Supplementary Information for the Paper

Pd-Catalyzed C(sp^3)–C(sp) Bond Formation in Iodocyclobutenes

Carlos Lázaro-Milla,[†] M. Teresa Quirós,[§,II] Diego J. Cárdenas,*[,§] and Pedro Almendros*[,‡]

[†]*Grupo de Lactamas y Heterociclos Bioactivos, Departamento de Química Orgánica, Unidad Asociada al CSIC, Facultad de Química, Universidad Complutense de Madrid, 28040-Madrid, Spain*

[§]*Departamento de Química Orgánica, Facultad de Ciencias, Institute for Advanced Research in Chemical Sciences (IAdChem), Universidad Autónoma de Madrid, Av. Francisco Tomás y Valiente 7, Cantoblanco, 28049 Madrid, Spain*

[II]*Current address: Departamento de Química Orgánica y Química Inorgánica, Facultad de Farmacia, Universidad de Alcalá de Henares, Alcalá de Henares, 28871 Madrid, Spain*

[‡]*Instituto de Química Orgánica General, IQOG-CSIC, Juan de la Cierva 3, 28006-Madrid, Spain*

E-mail: diego.cardenas@uam.es; palmendros@iqog.csic.es

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COMPUTATIONAL METHODS

Calculations were performed with Gaussian 09 at DFT level.[1] The geometries of all complexes here reported were optimized using the B3LYP hybrid functional.[2] Optimizations were carried out using the standard 6-31G(d) basis set for C, H, O, S, F, P and N. The LANL2DZ basis set, which includes the relativistic effective core potential (ECP) of Hay and Wadt and employs a split-valence (double-ζ) basis set, was used for Pd, Cu and I.[3] The starting approximate geometries for the transition states (TS) were graphically located. Harmonic frequencies were calculated at the same level to characterize the stationary points and to determine the zero-point energies (ZPE). Intrinsic reaction coordinate (IRC) studies were performed to confirm the relation of the transition states with the corresponding minima. In order to obtain more reliable energy values, single-point energies for all stationary points were calculated with the M06 functional,[4] which models dispersion forces, using:

(1) 6-31G(d) basis set for C, H, O, S, F, P and N, and LANL2DZ basis set for Pd, Cu and I. Solvent effects were considered in the single-point calculations using the polarized continuum model (PCM) with triethylamine as solvent.[5]

(2) 6-311+G** basis set for C, H, O, S, F, P and N, and SDD basis set for Pd, Cu and I.[6] Solvent effects were considered in the single-point calculations using the Solvation Model Based on Density (SMD) with triethylamine as solvent.[7]

To assess the validity of the obtained energies, all the minima and one of the transition states were re-optimized using M06 hybrid functional, LANL2DZ for Pd, Cu and I, and 6-31G(d) for all other atoms, using PCM with triethylamine as solvent. The obtained energies were similar in all cases and have been summarized in Supplementary Table 1.

Gibbs free energy has been used throughout the schemes.

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[1] Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, 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, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

[2] (a) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623-11627. (b) Kohn, W.; Becke, A. D.; Parr, R. G. *J. Phys. Chem.* **1996**, *100*, 12974-12980. (c) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 270-283. (d) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 284-298. (e) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299-310.

[3] (a) Becke, A. D. *J. Chem. Phys*. **1993**, *98*, 5648- 5653. (b) Becke, A. D. *Phys. Rev. A* **1988**, *38*, 3098-3100. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785-789.

