1.28845200	-1.45980000	2.30553700
H	6.59874300	-0.73780100	-2.65461100
H	7.71868800	-0.70755200	-0.40724400
H	4.07950500	-1.00023200	-2.72527300
H	0.84105700	-1.55783600	4.39617400
H	0.26559600	-1.54798000	1.96363900
H	4.97552200	-1.11719000	3.28303600
H	6.34574500	-0.93057300	1.64125600
N	2.22733800	-1.34634100	1.34876400
N	3.91512700	-1.09999100	-0.68157000
Pt	1.82014400	-1.30471700	-0.66518700
C	-0.15604800	-1.46081500	-0.56106300
C	-1.33497900	-1.78862500	-0.47508600
C	-2.69835300	-2.15019800	-0.35751600
C	-3.49311500	-2.37181000	-1.49953500
C	-3.29608100	-2.29297800	0.91455900
C	-4.83418400	-2.72307100	-1.37003000
H	-3.05078400	-2.26777000	-2.48556900
C	-4.63449000	-2.64076500	1.02416500
H	-2.70015400	-2.12605700	1.80670300
C	-5.43962000	-2.86608300	-0.11071000
H	-5.40786500	-2.88582600	-2.27462300
H	-5.06154400	-2.73974900	2.01720600
F	1.74886600	-1.23816100	-2.63254500
C	-0.09483200	2.82790500	-0.26121000
C	-0.21774400	3.43426400	1.00623700
C	-0.66375100	4.74520800	1.11690900
C	-1.00721800	5.51339600	-0.01231900
C	-0.87964800	4.89907100	-1.26759500
C	-0.43368000	3.58480100	-1.39753900

H	0.03852300	2.86775900	1.89661800
H	-0.74655300	5.17861400	2.10899800
H	-1.13035600	5.44213100	-2.17135000
H	-0.34659600	3.13704800	-2.38303300
C	0.35401100	1.48376800	-0.38509300
C	0.71946000	0.32549500	-0.49380300
C	-6.91598700	-3.24944200	0.06742600
C	-7.00661200	-4.56369200	0.87958500
C	-7.64472700	-2.11954500	0.83393000
C	-7.63482100	-3.46287100	-1.27755600
H	-6.49779000	-5.38111600	0.35593500
H	-6.55453100	-4.46316700	1.87172800
H	-8.05654300	-4.84748700	1.01815300
H	-7.59721600	-1.17727000	0.27608700
H	-8.70011100	-2.38150400	0.97404100
H	-7.20807600	-1.95006500	1.82354500
H	-8.67969500	-3.73538800	-1.09361400
H	-7.63201000	-2.55365900	-1.88937400
H	-7.17795200	-4.27223200	-1.85827700
C	-1.49947600	6.95777300	0.16727000
C	-1.82719300	7.63768000	-1.17532800
C	-2.78139900	6.95594900	1.03396000
C	-0.40268800	7.78809200	0.87544700
H	-0.94825100	7.69506200	-1.82754200
H	-2.62313200	7.11091800	-1.71399700
H	-2.17182700	8.66147500	-0.99270500
H	-2.60338300	6.52387700	2.02427200
H	-3.14121700	7.98191900	1.17630400
H	-3.57750300	6.37829400	0.55014600
H	-0.74355400	8.82090100	1.01539100

H	-0.15586000	7.38126100	1.86173900
H	0.51627300	7.80947700	0.27824800

5_{bipy}(t-Bu)

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1644.516047 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1643.883287 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1643.993912 hartrees

C	1.81362200	4.06925700	-2.45553400
C	1.45754900	5.01463100	-1.49349600
C	0.93945300	4.59559100	-0.26749400
C	0.78414000	3.23195500	-0.02549600
C	1.63643800	2.72111100	-2.16479200
C	0.26306800	2.63923700	1.21991300
C	-0.14115200	3.37978100	2.32837900
C	-0.60520600	2.72162300	3.46601200
H	-0.92138200	3.29195400	4.33256700
C	-0.65238300	1.32957800	3.47243600
C	-0.23847200	0.63678300	2.34038300
H	2.22060400	4.36297200	-3.41590400
H	1.58182800	6.07390400	-1.69128600
H	1.88447400	1.91600200	-2.84689200
H	-1.00178800	0.77602500	4.33598900
H	-0.25123600	-0.44402600	2.29693000
H	-0.09306900	4.46110000	2.30745900
H	0.66389000	5.32441600	0.48408800
N	0.20377800	1.27223700	1.24015100
N	1.13436100	2.33144800	-0.98234000
Pt	0.84188000	0.36878600	-0.47637500
C	-0.00433100	-1.63767900	-0.01289900

C	1.22190300	-1.68720500	0.24930800
C	2.55776200	-2.06831000	0.59055000
C	3.62139600	-1.76692000	-0.27911000
C	2.82179900	-2.73934100	1.79968800
C	4.92015500	-2.13553500	0.05979400
H	3.40318900	-1.24899300	-1.20765900
C	4.12597500	-3.09738200	2.11656500
H	2.00691100	-2.97034900	2.47853300
C	5.20694400	-2.80380500	1.26192300
H	5.71577900	-1.89072300	-0.63363200
H	4.30340600	-3.61284400	3.05514800
F	1.54243800	-0.27675000	-2.21415200
C	-3.87923700	-2.50283300	-0.53095300
C	-4.54103600	-3.37398600	0.36078100
C	-5.88179200	-3.67841300	0.17086500
C	-6.62296200	-3.13938400	-0.89924200
C	-5.95274000	-2.27146800	-1.77602800
C	-4.60741100	-1.95448400	-1.60353900
H	-3.99426800	-3.80495900	1.19361300
H	-6.36141900	-4.35286900	0.87308600
H	-6.47631000	-1.82857900	-2.61468500
H	-4.11325900	-1.28282400	-2.29874200
C	-2.50781500	-2.19064000	-0.35129000
C	-1.32279500	-1.94328300	-0.19280800
C	6.63107700	-3.21054200	1.66877000
C	6.99710300	-2.51161500	3.00018700
C	6.68950900	-4.74508600	1.85981400
C	7.67920400	-2.81527200	0.61196800
H	6.96151400	-1.42160600	2.89056100
H	6.31631100	-2.79327700	3.81010900

H	8.01260400	-2.79189100	3.30402700
H	6.43590300	-5.26381000	0.92823400
H	7.70110300	-5.04717700	2.15541100
H	5.99864400	-5.08696500	2.63735800
H	8.67332600	-3.12845000	0.94884900
H	7.48733000	-3.30025600	-0.35190400
H	7.70862900	-1.73122400	0.45393100
C	-8.10302400	-3.51492100	-1.06554700
C	-8.74981400	-2.83311400	-2.28547100
C	-8.22128200	-5.04739400	-1.24704100
C	-8.88323000	-3.08599300	0.20016600
H	-8.72353200	-1.74064900	-2.20240000
H	-8.25722000	-3.12078500	-3.22122000
H	-9.80034900	-3.13488200	-2.35761500
H	-7.82130000	-5.59283200	-0.38601300
H	-9.27405200	-5.33097100	-1.36268800
H	-7.67815400	-5.37733900	-2.14007500
H	-9.94138900	-3.35392100	0.09661200
H	-8.50142300	-3.57688200	1.10135600
H	-8.81762500	-2.00223200	0.35001500

4_{dppe}(t-Bu)

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2837.064972 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2836.148984 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2836.294199 hartrees

P	3.08409400	0.25284700	-0.48663300
P	0.85919500	-0.82173700	1.62253700
C	2.08419000	0.47507600	2.11657700
H	1.63933300	1.44929400	1.89760200

H	2.25520600	0.40341800	3.19493600
C	3.39697700	0.28567500	1.33962800
H	4.11249500	1.06423000	1.61525900
H	3.85523400	-0.67693700	1.58966200
C	3.14173000	1.93382200	-1.17319300
C	2.53331600	2.13880900	-2.42451800
C	3.77701000	2.99516100	-0.51472900
C	2.57369000	3.40320300	-3.00942400
H	2.01724000	1.31820000	-2.91473100
C	3.80657200	4.25957100	-1.10804700
H	4.24650000	2.85538100	0.45301900
C	3.20798000	4.46372600	-2.35355600
H	2.10027900	3.56365600	-3.97344100
H	4.29415700	5.08190800	-0.59334900
H	3.22982900	5.44895100	-2.80997200
C	4.38353700	-0.75394600	-1.25756500
C	5.66624100	-0.84416000	-0.69321300
C	4.08111400	-1.43677600	-2.44826200
C	6.64104800	-1.62208600	-1.31824900
H	5.91124400	-0.31409300	0.22223400
C	5.06674500	-2.20930400	-3.06460500
H	3.08614300	-1.35933500	-2.87689300
C	6.34212200	-2.30475100	-2.50135100
H	7.63239700	-1.69415100	-0.88102200
H	4.83497800	-2.74058800	-3.98303600
H	7.10391700	-2.91111600	-2.98268500
C	-0.74126400	-0.47111700	2.38238200
C	-1.66561400	-1.52075300	2.52040900
C	-1.09403800	0.83144600	2.76813300
C	-2.92720500	-1.26617600	3.05486500