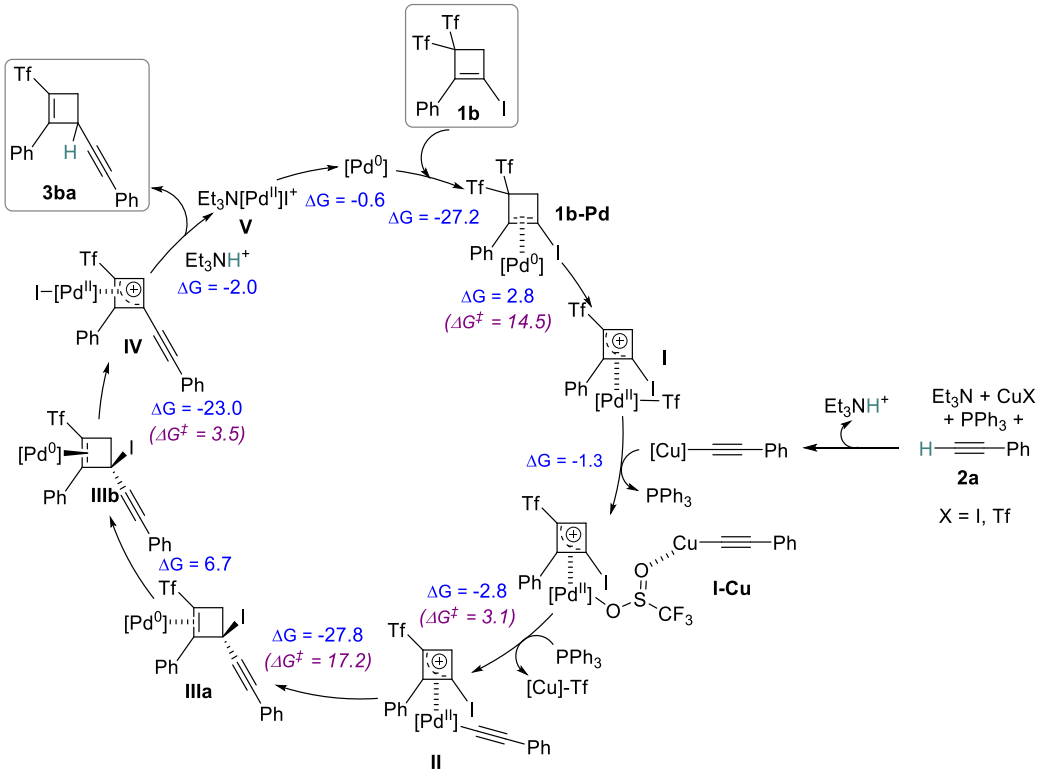
[4] Zhao, Y.; Truhlar, D.G. *Theor Chem Account.* **2006**, *120*: 215–241.

[5] Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev*., **2005**, *105*, 2999-3093.

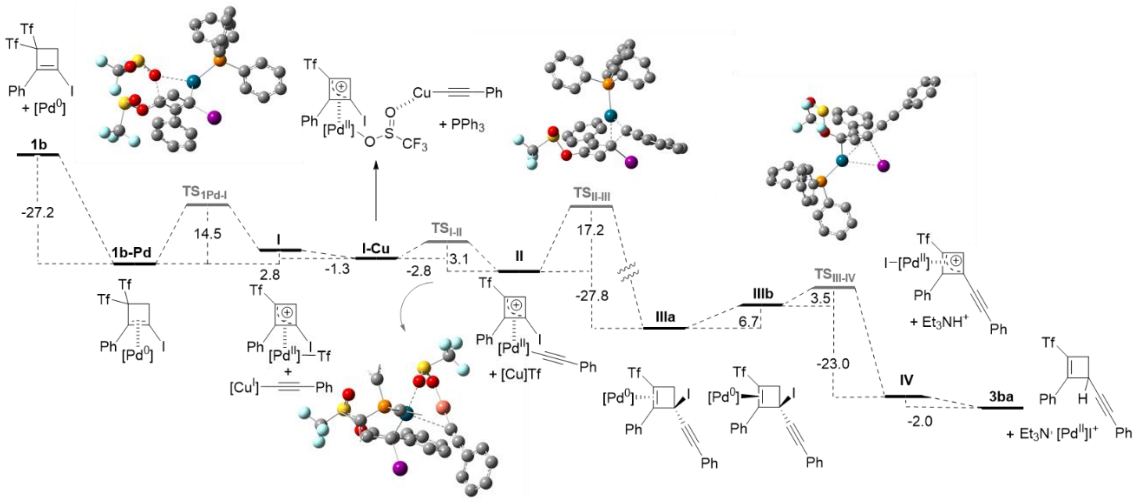
[6] (a) Dolg, M.; Stoll, H.; Preuss, H.; Pitzer, R. M. *J. Phys. Chem*., **1993**, *97*, 5852-5859; (b) Bergner, A.; Dolg, M.; Kuechle, W.; Stoll, H.; Preuss, H. *Mol. Phys.*, **1993**, *80*, 1431-1441; (c) Kaupp, M.; Schleyer, P. v. R.; Stoll, H.; Preuss, H. *J. Chem. Phys*., **1991**, *94*, 1360-1366.

[7] Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. J. *Phys. Chem. B* **2009**, *113*, 6378-6396

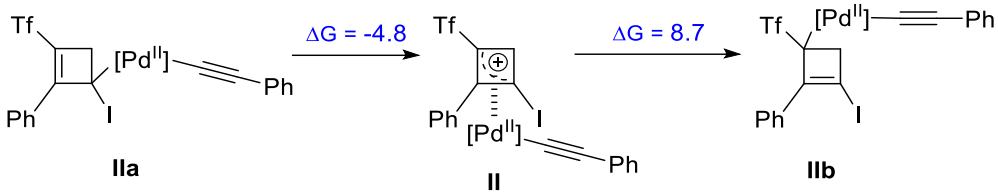
M06/6-311+G (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)**



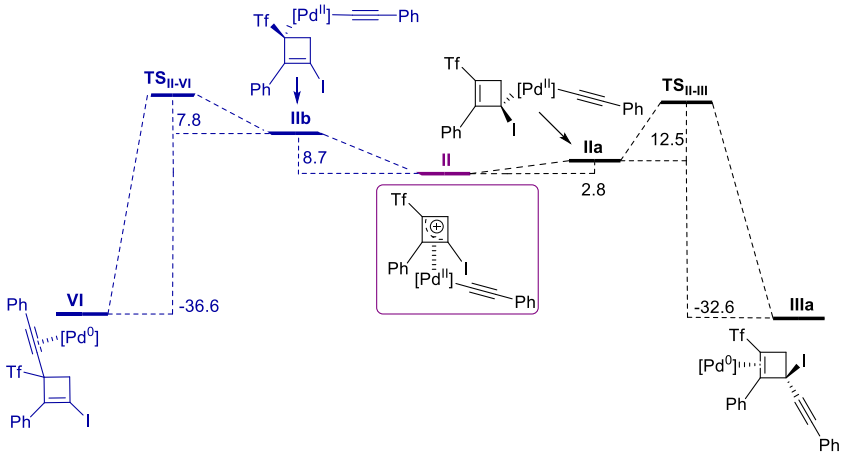
Supplementary Scheme 1. Mechanistic proposal for the Pd-catalyzed formation of 4-alkynyl-2-(triflyl)cyclobutenes **3**. Values of reaction free energies and activation energies (kcal/mol) are calculated at M06/6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I) with [Pd] = $(PPh_3)Pd$ and [Cu] = $(PPh_3)Cu$.



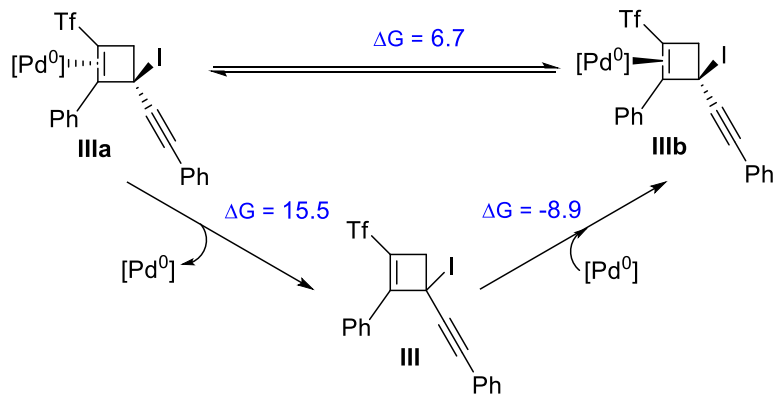
Supplementary Scheme 2. Energy profile for the Pd-catalyzed formation of 4-alkynyl-2-(triflyl)cyclobutenes **3**. Values of reaction free energies and activation energies (kcal/mol) are calculated M06/6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I) with [Pd] = $(PPh_3)Pd$ and [Cu] = $(PPh_3)Cu$. Ph in the PPh_3 ligand are omitted in some of the ball-and-stick models for clarity.