H	-1.40367400	-2.52810400	2.21494300
C	-2.36149700	1.07687700	3.29647900
H	-0.40313100	1.65810600	2.65454400
C	-3.27758900	0.03190900	3.43927500
H	-3.63764000	-2.07977700	3.16262600
H	-2.62987900	2.08675400	3.59027300
H	-4.26364500	0.22763000	3.84974300
C	1.45970800	-2.40962200	2.27342200
C	1.26836700	-2.65419200	3.64702600
C	2.15244400	-3.34860300	1.48987900
C	1.76522600	-3.82066900	4.22480200
H	0.72707400	-1.94298500	4.26305000
C	2.64342400	-4.51489600	2.08012100
H	2.32442000	-3.20676600	0.42922400
C	2.45192400	-4.75283500	3.44217400
H	1.61147500	-4.00100300	5.28416800
H	3.17473300	-5.23721700	1.46825400
H	2.83511100	-5.66316100	3.89335800
Pt	0.88450700	-0.75119100	-0.72348700
F	1.06840600	-0.68678200	-2.76472500
C	-0.95997400	-1.53614800	-0.89493800
C	-2.12207700	-1.89686800	-1.01737700
C	-3.47414000	-2.32072100	-1.16122300
C	-4.45167500	-1.93546200	-0.22537700
C	-3.87585500	-3.12220300	-2.24996100
C	-5.77899700	-2.33292800	-0.37786300
H	-4.16391000	-1.31774700	0.61915200
C	-5.20140600	-3.51482400	-2.38504400
H	-3.13832100	-3.43119300	-2.98489100
C	-6.18932900	-3.12984400	-1.45790200

H	-6.49660400	-2.00729500	0.36614100
H	-5.47210700	-4.13271700	-3.23576300
C	0.09980600	0.99666700	-0.50860800
C	-0.32057300	2.10213700	-0.23528400
C	-0.76663200	3.41106800	0.11309000
C	-2.03860800	3.61735500	0.67343600
C	0.08323500	4.52197700	-0.05619500
C	-2.44303300	4.89499800	1.05933700
H	-2.70276500	2.77082900	0.81673800
C	-0.33670800	5.78827300	0.33161000
H	1.06929100	4.37981800	-0.48623300
C	-1.60567900	6.00996200	0.90109800
H	-3.43034500	5.00778700	1.49185900
H	0.34438900	6.62219100	0.19033300
C	-2.01476100	7.42986000	1.32262200
C	-3.43435300	7.47978900	1.91730700
C	-1.02367900	7.94841500	2.39195100
C	-1.97261400	8.36218400	0.08860300
H	-4.18936300	7.14752400	1.19568000
H	-3.51988600	6.85902000	2.81647300
H	-3.67685000	8.50977600	2.20130600
H	0.00348000	7.97993500	2.01397100
H	-1.29877200	8.96438000	2.69949300
H	-1.03826600	7.30647600	3.28037000
H	-2.26103900	9.38028300	0.37594100
H	-0.97151400	8.41049100	-0.35239100
H	-2.66713700	8.01545200	-0.68528200
C	-7.64431900	-3.58014400	-1.66156800
C	-7.70612200	-5.12609900	-1.66980200
C	-8.57946800	-3.06585600	-0.55133400

C	-8.15953400	-3.03899300	-3.01677800
H	-7.09855800	-5.55450800	-2.47375600
H	-7.34691800	-5.53553900	-0.71856300
H	-8.73988700	-5.46097800	-1.81729700
H	-8.60250300	-1.97070500	-0.51461600
H	-9.60067700	-3.41287500	-0.74355000
H	-8.28231900	-3.43788900	0.43580900
H	-9.19697400	-3.35505200	-3.17891000
H	-8.12897700	-1.94344600	-3.03520300
H	-7.56242300	-3.40865000	-3.85692200

$TS_{C\text{-}C,dppe}$(t-Bu)

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2837.048593 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2836.134336 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2836.279034 hartrees

P	3.24748200	-0.04389700	-0.39363800
P	1.08995300	-1.07115200	1.71445900
C	2.26039300	0.28390200	2.17901200
H	1.79055900	1.23126300	1.89575900
H	2.41499600	0.27921800	3.26192700
C	3.58372500	0.08540200	1.42327800
H	4.28105100	0.89425200	1.65303700
H	4.06538400	-0.85062300	1.72381900
C	3.17753300	1.63317400	-1.10522100
C	2.54305700	1.78653800	-2.35143200
C	3.74856600	2.74395100	-0.46709300
C	2.50213900	3.04300800	-2.95460900
H	2.07119400	0.93018400	-2.82407500
C	3.69069900	3.99989900	-1.07520500

H	4.23976200	2.65013300	0.49516900
C	3.07443700	4.15008700	-2.31970000
H	2.01117700	3.15951300	-3.91625500
H	4.12919300	4.85778200	-0.57444800
H	3.03235300	5.12840800	-2.78950400
C	4.59872800	-0.97725100	-1.16440300
C	5.89462800	-0.98142600	-0.62549100
C	4.30824900	-1.71129000	-2.32727200
C	6.89643900	-1.72793600	-1.24694200
H	6.12698500	-0.41166300	0.26931700
C	5.32078500	-2.44869300	-2.94249200
H	3.30171700	-1.69228900	-2.73624900
C	6.61019000	-2.46097100	-2.40252300
H	7.89822800	-1.73717400	-0.82798000
H	5.10018600	-3.01878000	-3.84020400
H	7.39294600	-3.04230600	-2.88120000
C	-0.50793300	-0.79042500	2.51154100
C	-1.40868400	-1.86302100	2.62566900
C	-0.88867000	0.49265100	2.93390400
C	-2.66939500	-1.65358000	3.18213800
H	-1.12761000	-2.85599800	2.28961900
C	-2.15681400	0.69491700	3.47929500
H	-0.21719300	1.33785600	2.83626200
C	-3.04627500	-0.37493300	3.60485100
H	-3.35813900	-2.48719200	3.27910500
H	-2.44647100	1.68993000	3.80224400
H	-4.03188300	-0.21387300	4.03111400
C	1.78847000	-2.62767300	2.34035000
C	1.50171400	-3.03376200	3.65599200
C	2.67448600	-3.38583400	1.55512700

C	2.09119800	-4.18679300	4.17245500
H	0.82056700	-2.45745700	4.27313900
C	3.26093900	-4.53688600	2.08231500
H	2.92157300	-3.09391100	0.54038300
C	2.96851400	-4.93975500	3.38725400
H	1.86304900	-4.49560500	5.18794900
H	3.94385800	-5.11711300	1.46968400
H	3.42383500	-5.83837700	3.79260300
Pt	1.06198100	-1.01602800	-0.61136700
F	1.24766100	-1.00242700	-2.66248200
C	-0.92543500	-1.34149400	-0.81475200
C	-2.09273300	-1.68638000	-0.98669200
C	-3.44268500	-2.06204100	-1.17716600
C	-4.36323500	-2.00243400	-0.11152300
C	-3.90590200	-2.49170000	-2.44099500
C	-5.69480500	-2.35841500	-0.30648200
H	-4.02461100	-1.66864400	0.86360300
C	-5.23513900	-2.84753200	-2.61537400
H	-3.21113100	-2.54309700	-3.27381300
C	-6.16526500	-2.79067000	-1.55742000
H	-6.36873200	-2.29380700	0.53951600
H	-5.55699200	-3.17544500	-3.59880700
C	-0.21539300	0.49649000	-0.52019200
C	-0.59792400	1.63108700	-0.28447500
C	-1.01188800	2.96109700	0.00881200
C	-2.18680200	3.21367500	0.73887700
C	-0.22937700	4.05914100	-0.40309600
C	-2.56392200	4.52137600	1.04362200
H	-2.79794600	2.38012900	1.07107800
C	-0.62167400	5.35510400	-0.09378300

H	0.68452100	3.88233300	-0.96035000
C	-1.79671300	5.62330300	0.63509800
H	-3.47689600	4.66911300	1.60893800
H	0.00733700	6.17571500	-0.42636500
C	-2.18544800	7.07631400	0.94909600
C	-3.49654000	7.17322100	1.75103400
C	-1.05983800	7.73777700	1.77934400
C	-2.37035700	7.85331400	-0.37606400
H	-4.34176500	6.74429300	1.20078700
H	-3.42041000	6.66313000	2.71817300
H	-3.72868500	8.22554300	1.94852600
H	-0.10638600	7.74321500	1.24092100
H	-1.32090500	8.77802500	2.00800800
H	-0.91128000	7.20638400	2.72654100
H	-2.64313500	8.89471700	-0.16752800
H	-1.45420700	7.86167500	-0.97589500
H	-3.16707400	7.40577500	-0.98148000
C	-7.62580500	-3.19339900	-1.80722200
C	-7.67321900	-4.66656400	-2.27941700
C	-8.49664000	-3.06234100	-0.54387900
C	-8.22419100	-2.28186800	-2.90553500
H	-7.10847300	-4.81683400	-3.20537200
H	-7.25697100	-5.33397600	-1.51610800
H	-8.71087700	-4.96663400	-2.46742300
H	-8.52478100	-2.03081100	-0.17490600
H	-9.52481000	-3.36021300	-0.77681500
H	-8.13934200	-3.70913700	0.26546800
H	-9.26849000	-2.55781600	-3.09356700
H	-8.19832900	-1.23070700	-2.59621500
H	-7.67987800	-2.37050700	-3.85128200

5_{dppe}(t-Bu)

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2837.151022 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2836.235595 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2836.381581 hartrees

P	0.20985100	-2.48635400	-0.37249500
P	-0.34927700	-0.04998000	1.47486500
C	0.55151100	-1.50833700	2.19439000
H	1.62591500	-1.34467600	2.07480600
H	0.33558400	-1.57994000	3.26413900
C	0.10848800	-2.77629800	1.45097300
H	0.69954800	-3.64497800	1.75347700
H	-0.94184000	-3.00443900	1.66156500
C	1.95161300	-2.60711600	-0.90144700
C	2.25548200	-2.16185600	-2.20166000
C	2.97366900	-3.06010500	-0.05614500
C	3.57478200	-2.18731900	-2.64912500
H	1.46298400	-1.76150900	-2.82869400
C	4.29537200	-3.06916200	-0.51140000
H	2.76043200	-3.40145800	0.95142900
C	4.59601500	-2.63747000	-1.80487600
H	3.80938600	-1.83728900	-3.64992000
H	5.08686100	-3.41200700	0.14817600
H	5.62522000	-2.64109500	-2.15162600
C	-0.77624400	-3.76002900	-1.20730200
C	-0.89045000	-5.04401900	-0.64900800
C	-1.41142400	-3.45326400	-2.42211900
C	-1.64654500	-6.01599700	-1.30473700
H	-0.39876800	-5.29316400	0.28647500