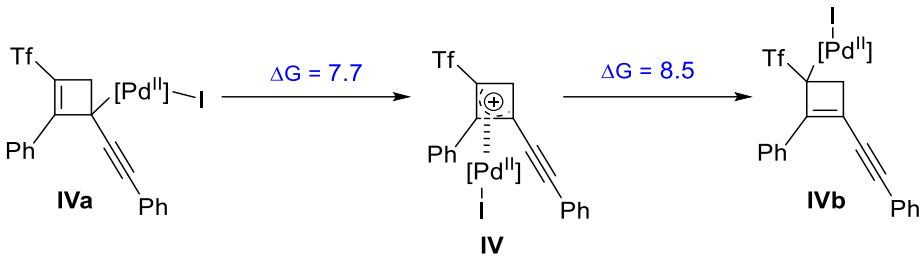
Supplementary Scheme 3. Π- and σ- allyl palladium complexes **II**. Values of reaction free energies and activation energies (kcal/mol) are calculated at M06/6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I) with [Pd] = $(PPh_3)Pd$ and [Cu] = $(PPh_3)Cu$.



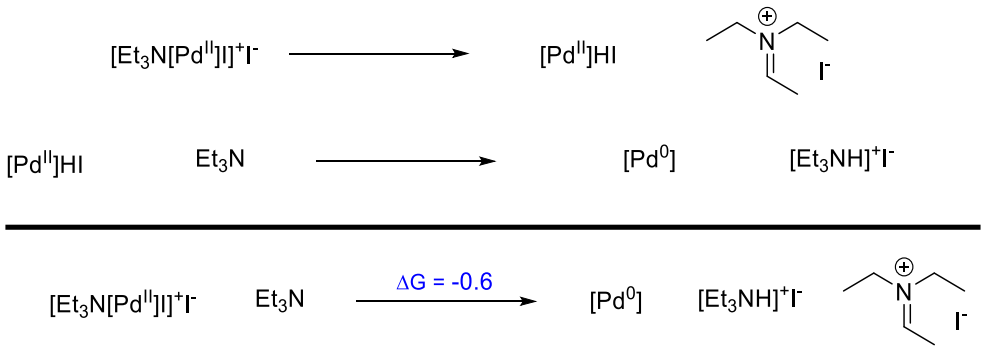
Supplementary Scheme 4. Energy profile for the comparison between the competitive reductive eliminations from **II**. The reductive elimination to give **IIIa** is energetically favoured, which matches the experimental results. Values of reaction free energies and activation energies (kcal/mol) are calculated at M06/6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I) with [Pd] = $(PPh_3)Pd$ and [Cu] = $(PPh_3)Cu$.