C	-2.16187700	-4.43677200	-3.06859900
H	-1.30071800	-2.45919600	-2.84596700
C	-2.28323700	-5.71299300	-2.51189100
H	-1.73893900	-7.00732400	-0.87123000
H	-2.65583600	-4.20268400	-4.00722900
H	-2.87322500	-6.47219700	-3.01726400
C	0.52507100	1.45333300	1.99764900
C	-0.18954600	2.62954700	2.27714800
C	1.92866200	1.47862900	1.98497900
C	0.49753500	3.80945600	2.56299000
H	-1.27481400	2.62498800	2.27327700
C	2.60883600	2.66027200	2.27553500
H	2.50128000	0.59529500	1.72254300
C	1.89522000	3.82580100	2.56566700
H	-0.06004400	4.71530500	2.78141800
H	3.69414100	2.67206500	2.25334100
H	2.42674500	4.74703200	2.78559800
C	-1.99155400	-0.06323700	2.26015700
C	-2.12523600	0.28056700	3.61738500
C	-3.11975900	-0.46308600	1.52821100
C	-3.37701100	0.23079900	4.22815100
H	-1.25921300	0.59846900	4.19064500
C	-4.36983700	-0.51212600	2.14806600
H	-3.02678900	-0.72546500	0.48003600
C	-4.50042000	-0.16395800	3.49326200
H	-3.47646000	0.50256500	5.27475600
H	-5.23909800	-0.81413100	1.57320300
H	-5.47556900	-0.19710500	3.97044800
Pt	-0.41350400	-0.34361400	-0.77479200
F	-0.46000700	-0.60744400	-2.81936500

C	-0.31032200	2.05139600	-1.27473600
C	-1.52563500	1.81605500	-1.25980800
C	-2.93652100	1.62158500	-1.27681500
C	-3.77800000	2.33911200	-0.41196600
C	-3.48964600	0.63120500	-2.11657200
C	-5.14358300	2.06384400	-0.38377800
H	-3.35737900	3.09213400	0.24685700
C	-4.85143400	0.37243400	-2.07046900
H	-2.82463400	0.06665700	-2.76311700
C	-5.71178300	1.07313400	-1.20011400
H	-5.76225400	2.62782000	0.30330000
H	-5.25204600	-0.39770700	-2.72162400
C	1.02253800	2.32576500	-1.29734600
C	2.24047200	2.36132600	-1.21439500
C	3.63551800	2.20687800	-1.02253800
C	4.13111200	0.90758100	-0.79359400
C	4.53213200	3.29186400	-0.99470700
C	5.48425700	0.70723900	-0.53952100
H	3.44832400	0.06397500	-0.80942800
C	5.88003500	3.07035400	-0.74015800
H	4.16390800	4.29872100	-1.16434500
C	6.39103900	1.77864300	-0.50392700
H	5.82098400	-0.30758500	-0.36760700
H	6.54783200	3.92599000	-0.72193000
C	7.88790300	1.58818300	-0.21798700
C	8.25653200	0.11077200	0.01335400
C	8.70877200	2.11030500	-1.42112100
C	8.26776300	2.38826700	1.05099200
H	7.72748400	-0.30994700	0.87602100
H	8.03170600	-0.50668800	-0.86391800

H	9.33096800	0.02875900	0.21025600
H	8.52763500	3.17372300	-1.60832100
H	9.78041400	1.98234000	-1.22778100
H	8.45737200	1.55754600	-2.33363100
H	9.33608100	2.26732500	1.26584800
H	8.06951000	3.45862000	0.93292400
H	7.70132600	2.03238800	1.91934100
C	-7.21161200	0.74219000	-1.18359100
C	-7.41014600	-0.76399500	-0.89021400
C	-7.97710000	1.54298400	-0.11398200
C	-7.81194100	1.07589200	-2.57071000
H	-6.92482800	-1.39876500	-1.63818000
H	-7.00436700	-1.02820000	0.09285900
H	-8.47920700	-1.00648700	-0.89103600
H	-7.92456400	2.62212100	-0.29652000
H	-9.03416300	1.25653600	-0.13004500
H	-7.59234200	1.34310000	0.89277100
H	-8.88382700	0.84529500	-2.58157200
H	-7.68800100	2.13963300	-2.80353800
H	-7.33542500	0.49620200	-3.36836400

$4_{bipy}(NO_2)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1738.911498 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1738.506584 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1738.607520 hartrees

C	5.18950800	-0.70944500	-1.81630200
C	5.84992900	-0.75270500	-0.58873800
C	5.12182800	-0.93668600	0.58828900
C	3.73737400	-1.07389400	0.51220900

C	3.80559700	-0.85230500	-1.83378100
C	2.83739700	-1.26497300	1.66605300
C	3.26728400	-1.33057700	2.98890200
C	2.33631900	-1.50357700	4.01232300
H	2.66956700	-1.55149000	5.04318900
C	0.98337400	-1.60916300	3.69787000
C	0.59665900	-1.53801400	2.36564300
H	5.72787700	-0.56660500	-2.74560000
H	6.92787600	-0.64272300	-0.54106500
H	3.20827900	-0.82959000	-2.73839900
H	0.22820800	-1.74059600	4.46344900
H	-0.43761100	-1.60568200	2.05544600
H	4.32080500	-1.24451200	3.22165600
H	5.63147900	-0.97030900	1.54265100
N	1.50375600	-1.37808100	1.38514600
N	3.12204600	-1.02970100	-0.69604000
Pt	1.02295500	-1.23654700	-0.61226500
C	-0.94241000	-1.43259900	-0.44472800
C	-2.14768300	-1.54384700	-0.30232300
C	-3.55213100	-1.70736900	-0.13684800
C	-4.40110000	-1.76595000	-1.26267400
C	-4.10808300	-1.81908600	1.15571900
C	-5.77002800	-1.93484400	-1.10389400
H	-3.97680500	-1.68046500	-2.25703300
C	-5.47605800	-1.98781800	1.32163300
H	-3.45957000	-1.77433500	2.02383000
C	-6.28923000	-2.04456500	0.18780200
H	-6.43182400	-1.98325000	-1.95910900
H	-5.91459300	-2.07625000	2.30735800
F	0.86965500	-1.11661000	-2.56315700

C	0.53944100	3.27111400	-0.17990200
C	0.99872400	3.94513800	0.97012000
C	0.84303700	5.32039000	1.08598900
C	0.22646600	6.01820400	0.04564400
C	-0.23696900	5.37766600	-1.10515600
C	-0.07880100	4.00257600	-1.21512100
H	1.47458300	3.38367800	1.76667600
H	1.18969500	5.85157200	1.96314700
H	-0.71015200	5.95176400	-1.89145000
H	-0.43237600	3.48456000	-2.09984200
C	0.69297700	1.85878900	-0.29788300
C	0.80918300	0.65896600	-0.41952200
N	-7.73251100	-2.22670100	0.35889600
N	0.05996500	7.46872100	0.16490500
O	-8.43558700	-2.27882700	-0.65314800
O	-8.17420400	-2.31957900	1.50678500
O	-0.48876400	8.06852900	-0.76256600
O	0.47652000	8.01916500	1.18697800

$TS_{C\text{-}C,bipy}(NO_2)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1738.894359 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1738.491268 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1738.591145 hartrees

C	5.44959700	-0.96834100	-1.91821700
C	6.12973200	-0.95714600	-0.70059700
C	5.41574200	-1.03856000	0.49625500
C	4.02633900	-1.13415300	0.45047900
C	4.06177900	-1.06504800	-1.90540900
C	3.14099000	-1.22450700	1.62707700

C	3.59262500	-1.22177900	2.94476300
C	2.67655900	-1.31113300	3.99176500
H	3.02606600	-1.30794300	5.01834500
C	1.31670800	-1.40249200	3.70414300
C	0.91046800	-1.40010800	2.37566000
H	5.97632600	-0.90634000	-2.86303900
H	7.21171500	-0.88547500	-0.67638200
H	3.44972300	-1.08194700	-2.80032900
H	0.57108300	-1.47210700	4.48710900
H	-0.13171700	-1.46141500	2.09136100
H	4.65212800	-1.14975000	3.15423900
H	5.94006300	-1.02931400	1.44327500
N	1.80049100	-1.31733200	1.37023900
N	3.39003600	-1.14313500	-0.74866600
Pt	1.29004600	-1.28300900	-0.62063100
C	-0.68898800	-1.17708000	-0.41012100
C	-1.90231800	-1.30320800	-0.27679700
C	-3.30573700	-1.38086500	-0.11890500
C	-4.15141300	-1.34674100	-1.25114600
C	-3.87302400	-1.46179500	1.17341900
C	-5.52973900	-1.38536500	-1.09644000
H	-3.71626900	-1.28467400	-2.24235700
C	-5.25086000	-1.50056200	1.33167900
H	-3.22549000	-1.48786700	2.04277100
C	-6.05980000	-1.45980700	0.19371600
H	-6.19137000	-1.35519000	-1.95253400
H	-5.70115000	-1.55751500	2.31430100
F	1.11268300	-1.23662100	-2.57961700
C	0.04791600	3.04588200	-0.15986400
C	0.03080100	3.63904000	1.12278500

C	-0.11439800	5.01194100	1.25890200
C	-0.24406200	5.79528700	0.10894000
C	-0.23615100	5.23660500	-1.17191200
C	-0.09138000	3.86331500	-1.30413500
H	0.13662200	3.01370400	2.00255500
H	-0.12552000	5.47930800	2.23525200
H	-0.33923200	5.87447300	-2.04041900
H	-0.07919300	3.41082800	-2.28961800
C	0.22215100	1.64658800	-0.29619200
C	0.37182300	0.44068800	-0.41312800
N	-7.51657300	-1.49175300	0.35968600
N	-0.38859500	7.24312800	0.24988900
O	-8.21621700	-1.45687800	-0.65484500
O	-7.96787200	-1.55066000	1.50552300
O	-0.49774600	7.92004800	-0.77635900
O	-0.39339100	7.71961800	1.38845500

$5_{bipy}(NO_2)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1738.982105 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1738.577126 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1738.677199 hartrees

C	3.40506800	-2.94536900	-2.48260700
C	4.32100000	-3.08799600	-1.44031700
C	4.01352700	-2.59082600	-0.17315600
C	2.78999500	-1.95571400	0.02907800
C	2.19994000	-2.29975200	-2.22943400
C	2.31774400	-1.40126500	1.31047800
C	3.04373700	-1.45238900	2.49814100
C	2.49707500	-0.92109700	3.66496300

H	3.05713100	-0.95757500	4.59286300
C	1.22679300	-0.35182600	3.62060400
C	0.54417800	-0.32332800	2.40994700
H	3.61333700	-3.32334500	-3.47651000
H	5.27061200	-3.58496300	-1.60718000
H	1.42829200	-2.14351900	-2.97420500
H	0.75916800	0.06707500	4.50374700
H	-0.44646200	0.10268400	2.32788900
H	4.02686800	-1.90519400	2.51570400
H	4.71919400	-2.70180000	0.64027100
N	1.07575200	-0.82736700	1.28154800
N	1.91786400	-1.82336300	-1.00633400
Pt	0.17324000	-0.85624300	-0.55310500
C	-1.30154600	0.74312400	-0.03320600
C	-1.87749300	-0.37403300	-0.05008700
C	-2.93515000	-1.34368100	-0.01283600
C	-2.97365100	-2.38039300	-0.96637800
C	-3.93454900	-1.24109700	0.97431700
C	-4.00566200	-3.30856000	-0.93183600
H	-2.20448200	-2.41905800	-1.72927800
C	-4.96647100	-2.17044400	1.00977700
H	-3.89444400	-0.44093300	1.70490100
C	-4.98384200	-3.19094800	0.05750000
H	-4.06162700	-4.11042000	-1.65673400
H	-5.74577300	-2.11382100	1.75876700
F	-0.51810400	-1.07713600	-2.39391700
C	-0.08525700	4.53293200	0.34331200
C	-0.80218100	5.44006500	1.15357200
C	-0.35132400	6.74441700	1.30395900
C	0.81586500	7.13280300	0.64391300

C	1.54404800	6.25755700	-0.16387800
C	1.09064300	4.95428300	-0.31514700
H	-1.70470600	5.11433000	1.65825000
H	-0.88671400	7.45426100	1.92119100
H	2.44423300	6.59822500	-0.65898600
H	1.63881700	4.25596900	-0.93759300
C	-0.53644600	3.19738000	0.19714900
C	-0.92508700	2.04663600	0.07881000
N	-6.07325100	-4.17508600	0.09669900
N	1.29571000	8.51054300	0.80669800
O	-6.06586000	-5.07934100	-0.74035100
O	-6.93881400	-4.04590100	0.96427800
O	2.32893900	8.83637400	0.21927700
O	0.64098200	9.27026100	1.52285400

$4_{dppe}(NO_2)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2931.537241 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2930.850237 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2930.983963 hartrees

P	2.77203700	-1.19151100	-0.02613200
P	-0.00973900	-1.11732600	1.63462800
C	1.55629100	-0.54782900	2.42433400
H	1.62351500	0.52795300	2.23970700
H	1.49889500	-0.69272600	3.50720200
C	2.76763500	-1.28249900	1.82639300
H	3.69097500	-0.87673600	2.24579400
H	2.73428100	-2.34541700	2.08136500
C	3.78137400	0.20109500	-0.60764900
C	3.56245800	0.64158200	-1.92544200

C	4.76792100	0.80397700	0.18489800
C	4.34042100	1.67649500	-2.44171900
H	2.77573600	0.18800200	-2.52127700
C	5.53716500	1.84431300	-0.34199500
H	4.94834000	0.47885100	1.20378600
C	5.32709400	2.27811000	-1.65333900
H	4.16903000	2.02062300	-3.45718900
H	6.29730600	2.31369100	0.27482500
H	5.92596000	3.08854900	-2.05805300
C	3.45970000	-2.75002900	-0.65797000
C	4.39321000	-3.48810100	0.08814700
C	3.04008600	-3.20438000	-1.92068600
C	4.89520600	-4.68390300	-0.42545900
H	4.73588100	-3.13917600	1.05763700
C	3.55139600	-4.40236000	-2.42220100
H	2.32405300	-2.62456300	-2.49585300
C	4.47238000	-5.14290100	-1.67664800
H	5.61528800	-5.25557900	0.15212900
H	3.22480100	-4.75833100	-3.39480300
H	4.86222500	-6.07733900	-2.06967100
C	-1.39678800	-0.11247000	2.20570100
C	-2.64511200	-0.71716200	2.42718800
C	-1.24496800	1.27440200	2.37630200
C	-3.73181600	0.06391500	2.81798700
H	-2.77209900	-1.78632500	2.29805000
C	-2.33851600	2.04523900	2.76772500
H	-0.29231300	1.75872100	2.20082900
C	-3.58111900	1.44282600	2.98689000
H	-4.69587500	-0.40570300	2.98492400
H	-2.21682200	3.11570200	2.90073900

H	-4.43107700	2.04811100	3.28716800
C	-0.28547600	-2.86480100	2.00489900
C	0.29400800	-3.45715600	3.13966400
C	-1.08829100	-3.63026300	1.13854700
C	0.06933100	-4.80816500	3.40084800
H	0.90749100	-2.87934300	3.82265400
C	-1.30784200	-4.97941100	1.41322500
H	-1.53991100	-3.17366600	0.26280700
C	-0.72786400	-5.56823600	2.54003300
H	0.51705500	-5.26509900	4.27767200
H	-1.92918200	-5.56809000	0.74582700
H	-0.89693000	-6.62029700	2.74836300
Pt	0.44444200	-1.00566200	-0.66397800
F	0.96697100	-0.97314400	-2.66057300
C	-1.52674300	-0.86937300	-1.08920300
C	-2.72395400	-0.66259500	-1.21841600
C	-4.11703200	-0.39243200	-1.30615100
C	-4.66745300	0.64731800	-0.52387900
C	-4.96156700	-1.14330000	-2.15058500
C	-6.02459800	0.92989500	-0.58181600
H	-4.02077800	1.22170900	0.12912200
C	-6.32117100	-0.86751200	-2.21088900
H	-4.54302000	-1.94154600	-2.75382700
C	-6.83551200	0.16695300	-1.42563500
H	-6.45737600	1.72274200	0.01487200
H	-6.98057800	-1.43703700	-2.85329400
C	0.57191700	0.89909100	-0.47200900
C	0.72646300	2.09126600	-0.31298300
C	0.96411400	3.47928500	-0.10347400
C	-0.10445300	4.36354200	0.14882900

C	2.28668600	3.96919800	-0.12935300
C	0.14152200	5.71294700	0.36871100
H	-1.12042100	3.98446600	0.17298300
C	2.53755500	5.31710500	0.08724500
H	3.10685900	3.28684400	-0.31915900
C	1.46012600	6.17115500	0.33324700
H	-0.66688600	6.40566500	0.56449000
H	3.54665200	5.70860300	0.06885400
N	1.72239300	7.59403500	0.56279200
N	-8.26745600	0.45999600	-1.48778200
O	-8.97074800	-0.22603800	-2.23438900
O	-8.70399900	1.37959300	-0.79019600
O	2.89296200	7.98145800	0.52982700
O	0.76028500	8.33523900	0.77780600

$TS_{C\text{-}C,dppe}(NO_2)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2931.519552 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2930.833108 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2930.968155 hartrees

P	3.23773400	0.15969000	-0.07304400
P	0.88526300	-1.06155000	1.71602900
C	2.17988600	-0.00097100	2.49408100
H	1.80640000	1.02677100	2.45571600
H	2.28948600	-0.26421100	3.55021800
C	3.50774900	-0.12808200	1.73345000
H	4.25216400	0.55779800	2.14587800
H	3.91570200	-1.13982500	1.82171600
C	3.18907800	1.94724500	-0.40457200

C	2.69137700	2.34943400	-1.65722900
C	3.61593100	2.90515300	0.52582500
C	2.65141600	3.70523100	-1.97883300
H	2.31515400	1.60351200	-2.35153800
C	3.55138400	4.26182200	0.20026900
H	3.99807000	2.61394400	1.49843800
C	3.07657400	4.66209800	-1.05074400
H	2.27344700	4.01578700	-2.94855700
H	3.87619700	5.00240600	0.92479200
H	3.03157100	5.71799300	-1.30089100
C	4.61943200	-0.59301000	-0.97433900
C	5.89777400	-0.66993500	-0.39785300
C	4.39272700	-1.08418100	-2.27090600
C	6.94493300	-1.24521000	-1.11802000
H	6.08365900	-0.28819900	0.60158700
C	5.45061100	-1.65342500	-2.98171800
H	3.40127000	-1.01065800	-2.70772100
C	6.72214400	-1.73672600	-2.40773900
H	7.93255600	-1.30905900	-0.67120700
H	5.27885800	-2.03542900	-3.98375400
H	7.54043500	-2.18454700	-2.96413100
C	-0.71056100	-0.70483100	2.49076200
C	-1.59119100	-1.75062700	2.81049600
C	-1.08519300	0.62822200	2.73122200
C	-2.83730700	-1.46091700	3.36787500
H	-1.31119200	-2.78282600	2.63132300
C	-2.32923800	0.90605100	3.29528800
H	-0.42591500	1.44937600	2.47280500
C	-3.20796200	-0.13539000	3.60848000
H	-3.51434300	-2.27260200	3.61591100