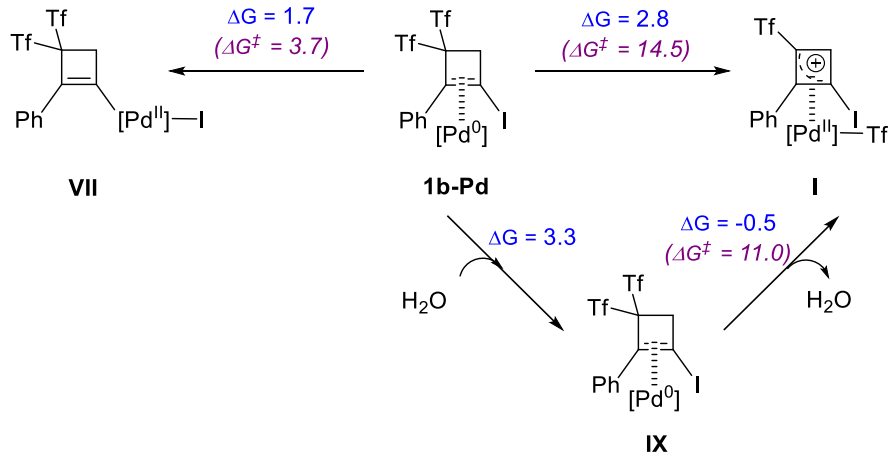
Supplementary Scheme 5. Interconversion between **IIIa** and **IIIb**. Values of reaction free energies and activation energies (kcal/mol) are calculated at M06/6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I) with [Pd] = $(PPh_3)Pd$ and [Cu] = $(PPh_3)Cu$.



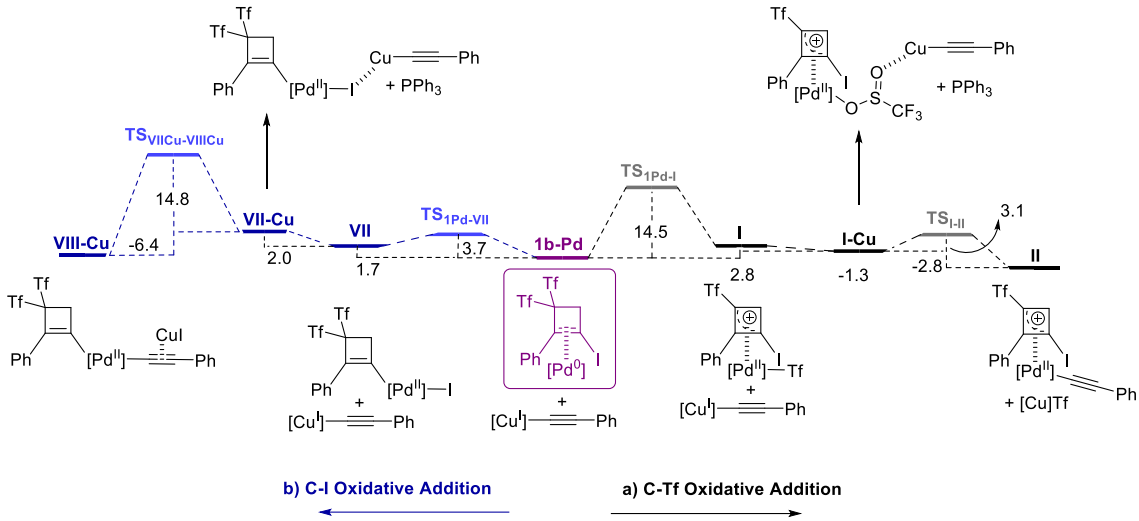
Supplementary Scheme 6. Π- and σ- allyl palladium complexes **IV**. Values of reaction free energies and activation energies (kcal/mol) are calculated at M06/6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I) with [Pd] = $(PPh_3)Pd$ and [Cu] = $(PPh_3)Cu$.



Supplementary Scheme 7. Reductive elimination from Pd(II) species to Pd(0). Values of reaction free energies and activation energies (kcal/mol) are calculated at M06/6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I) with [Pd] = $(PPh_3)Pd$ and [Cu] = $(PPh_3)Cu$.



Supplementary Scheme 8. Comparison between the competitive oxidative additions of the C-Tf or C-I bonds in **1b-Pd**. Values of reaction free energies and activation energies (kcal/mol) are calculated at M06/6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I) with [Pd] = $(PPh_3)Pd$ and [Cu] = $(PPh_3)Cu$.