H	-2.61217800	1.93674100	3.48448800
H	-4.17834200	0.08643000	4.04206300
C	1.31201500	-2.80655900	1.94698400
C	2.21368300	-3.21277200	2.94422700
C	0.72201500	-3.76298200	1.09900500
C	2.52156100	-4.56574000	3.08738500
H	2.67370200	-2.49205200	3.61166800
C	1.03188400	-5.11302400	1.25629700
H	0.02218000	-3.45579000	0.32731300
C	1.93347100	-5.51409000	2.24609800
H	3.22021700	-4.87683400	3.85766800
H	0.57216500	-5.84837900	0.60349500
H	2.17824000	-6.56558600	2.36176000
Pt	1.03619000	-0.67148600	-0.58213000
F	1.39039900	-0.38190100	-2.58219700
C	-0.93733900	-0.99466000	-0.93615900
C	-2.07280100	-1.41954600	-1.12019100
C	-3.39187500	-1.90011500	-1.29888800
C	-4.22430200	-2.09974600	-0.17392100
C	-3.88911500	-2.17754600	-2.59196300
C	-5.52056000	-2.56679300	-0.33656900
H	-3.84203100	-1.88285700	0.81743800
C	-5.18478000	-2.64530100	-2.75871500
H	-3.25069900	-2.02351900	-3.45496600
C	-5.98271500	-2.83423500	-1.62764500
H	-6.17060900	-2.72484900	0.51444300
H	-5.58024700	-2.86338200	-3.74244200
C	-0.26333900	0.80235100	-0.52162500
C	-0.75889500	1.90794100	-0.37513400
C	-1.38288700	3.16495600	-0.16415100

C	-2.59412900	3.23622900	0.55976500
C	-0.79935400	4.35132100	-0.65862100
C	-3.20462200	4.46116200	0.78903700
H	-3.04482700	2.32510900	0.93620800
C	-1.40762800	5.57841900	-0.43460400
H	0.13571400	4.29818500	-1.20396700
C	-2.60310900	5.61829900	0.28767200
H	-4.13263700	4.52961200	1.34224600
H	-0.96848600	6.49626400	-0.80435600
N	-7.35035200	-3.33009500	-1.80182900
N	-3.24420600	6.91084300	0.52741500
O	-2.70433100	7.92221000	0.07068800
O	-4.29456800	6.92842100	1.17509700
O	-8.04044000	-3.49592900	-0.79311500
O	-7.74385700	-3.55729800	-2.94842900

$5_{dppe}(NO_2)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2931.614915 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2930.926287 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2931.062575 hartrees

P	0.75852300	2.35999600	0.68747900
P	0.30179600	-0.57569000	1.63779100
C	0.01858700	0.79271000	2.85980300
H	-1.02909600	1.10144200	2.80445000
H	0.21616500	0.43113200	3.87294500
C	0.94297000	1.96074600	2.49266200
H	0.71645100	2.84539900	3.09412900
H	1.99242300	1.69224800	2.65421100
C	-0.69659700	3.44215900	0.51297300

C	-0.56004800	4.83354800	0.64502800
C	-1.96723200	2.88081100	0.29857900
C	-1.68799900	5.65160400	0.57333700
H	0.41883500	5.27765600	0.79845400
C	-3.08991700	3.70645800	0.23177600
H	-2.08156200	1.80911300	0.17125300
C	-2.95175100	5.09026600	0.36895900
H	-1.57783100	6.72722800	0.67314400
H	-4.06936700	3.26717600	0.06656700
H	-3.82654800	5.73123600	0.31098400
C	2.24216400	3.26810800	0.17538500
C	2.97982300	4.02138600	1.10403800
C	2.63883500	3.21578700	-1.17189200
C	4.11132300	4.72095100	0.68177600
H	2.68297300	4.07009000	2.14705300
C	3.77341600	3.91788100	-1.57916100
H	2.06238300	2.62130600	-1.87513900
C	4.50892000	4.66819800	-0.65680600
H	4.68153000	5.30252800	1.39983500
H	4.08551800	3.87483600	-2.61856600
H	5.39303700	5.21023000	-0.97978200
C	-1.05183200	-1.77879700	1.76813300
C	-0.81578200	-3.13545600	1.49025600
C	-2.36585500	-1.33287500	1.98620700
C	-1.88065800	-4.03551800	1.45237800
H	0.19340400	-3.48971000	1.30831500
C	-3.42423600	-2.23974800	1.95322300
H	-2.57819100	-0.28510000	2.16988900
C	-3.18414000	-3.59025100	1.68580100
H	-1.69001100	-5.08302400	1.23982600

H	-4.43721500	-1.88838900	2.12254000
H	-4.01217200	-4.29220700	1.65435600
C	1.85347500	-1.37864000	2.15576700
C	1.85330500	-2.29494600	3.22261500
C	3.06671900	-1.03923400	1.53357600
C	3.04859800	-2.87553500	3.64456200
H	0.92370100	-2.56336300	3.71540100
C	4.25946900	-1.62254900	1.96437400
H	3.09117700	-0.33077000	0.71290600
C	4.25151900	-2.54374800	3.01338900
H	3.03955700	-3.58835300	4.46359200
H	5.19082600	-1.36125600	1.47143400
H	5.17989800	-3.00281900	3.34029900
Pt	0.44360200	0.39592200	-0.41594100
F	0.63445200	1.22935200	-2.27570600
C	-0.45041100	-1.62787600	-1.58679600
C	0.78627300	-1.66680200	-1.61050800
C	2.18712800	-1.92219300	-1.73042500
C	2.72226800	-3.13669100	-1.26101200
C	3.03198000	-0.92119100	-2.25600900
C	4.09533800	-3.34440200	-1.29914000
H	2.06582300	-3.89721600	-0.85380800
C	4.40317600	-1.12905900	-2.29443100
H	2.58964700	0.00955300	-2.59504600
C	4.91359700	-2.33532900	-1.80831600
H	4.53271400	-4.26278800	-0.92975400
H	5.07352100	-0.37258700	-2.68145800
C	-1.80573000	-1.56694500	-1.55881500
C	-3.01785800	-1.45844500	-1.47639100
C	-4.41264600	-1.26724600	-1.32294100

C	-5.25863900	-2.35916100	-1.03508000
C	-4.95036500	0.03452400	-1.42346000
C	-6.61820500	-2.15377500	-0.84479100
H	-4.84017200	-3.35535900	-0.95242100
C	-6.30907200	0.24281900	-1.22963700
H	-4.29682100	0.87033500	-1.64781900
C	-7.12211600	-0.85523900	-0.94242900
H	-7.28314800	-2.97753700	-0.61956600
H	-6.73923200	1.23375100	-1.29686800
N	6.36730500	-2.54392000	-1.82028200
N	-8.55823000	-0.63598400	-0.73306300
O	-8.98549100	0.51706200	-0.81606400
O	-9.26292800	-1.61599900	-0.48439700
O	6.80369000	-3.60180700	-1.36335800
O	7.07544100	-1.64849900	-2.28387900

$4_{bipy}(CF_3)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2003.980396 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2003.569067 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2003.675050 hartrees

C	5.17392100	-1.95779900	-1.80065700
C	5.78670300	-2.20800800	-0.57307700
C	5.01736100	-2.26312400	0.59054100
C	3.64089400	-2.06547800	0.50121900
C	3.79584100	-1.76836000	-1.83119000
C	2.70576200	-2.08871600	1.64266000
C	3.09425500	-2.28063100	2.96628600
C	2.13451800	-2.27475400	3.97759500
H	2.43583100	-2.41987300	5.00923200

C	0.79505900	-2.07632300	3.65012500
C	0.45069900	-1.88825000	2.31759700
H	5.74502400	-1.90790000	-2.72000100
H	6.85914500	-2.35927300	-0.51509300
H	3.23538900	-1.56821200	-2.73756100
H	0.01910800	-2.06085700	4.40608100
H	-0.56962800	-1.72392100	1.99699500
H	4.13846100	-2.42861000	3.20943600
H	5.48887500	-2.45819800	1.54519300
N	1.38395600	-1.90274500	1.34878400
N	3.07065400	-1.82722000	-0.70665400
Pt	0.97496600	-1.58751500	-0.64961300
C	-0.98892500	-1.49039500	-0.50060700
C	-2.19988700	-1.40956600	-0.38294500
C	-3.61740100	-1.34249100	-0.25023800
C	-4.44670700	-1.44896800	-1.38532400
C	-4.20692200	-1.16086000	1.01729300
C	-5.82922700	-1.37788400	-1.25390100
H	-3.99786700	-1.58497700	-2.36367100
C	-5.58972900	-1.08724200	1.14397700
H	-3.57403600	-1.07342500	1.89430800
C	-6.40023400	-1.19552300	0.00957800
H	-6.46378400	-1.45540500	-2.13015800
H	-6.03972500	-0.93914700	2.11962800
F	0.87208500	-1.33232200	-2.58783100
C	1.39298600	2.91366400	-0.06953400
C	1.56184000	3.48471800	1.20606900
C	1.69712400	4.86278700	1.34358800
C	1.66314100	5.68306900	0.21229400
C	1.49705600	5.12703600	-1.06023800

C	1.36212400	3.75052200	-1.20257600
H	1.58259200	2.84420600	2.08157600
H	1.82066900	5.30135000	2.32767900
H	1.46526900	5.76946600	-1.93380100
H	1.22854200	3.31370700	-2.18668400
C	1.24956400	1.50092300	-0.21984100
C	1.12318400	0.30588400	-0.37500600
C	-7.89582800	-1.17591700	0.15722200
C	1.86156600	7.16615800	0.35156800
F	-8.50811600	-0.67843600	-0.94133000
F	-8.29186500	-0.43156900	1.21482100
F	-8.39485300	-2.42255700	0.34982800
F	1.48805100	7.61839800	1.56994000
F	1.15641600	7.85909700	-0.57235700
F	3.16215200	7.51520600	0.18705800

$TS_{C\text{-}C,bipy}(CF_3)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2003.964728 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2003.555275 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2003.661442 hartrees

C	5.41233800	-2.48522000	-1.82971600
C	6.01329900	-2.72212700	-0.59356100
C	5.24460200	-2.68789800	0.57119800
C	3.88113100	-2.41716300	0.47525300
C	4.04779800	-2.21739300	-1.86716900
C	2.94886300	-2.34555000	1.61669500
C	3.31991500	-2.56025600	2.94202800
C	2.36454000	-2.46524900	3.95290200
H	2.65174200	-2.62952800	4.98569900

C	1.04714700	-2.15675400	3.62187600
C	0.72143700	-1.95206600	2.28675900
H	5.98267300	-2.50560600	-2.75072700
H	7.07544500	-2.93249700	-0.53011100
H	3.49726500	-2.01879300	-2.77984500
H	0.27450800	-2.07082900	4.37652100
H	-0.28258900	-1.70615300	1.96713800
H	4.34704800	-2.79883300	3.18641400
H	5.70741200	-2.86881000	1.53290000
N	1.64764500	-2.05003600	1.31665400
N	3.32148800	-2.18583000	-0.74094800
Pt	1.26747100	-1.75565400	-0.68622300
C	-0.65080600	-1.25145300	-0.53462500
C	-1.87025900	-1.17360400	-0.43332200
C	-3.27564600	-1.05088700	-0.30235000
C	-4.09027500	-0.89794300	-1.44545900
C	-3.87348300	-1.06401900	0.97665900
C	-5.46642800	-0.76345900	-1.30897800
H	-3.63356900	-0.88304100	-2.42926100
C	-5.25034100	-0.92832200	1.10579300
H	-3.25094700	-1.17538700	1.85806400
C	-6.04540100	-0.77799700	-0.03516000
H	-6.09046700	-0.63927400	-2.18738000
H	-5.70740500	-0.93109400	2.08912100
F	1.19946000	-1.58159000	-2.63925800
C	0.85658800	2.74800200	-0.16796700
C	0.97768800	3.34216600	1.10525000
C	1.04188600	4.72567900	1.22914800
C	0.98280500	5.53297300	0.08888400
C	0.85960400	4.95607700	-1.17979500

C	0.79554400	3.57401500	-1.31048900
H	1.02061900	2.71221900	1.98761100
H	1.13189300	5.17945000	2.21002900
H	0.80748000	5.58752900	-2.06044800
H	0.69748500	3.12220400	-2.29201000
C	0.79902500	1.33459000	-0.30281900
C	0.73774800	0.12328000	-0.43103600
C	-7.54075900	-0.69005700	0.10153200
C	1.11415100	7.02402100	0.21531600
F	-8.09247200	0.07585500	-0.86647500
F	-7.91210100	-0.17030900	1.29272300
F	-8.11950200	-1.91259000	0.00929600
F	0.70359400	7.47191900	1.42358300
F	0.39412400	7.67757700	-0.72583400
F	2.40110800	7.42775700	0.06633000

$5_{bipy}(CF_3)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2004.053742 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2003.642303 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -2003.748071 hartrees

C	2.87643900	-3.82129200	-2.51164700
C	3.63068400	-4.30960600	-1.44459500
C	3.38596100	-3.84520000	-0.15162600
C	2.38807500	-2.89410800	0.05147200
C	1.89323000	-2.87211000	-2.25532600
C	2.00745500	-2.31980500	1.35461900
C	2.61297100	-2.65504200	2.56350700
C	2.16849500	-2.06424700	3.74506700
H	2.63602800	-2.31985800	4.68962000

C	1.12037300	-1.14843900	3.69294100
C	0.55149100	-0.84608100	2.46105700
H	3.04089000	-4.16434400	-3.52622800
H	4.40545100	-5.04995800	-1.61248600
H	1.25616900	-2.43801900	-3.01735400
H	0.73971900	-0.66739400	4.58615600
H	-0.26589100	-0.14357600	2.36944600
H	3.42424700	-3.37167900	2.58511700
H	3.96526100	-4.22336100	0.68111800
N	0.98462400	-1.41156300	1.31995700
N	1.67051400	-2.43122500	-1.00690000
Pt	0.23809700	-1.04343600	-0.54786300
C	-0.84500000	0.82908800	0.00682900
C	-1.67157500	-0.11350600	-0.04852600
C	-2.88328100	-0.88214000	-0.06307400
C	-3.14342300	-1.74819500	-1.14318000
C	-3.80051000	-0.76987900	0.99708700
C	-4.31594700	-2.49370800	-1.15624200
H	-2.42250500	-1.80536200	-1.95175600
C	-4.96997700	-1.52336300	0.97514400
H	-3.59216800	-0.10119000	1.82524800
C	-5.22424500	-2.38369400	-0.09718100
H	-4.52955300	-3.15528400	-1.98863800
H	-5.68386700	-1.44103300	1.78717200
F	-0.35129800	-0.88414200	-2.43293700
C	1.02287000	4.34932900	0.38270900
C	0.75562200	5.17814000	1.49199700
C	1.39767800	6.40533400	1.61340100
C	2.30754400	6.81491000	0.63401700
C	2.58100200	6.00021500	-0.46971800

C	1.94294300	4.77243500	-0.59946800
H	0.04554200	4.85510800	2.24553200
H	1.18795100	7.04660000	2.46221600
H	3.28292300	6.33036600	-1.22772000
H	2.14492100	4.13764500	-1.45549800
C	0.36411000	3.09915800	0.25041200
C	-0.22057400	2.03474200	0.13478700
C	-6.45664000	-3.24721100	-0.08408800
C	3.04580600	8.11642400	0.79218700
F	-6.91103300	-3.49837700	-1.33214600
F	-7.46689800	-2.67881100	0.61070300
F	-6.21116600	-4.44937800	0.49204500
F	2.35328200	9.00674800	1.53610800
F	3.30464500	8.69637000	-0.40149900
F	4.24096800	7.93632000	1.40573600

$4_{dppe}(CF_3)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -3196.606389 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -3195.911998 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -3196.054926 hartrees

P	3.12901000	0.28975500	-0.10600400
P	0.71765500	-1.07491100	1.57000900
C	1.75401200	0.22619900	2.36900100
H	1.21291600	1.16473600	2.21284400
H	1.80324500	0.04844000	3.44761100
C	3.16455600	0.28401800	1.75279500
H	3.69228600	1.16085600	2.13380600
H	3.74191500	-0.59560200	2.04586000
C	3.41606100	1.96464400	-0.74792400

C	2.95406000	2.24888800	-2.04514900
C	4.11153300	2.93852500	-0.01703600
C	3.18892700	3.50691100	-2.59854000
H	2.40410400	1.49339600	-2.59800700
C	4.33784000	4.19624100	-0.58098700
H	4.48308300	2.73508900	0.98161300
C	3.87754400	4.48123300	-1.86903500
H	2.82499200	3.72913500	-3.59715300
H	4.87089300	4.95073000	-0.01061600
H	4.05110600	5.46216900	-2.30141100
C	4.44421600	-0.81602400	-0.69862100
C	5.60606300	-1.06014700	0.05082100
C	4.26618500	-1.43141600	-1.95050700
C	6.57954900	-1.92656900	-0.44708800
H	5.76312200	-0.57912500	1.01127500
C	5.24876600	-2.29461000	-2.43760200
H	3.37319700	-1.23061700	-2.53552500
C	6.40037200	-2.54638800	-1.68737100
H	7.47691500	-2.11596300	0.13418000
H	5.11044800	-2.77314000	-3.40260000
H	7.15917600	-3.22355600	-2.06844800
C	-0.95311900	-1.06644300	2.26108300
C	-1.34392300	-2.11060900	3.11647800
C	-1.84440900	-0.01988700	1.97175600
C	-2.61869200	-2.09629300	3.68552100
H	-0.66557200	-2.92706900	3.33870500
C	-3.11435200	-0.01822000	2.54365900
H	-1.55494800	0.77419200	1.29563900
C	-3.50285300	-1.05336900	3.40041200
H	-2.91854300	-2.90419600	4.34555500

H	-3.80293400	0.78878000	2.31325200
H	-4.49633600	-1.05024400	3.83855200
C	1.46288200	-2.70359600	1.83250600
C	2.41425900	-2.92284200	2.84245200
C	1.06728300	-3.76384400	0.99401400
C	2.97367900	-4.19069000	2.99998700
H	2.71166300	-2.12610600	3.51556900
C	1.63335500	-5.02605400	1.16110300
H	0.32401200	-3.59826700	0.21897100
C	2.58901700	-5.23849100	2.15898400
H	3.70813800	-4.35792600	3.78142700
H	1.32879700	-5.84101100	0.51208000
H	3.03182100	-6.22197900	2.28367800
Pt	0.97820200	-0.65722900	-0.72460400
F	1.37326300	-0.36386700	-2.71392300
C	-0.84494300	-1.43966500	-1.09652400
C	-1.99754200	-1.84162200	-1.15155800
C	-3.33678400	-2.32424100	-1.12121700
C	-3.89980800	-2.71145100	0.11333100
C	-4.11942400	-2.40990800	-2.28970600
C	-5.21203700	-3.16455500	0.17586500
H	-3.29963000	-2.65155200	1.01398400
C	-5.43264000	-2.86410400	-2.22288000
H	-3.69123000	-2.11765400	-3.24291900
C	-5.97900900	-3.24059100	-0.99158700
H	-5.63925400	-3.46267000	1.12739200
H	-6.03122400	-2.93174700	-3.12499700
C	0.25552600	1.10809300	-0.47199900
C	-0.10326300	2.24969900	-0.27039600
C	-0.46292100	3.60700600	-0.01640800