Supplementary Scheme 9. Energy profile for the comparison between the competitive oxidative additions of the C-Tf or C-I bonds in **1b-Pd**. Although the oxidative addition of the C-I bond is energetically more favoured, it is reversible, and the next transmetallation step is more favoured from **I-Cu** than from **VII-Cu**. Values of reaction free energies and activation energies (kcal/mol) are calculated at M06/6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I) with [Pd] = (PPh_3)Pd and [Cu] = (PPh_3)Cu.

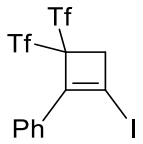
Comparison of energies obtained using different functionals

Supplementary Table 1: Values of reaction free energies and activation energies (kcal/mol) for the different mechanistic steps calculated with: (1) B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I); (2) M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I); (3) M06/6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I); (4) M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine).

Step	**(1) B3LYP / Gas phase**		**(2) M06//B3LYP / Et_3N (PCM)**		**(3) M06//B3LYP / Et_3N (SMD)**		**(4) M06 / Et_3N (PCM)**	
	ΔG	**E_a(G)**	**ΔG**	**E_a(G)**	**ΔG**	**E_a(G)**	**ΔG**	**E_a(G)**
Pd+1b → 1b-Pd	-20.7	--	-25.3	--	-27.2	--	-29.3	--
1b-Pd → I	7.9	16.4	8.0	16.7	2.8	14.5	8.8	--
I → I-Cu	-7.6	--	-7.0	--	-1.3	--	-6.2	--
I-Cu → II	-4.4	3.9	-0.7	2.8	-2.8	3.1	-1.2	--
II → IIIa	-28.4	16.1	-28.8	14.6	-27.8	17.2	-33.5	--
IIIa → IIIb	3.2	--	4.7	--	6.7	--	7.3	--
IIIb → IV	-24.8	2.4	-20.7	3.2	-23.0	3.5	-19.9	4.1
IV → 3ba + V	-11.3	--	-2.4	--	-2.0	--	-2.4	--
V → Pd	-2.9	--	-2.8	--	-0.6	--	0.6	--
II → IIa	1,8	--	2.3	--	2.8	--	1,1	--
II → IIb	-0,4	--	7.9	--	8.7	--	7,6	--
IIa → IIIa	-30.2	14.4	-31.5	12.3	-32.6	12.5	-34.6	--
IIb → VI	-30.6	15.6	-39.1	7.9	-36.6	7.8	-38.9	--
IIIa → III	6.2	--	11.8	--	15.5	--	18.7	--
III → IIIb	-3.0	--	-7.1	--	-8.9	--	-11.4	--
IV → IVa	-5.2	--	-9.9	--	-7.7	--	-8.3	--
IV → IVb	1.9	--	5.4	--	8.5	--	6.6	--
1b-Pd → VII	-3.0	3.4	4.2	4.6	1.7	3.7	3.9	--
VII → VII-Cu	5.9	--	2.7	--	2.0	--	4.1	--
VII-Cu → VIII-Cu	-12.3	15.2	-7.2	13.8	-6.4	14.8	-10.8	--
1b-Pd → IX	1.7	--			3.3	--		
IX → I	6.2	8.3			-0.5	11.0		

CARTESIAN COORDINATES

1b



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.319552	-2.706805	0.144364
2	6	0	0.012704	-1.889606	-0.511875
3	6	0	0.568345	-0.486986	-0.094453
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6	6	0	-1.318735	-1.264966	-0.175686
7	6	0	-1.463150	1.149891	0.801682
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9	6	0	-0.939296	1.710779	1.979429
10	6	0	-2.589137	1.739210	0.203304
11	6	0	-3.181091	2.863259	0.775992
12	6	0	-1.536467	2.834708	2.547385
13	1	0	-0.074130	1.255625	2.449276
14	1	0	-2.976105	1.327309	-0.722195
15	1	0	-4.047815	3.314642	0.301193
16	1	0	-1.126678	3.257539	3.460617
17	1	0	-3.120868	4.290123	2.392661
18	53	0	-3.238363	-2.120155	-0.271473
19	8	0	1.296847	0.111964	-1.166821
20	8	0	1.373481	-0.464790	1.096413
21	16	0	3.061747	-0.564358	1.213223
22	8	0	3.795616	0.343686	0.305915
23	6	0	3.276232	-2.280532	0.423911
24	9	0	2.952201	-2.311098	-0.869027
25	9	0	4.566728	-2.602769	0.560958
26	9	0	2.533820	-3.175374	1.092682
27	16	0	0.914342	1.480287	-2.071321
28	8	0	-0.538062	1.604622	-2.328654
29	6	0	1.284611	2.838964	-0.751624
30	9	0	0.226167	3.635114	-0.638787
31	9	0	2.318391	3.537487	-1.239411
32	9	0	1.615999	2.356725	0.445790