C	-1.79076500	3.96045400	0.28973000
C	0.52988400	4.60607700	-0.05309600
C	-2.11617900	5.28574800	0.56157100
H	-2.55935900	3.19461900	0.31258100
C	0.19868600	5.92921500	0.21612800
H	1.55219100	4.33662200	-0.29144900
C	-1.12256800	6.26892300	0.52464600
H	-3.14001400	5.55688100	0.79556900
H	0.96376700	6.69744900	0.18201700
C	-7.41727700	-3.66717700	-0.91107500
C	-1.46052300	7.68910700	0.88128600
F	-7.63427700	-4.53427200	0.10471900
F	-7.83634300	-4.26429800	-2.05010600
F	-8.24120300	-2.60956100	-0.70104200
F	-2.74201900	7.99958700	0.58044700
F	-1.30568000	7.92051800	2.20919200
F	-0.66651900	8.57604700	0.23855100

$TS_{C\text{-}C,dppe}(CF_3)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -3196.589231 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -3195.896442 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -3196.039003 hartrees

P	3.48179900	-0.11528000	-0.11355200
P	1.09023700	-1.14823500	1.72647300
C	2.46304000	-0.16137600	2.46851700
H	2.16069500	0.88894300	2.41427300
H	2.57182100	-0.41137300	3.52782900
C	3.76527800	-0.39842500	1.69078600
H	4.56631900	0.23474400	2.08047100

H	4.09660100	-1.43705700	1.78823700
C	3.56604500	1.66810900	-0.46801900
C	3.05424200	2.09428000	-1.70712500
C	4.09935400	2.60058900	0.43285500
C	3.10153200	3.44630400	-2.04351300
H	2.60068300	1.37146800	-2.37937700
C	4.12373000	3.95507100	0.09261800
H	4.49619400	2.29149400	1.39401500
C	3.63043700	4.37786000	-1.14376700
H	2.71169300	3.77447400	-3.00274000
H	4.53104900	4.67635000	0.79464900
H	3.65311900	5.43188100	-1.40471800
C	4.78482700	-0.98119600	-1.02985600
C	6.07051200	-1.13057700	-0.48503600
C	4.48869600	-1.48791400	-2.30619800
C	7.05583800	-1.79375700	-1.21664300
H	6.30863600	-0.73706400	0.49879200
C	5.48543500	-2.14563300	-3.02913300
H	3.49327500	-1.35433300	-2.71941800
C	6.76396500	-2.30111500	-2.48642900
H	8.04913000	-1.91396100	-0.79465700
H	5.26059100	-2.53993800	-4.01578700
H	7.53414600	-2.81775200	-3.05183900
C	-0.46330600	-0.68476300	2.53023500
C	-1.37780800	-1.67407000	2.92404300
C	-0.77009800	0.67359100	2.72022200
C	-2.59117800	-1.30328000	3.50560400
H	-1.14893900	-2.72454200	2.78176700
C	-1.98273200	1.03288500	3.30610000
H	-0.08270000	1.45005100	2.40364900

C	-2.89560900	0.04724500	3.69398200
H	-3.29538900	-2.07107500	3.81110000
H	-2.21483500	2.08291400	3.45385400
H	-3.84133600	0.33228700	4.14486800
C	1.42008300	-2.91042200	1.98916200
C	2.27866500	-3.34338000	3.01301900
C	0.79841000	-3.85190900	1.14785600
C	2.51371300	-4.70700000	3.18845500
H	2.76080400	-2.63392500	3.67683300
C	1.03507000	-5.21287700	1.33709900
H	0.12942400	-3.52516200	0.35737000
C	1.89470000	-5.64040000	2.35270100
H	3.17965200	-5.03778200	3.97928300
H	0.55081200	-5.93651400	0.68890800
H	2.08235800	-6.70060900	2.49315100
Pt	1.21583600	-0.78618500	-0.57637700
F	1.53792100	-0.53727700	-2.58550000
C	-0.77297800	-1.03486800	-0.87279600
C	-1.92555100	-1.43208800	-1.00378600
C	-3.26172300	-1.89122400	-1.11774700
C	-4.06996800	-1.99217600	0.03564400
C	-3.79687200	-2.25528900	-2.37169400
C	-5.37937500	-2.44574700	-0.06674100
H	-3.65880200	-1.71422700	1.00008900
C	-5.10647000	-2.71043200	-2.46670200
H	-3.17682300	-2.18244000	-3.25895500
C	-5.89624500	-2.80653200	-1.31587500
H	-5.99727300	-2.52807100	0.82091900
H	-5.51443400	-2.99787300	-3.42958000
C	-0.00895200	0.75617100	-0.52772900

C	-0.44555700	1.88937200	-0.41634200
C	-0.99767000	3.18916800	-0.24566400
C	-2.18785400	3.35713000	0.49272100
C	-0.36705200	4.32029800	-0.80201100
C	-2.72855100	4.62539000	0.67259900
H	-2.67868400	2.48794700	0.91683900
C	-0.91470900	5.58581500	-0.62284500
H	0.55193600	4.19579100	-1.36409400
C	-2.09430600	5.73952500	0.11304700
H	-3.64698200	4.74941300	1.23643600
H	-0.42953600	6.45355100	-1.05701500
C	-7.33039600	-3.24300100	-1.43220400
C	-2.64951100	7.11397800	0.35583200
F	-7.76456500	-3.86248200	-0.31147700
F	-7.51925400	-4.09396200	-2.46611400
F	-8.15608200	-2.18744100	-1.63956800
F	-3.99431400	7.10037300	0.50369000
F	-2.14077800	7.66758400	1.48566500
F	-2.36142100	7.96539100	-0.65518100

$5_{dppe}(CF_3)$

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -3196.688943 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -3195.994612 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -3196.135856 hartrees

P	-0.25158700	-2.36482200	0.79223200
P	-0.41297500	0.64717200	1.54916400
C	0.24282400	-0.54358200	2.81675100
H	1.32976900	-0.59747900	2.71235700
H	0.01740600	-0.16873300	3.81909500

C	-0.39333300	-1.91928800	2.58113300
H	0.05760900	-2.68114600	3.22253800
H	-1.46646600	-1.89606700	2.79900500
C	1.45923400	-2.89052700	0.43528100
C	1.84255800	-2.95991600	-0.91749600
C	2.38899800	-3.17067000	1.44596800
C	3.14857800	-3.31895200	-1.24630900
H	1.12463200	-2.70579200	-1.69306800
C	3.69959300	-3.51563600	1.10458800
H	2.11217700	-3.12057500	2.49375000
C	4.07944800	-3.59205800	-0.23705400
H	3.44518100	-3.36886900	-2.28972600
H	4.42057300	-3.72304300	1.88947200
H	5.09966600	-3.85838100	-0.49748500
C	-1.40405600	-3.72541200	0.45675600
C	-1.68615000	-4.66851300	1.45906300
C	-1.99330600	-3.83840800	-0.81325100
C	-2.56227400	-5.71999100	1.18898400
H	-1.23223900	-4.59203200	2.44222600
C	-2.86617100	-4.89708200	-1.06968700
H	-1.75542100	-3.10586800	-1.57884900
C	-3.15291200	-5.83384400	-0.07300400
H	-2.78385000	-6.44703900	1.96450700
H	-3.32506800	-4.98703900	-2.05003900
H	-3.83614600	-6.65300100	-0.27802700
C	0.71123600	2.07396000	1.51333700
C	0.21277700	3.37382700	1.33101300
C	2.09879700	1.85797600	1.54075400
C	1.09653600	4.44580600	1.20089800
H	-0.85726100	3.55093800	1.29472900

C	2.97534400	2.93521200	1.42145000
H	2.50499800	0.85526700	1.62731800
C	2.47611400	4.22919400	1.25064000
H	0.70532500	5.44916500	1.06204500
H	4.04632700	2.75955700	1.44053400
H	3.16123600	5.06567300	1.14910700
C	-2.02427800	1.20435800	2.19148100
C	-2.07037300	2.00576700	3.34684600
C	-3.21961800	0.82272600	1.56312800
C	-3.29843700	2.42513200	3.85517700
H	-1.15233100	2.31259400	3.84011900
C	-4.44666600	1.25301900	2.07290700
H	-3.20029300	0.19953900	0.67688300
C	-4.48620300	2.05406900	3.21528200
H	-3.32832200	3.04647500	4.74518200
H	-5.36392800	0.97884900	1.56168700
H	-5.44063100	2.39275400	3.60791000
Pt	-0.55214900	-0.47110100	-0.42340500
F	-0.72549700	-1.48595800	-2.20550300
C	0.02640200	1.51313300	-1.80985000
C	-1.20810900	1.44786700	-1.77023900
C	-2.63327400	1.54431000	-1.79370500
C	-3.26742400	2.71847900	-1.35040600
C	-3.39682100	0.41777000	-2.16490100
C	-4.65440900	2.75327300	-1.24858900
H	-2.67231000	3.57762000	-1.06122600
C	-4.78066100	0.46285000	-2.05893700
H	-2.87873400	-0.47967000	-2.48718800
C	-5.40486900	1.62474500	-1.58888100
H	-5.15034000	3.64757100	-0.88883000

H	-5.37527000	-0.40347500	-2.32782400
C	1.38364600	1.56669600	-1.83478300
C	2.59938300	1.53599300	-1.73985400
C	3.98327000	1.38111800	-1.47253600
C	4.89615600	2.43696200	-1.65568300
C	4.42967700	0.14881200	-0.94829700
C	6.23293900	2.26256100	-1.31272500
H	4.55092000	3.38474300	-2.05395800
C	5.76582700	-0.01595700	-0.60709600
H	3.72507900	-0.66361200	-0.80920500
C	6.66538100	1.04048200	-0.78785800
H	6.93951800	3.07311900	-1.45249700
H	6.10801100	-0.96391600	-0.20592700
C	-6.89058900	1.61643100	-1.35908200
C	8.09589800	0.87617400	-0.35242100
F	-7.19294500	1.07466400	-0.14752900
F	-7.54385900	0.87924800	-2.28297500
F	-7.42020000	2.85727200	-1.37413600
F	8.93392500	1.67934600	-1.04424400
F	8.25188100	1.18184300	0.95922900
F	8.52804600	-0.39538300	-0.50959200

4,4'-(buta-1,3-diyne-1,4-diyl)bis(N,N-dimethylaniline)

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -883.603064 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -883.230870 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -883.310272 hartrees

C	-5.44212400	-0.88221600	-0.83173400
C	-4.05680800	-0.87755700	-0.82776600
C	-3.32274500	0.00014300	-0.00011000

C	-4.05679700	0.87780200	0.82758400
C	-5.44212000	0.88242000	0.83160900
C	-6.18274400	0.00012100	-0.00007400
H	-5.95333800	-1.57690300	-1.48688100
H	-3.52209200	-1.56532700	-1.47661000
H	-3.52208500	1.56555900	1.47644600
H	-5.95331800	1.57703400	1.48684600
C	-1.90500000	0.00013800	-0.00013300
C	-0.67995100	0.00011200	-0.00015600
C	0.67994600	0.00008600	-0.00016400
C	1.90499500	0.00004300	-0.00015900
C	3.32274100	-0.00002200	-0.00013900
C	4.05673900	-0.87774200	0.82754600
C	4.05685600	0.87763600	-0.82778500
C	5.44205900	-0.88243200	0.83158200
H	3.52197900	-1.56548800	1.47637800
C	5.44217600	0.88221500	-0.83174400
H	3.52218800	1.56543200	-1.47664100
C	6.18273800	-0.00014200	-0.00006500
H	5.95321700	-1.57711600	1.48677700
H	5.95342800	1.57685200	-1.48691500
N	-7.55593800	0.00014300	-0.00011200
N	7.55594200	-0.00021500	-0.00004700
C	8.28779900	0.91983500	-0.85949400
H	8.05161200	1.96655700	-0.62549500
H	9.35816400	0.77452900	-0.71238000
H	8.06384300	0.74801100	-1.92098400
C	8.28768100	-0.91967900	0.86012500
H	9.35806600	-0.77452900	0.71299900
H	8.06362100	-0.74716900	1.92149200

H	8.05148200	-1.96653300	0.62677100
C	-8.28771500	-0.92003200	-0.85948900
H	-8.05148100	-1.96672100	-0.62538300
H	-9.35809300	-0.77477000	-0.71243100
H	-8.06372800	-0.74830000	-1.92098700
C	-8.28774000	0.91953700	0.86007000
H	-9.35811400	0.77452000	0.71272700
H	-8.06388900	0.74686900	1.92145800
H	-8.05139900	1.96639700	0.62689300

1,4-bis(4-(tert-butyl)phenyl)buta-1,3-diyne

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -930.184338 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -929.730171 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -929.810511 hartrees

C	5.43253500	1.22756500	0.07924800
C	4.03938200	1.22920800	0.06136800
C	3.32292000	0.02131800	-0.03193700
C	4.05266900	-1.18399800	-0.10960300
C	5.44087600	-1.16630300	-0.09121700
C	6.16880100	0.03531800	0.00501900
H	5.94147100	2.18132000	0.15444300
H	3.49756400	2.16821300	0.12182200
H	3.51997700	-2.12723200	-0.18320400
H	5.96840700	-2.11337300	-0.15235200
C	1.90232500	0.01407200	-0.04338900
C	0.67988500	0.00466900	-0.04751400
C	-0.67988800	-0.00460200	-0.04746100
C	-1.90232700	-0.01402100	-0.04332200
C	-3.32292000	-0.02130000	-0.03187600

C	-4.03936700	-1.22919400	0.06140700
C	-4.05268400	1.18401400	-0.10954900
C	-5.43252400	-1.22756300	0.07927200
H	-3.49754700	-2.16819800	0.12185300
C	-5.44088800	1.16630500	-0.09118100
H	-3.51999500	2.12725000	-0.18314600
C	-6.16880100	-0.03532600	0.00505100
H	-5.94144100	-2.18132800	0.15445200
H	-5.96843600	2.11336600	-0.15233200
C	7.70477200	-0.00176400	0.02769100
C	-7.70477200	0.00173800	0.02767100
C	-8.32490600	-1.40329200	0.13869100
H	-8.05041400	-2.03729400	-0.71200700
H	-8.01859700	-1.91071500	1.06044300
H	-9.41713500	-1.32069300	0.15218400
C	-8.21960800	0.65637300	-1.27624600
H	-7.85217800	1.68126300	-1.39124800
H	-7.90028600	0.08153700	-2.15314800
H	-9.31550900	0.69260300	-1.27186600
C	-8.17610100	0.83665600	1.24210600
H	-7.80472400	1.86580000	1.19866700
H	-9.27147900	0.87733500	1.26887800
H	-7.82768100	0.39011400	2.18048600
C	8.21965500	-0.65640500	-1.27620300
H	7.85222700	-1.68129200	-1.39123800
H	7.90036900	-0.08156100	-2.15311600
H	9.31555500	-0.69263800	-1.27177900
C	8.17604300	-0.83668400	1.24214500
H	7.80464100	-1.86581700	1.19870100
H	9.27142000	-0.87738900	1.26895600

H	7.82759900	-0.39012200	2.18050700
C	8.32492300	1.40325900	0.13871900
H	8.05040200	2.03728200	-0.71195400
H	8.01864900	1.91066200	1.06049300
H	9.41715000	1.32065100	0.15217500

N-(4-((4-(hydroxy(λ^1-oxidaneyl)amino)phenyl)buta-1,3-diyn-1-yl)phenyl)-N-(λ^1-oxidaneyl)hydroxylamine

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1024.656198 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1024.430584 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1024.498020 hartrees

C	-5.41835100	0.86568200	0.86240100
C	-4.03052000	0.86431300	0.86095000
C	-3.31983500	-0.00000400	-0.00008900
C	-4.03055600	-0.86429500	-0.86110800
C	-5.41838400	-0.86570900	-0.86243800
C	-6.09361400	-0.00003500	0.00001800
H	-5.97663500	1.52269900	1.51689000
H	-3.48647300	1.52877400	1.52288400
H	-3.48654100	-1.52873200	-1.52309200
H	-5.97670700	-1.52270700	-1.51691500
C	-1.90018600	0.00003200	-0.00008700
C	-0.67915900	0.00005100	-0.00006800
C	0.67916200	0.00009900	-0.00003500
C	1.90019200	0.00014600	-0.00003300
C	3.31983500	0.00010400	-0.00003600
C	4.03059800	0.86442900	-0.86098200
C	4.03048900	-0.86428100	0.86097200
C	5.41843200	0.86575200	-0.86234100
H	3.48662900	1.52898300	-1.52288700

C	5.41830500	-0.86574100	0.86238800
H	3.48640300	-1.52875500	1.52286100
C	6.09363300	-0.00002200	0.00002900
H	5.97677400	1.52276800	-1.51678400
H	5.97656400	-1.52278500	1.51687000
N	7.55874900	-0.00008100	0.00005100
N	-7.55876000	-0.00004500	0.00007000
O	8.14022800	0.77054300	-0.76782000
O	8.14019400	-0.77077800	0.76789100
O	-8.14025800	-0.77121400	-0.76724200
O	-8.14018700	0.77113800	0.76743100

1,4-bis(4-(trifluoromethyl)phenyl)buta-1,3-diyne

E (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1289.724472 hartrees

H (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1289.491638 hartrees

G (SMD/B3LYP-D3/LANL2DZ,6-31G(d)) = -1289.569165 hartrees

C	5.41351000	0.86013600	-0.86026600
C	4.02352700	0.84984900	-0.85596000
C	3.32291500	-0.04411200	-0.01992900
C	4.04771900	-0.92786100	0.80623300
C	5.43769700	-0.91244900	0.79723700
C	6.12015000	-0.01963500	-0.03468400
H	5.94942900	1.54572800	-1.50767600
H	3.47073700	1.52839400	-1.49683900
H	3.51378100	-1.62082500	1.44767200
H	5.99246100	-1.59645500	1.43031700
C	1.90093600	-0.05423900	-0.01175900
C	0.67992700	-0.05689900	-0.00441400
C	-0.67993400	-0.05694200	0.00419200

C	-1.90094300	-0.05424200	0.01160700
C	-3.32292200	-0.04414000	0.01987800
C	-4.02351000	0.84990500	0.85585100
C	-4.04774800	-0.92795400	-0.80618600
C	-5.41349000	0.86019800	0.86019300
H	-3.47069200	1.52849400	1.49665800
C	-5.43772800	-0.91253300	-0.79715500
H	-3.51383300	-1.62096100	-1.44759800
C	-6.12015100	-0.01964700	0.03471100
H	-5.94940000	1.54584100	1.50755900
H	-5.99251000	-1.59658200	-1.43017000
C	7.62146500	0.03903700	0.00621100
C	-7.62146200	0.03903600	-0.00614400
F	8.14663700	0.43741400	-1.17498100
F	8.06100800	0.91607200	0.94352500
F	8.16880000	-1.16010900	0.30967500
F	-8.16880400	-1.16002700	-0.30992500
F	-8.14660600	0.43710600	1.17516400
F	-8.06100400	0.91635800	-0.94319300