Zero-point correction=	0.184829	(Hartree/Particle)
Thermal correction to Energy=	0.209306	
Thermal correction to Enthalpy=	0.210251	
Thermal correction to Gibbs Free Energy=	0.126318	
Sum of electronic and zero-point Energies=	-2168.781002	
Sum of electronic and thermal Energies=	-2168.756524	
Sum of electronic and thermal Enthalpies=	-2168.755580	
Sum of electronic and thermal Free Energies=	-2168.839513	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.185613	(Hartree/Particle)
Thermal correction to Energy=	0.208475	
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Thermal correction to Gibbs Free Energy=	0.132032	
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Sum of electronic and thermal Energies=	-2168.066187	
Sum of electronic and thermal Enthalpies=	-2168.065243	
Sum of electronic and thermal Free Energies=	-2168.142630	

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.182575	(Hartree/Particle)
Thermal correction to Energy=	0.205668	
Thermal correction to Enthalpy=	0.206612	
Thermal correction to Gibbs Free Energy=	0.127933	
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Sum of electronic and thermal Energies=	-2168.543617	
Sum of electronic and thermal Enthalpies=	-2168.542673	
Sum of electronic and thermal Free Energies=	-2168.621352	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.499554	-2.667181	0.188064
2	6	0	0.158551	-1.870284	-0.481262
3	6	0	0.634357	-0.450042	-0.075686
4	1	0	0.352069	-2.135897	-1.526835
5	6	0	-0.810398	-0.095683	0.238067
6	6	0	-1.198440	-1.318897	-0.158315
7	6	0	-1.464111	1.076187	0.807982
8	6	0	-2.755226	3.285810	1.919396
9	6	0	-0.947821	1.691586	1.954743
10	6	0	-2.640067	1.569638	0.231346
11	6	0	-3.279245	2.670957	0.785079
12	6	0	-1.591720	2.792993	2.504320
13	1	0	-0.040558	1.297485	2.409766
14	1	0	-3.025584	1.105848	-0.674958
15	1	0	-4.186744	3.057074	0.324465
16	1	0	-1.185011	3.267088	3.395853
17	1	0	-3.255780	4.151539	2.349882
18	53	0	-3.068123	-2.250418	-0.237727
19	8	0	1.320717	0.186999	-1.139842
20	8	0	1.435848	-0.374463	1.102726
21	16	0	3.101236	-0.396496	1.213565
22	8	0	3.777922	0.522544	0.286403
23	6	0	3.370116	-2.072207	0.408491
24	9	0	2.962081	-2.106146	-0.848258
25	9	0	4.672996	-2.301711	0.448598
26	9	0	2.741042	-3.007352	1.108178
27	16	0	0.788683	1.448390	-2.071451
28	8	0	-0.660265	1.363696	-2.314354
29	6	0	0.977887	2.859973	-0.785706
30	9	0	-0.171073	3.484859	-0.629292
31	9	0	1.862379	3.693453	-1.320812
32	9	0	1.432223	2.451955	0.384838

Zero-point correction=	0.187740 (Hartree/Particle)
Thermal correction to Energy=	0.211086
Thermal correction to Enthalpy=	0.212031
Thermal correction to Gibbs Free Energy=	0.133486
Sum of electronic and zero-point Energies=	-2168.091261
Sum of electronic and thermal Energies=	-2168.067915
Sum of electronic and thermal Enthalpies=	-2168.066970
Sum of electronic and thermal Free Energies=	-2168.145515

[Pd^0] = Pd^0-PPh_3

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.019179	0.009727	2.580038
2	15	0	-0.001488	0.000871	0.354656
3	6	0	0.552073	-1.585635	-0.424249
4	6	0	1.313047	-4.063617	-1.515358
5	6	0	0.190918	-2.787639	0.206220
6	6	0	1.309475	-1.643392	-1.604313
7	6	0	1.688730	-2.875331	-2.143510
8	6	0	0.560728	-4.016824	-0.338881
9	1	0	-0.372399	-2.748890	1.135530
10	1	0	1.611718	-0.727142	-2.102145
11	1	0	2.280343	-2.903602	-3.055021
12	1	0	0.271432	-4.937612	0.160905
13	1	0	1.611069	-5.020797	-1.935153
14	6	0	1.101381	1.265031	-0.429768
15	6	0	2.875061	3.149733	-1.529358
16	6	0	0.785066	1.929836	-1.624543
17	6	0	2.314827	1.565525	0.210403
18	6	0	3.198677	2.493995	-0.338761
19	6	0	1.666397	2.867987	-2.167906
20	1	0	-0.152730	1.721395	-2.130301
21	1	0	2.552851	1.072747	1.150060
22	1	0	4.134452	2.713841	0.168474
23	1	0	1.405087	3.379517	-3.090786
24	1	0	3.557996	3.881728	-1.952503
25	6	0	-1.642792	0.315667	-0.444295
26	6	0	-4.156071	0.897150	-1.563673
27	6	0	-2.055571	-0.306546	-1.632428
28	6	0	-2.511867	1.225767	0.179444
29	6	0	-3.754793	1.521072	-0.379619
30	6	0	-3.305893	-0.018412	-2.185600
31	1	0	-1.404851	-1.022065	-2.125683
32	1	0	-2.208500	1.689951	1.114788
33	1	0	-4.414589	2.229068	0.115066
34	1	0	-3.614495	-0.512786	-3.103215
35	1	0	-5.129190	1.117943	-1.994434

Zero-point correction=	0.275503 (Hartree/Particle)
Thermal correction to Energy=	0.293428
Thermal correction to Enthalpy=	0.294373
Thermal correction to Gibbs Free Energy=	0.225563
Sum of electronic and zero-point Energies=	-1162.775972
Sum of electronic and thermal Energies=	-1162.758046
Sum of electronic and thermal Enthalpies=	-1162.757102

Sum of electronic and thermal Free Energies= -1162.825912

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction= 0.272967 (Hartree/Particle)
Thermal correction to Energy= 0.291004
Thermal correction to Enthalpy= 0.291948
Thermal correction to Gibbs Free Energy= 0.223857
Sum of electronic and zero-point Energies= -1162.201260
Sum of electronic and thermal Energies= -1162.183222
Sum of electronic and thermal Enthalpies= -1162.182278
Sum of electronic and thermal Free Energies= -1162.250370

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction= 0.270730 (Hartree/Particle)
Thermal correction to Energy= 0.288526
Thermal correction to Enthalpy= 0.289471
Thermal correction to Gibbs Free Energy= 0.223177
Sum of electronic and zero-point Energies= -1163.576017
Sum of electronic and thermal Energies= -1163.558221
Sum of electronic and thermal Enthalpies= -1163.557276
Sum of electronic and thermal Free Energies= -1163.623570

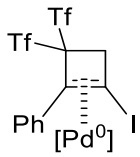
M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.031135	-0.076358	-2.611744
2	15	0	0.003055	-0.010074	-0.383990
3	6	0	-1.180860	-1.133662	0.461212
4	6	0	-2.907362	-2.970792	1.675384
5	6	0	-1.344492	-2.416524	-0.072292
6	6	0	-1.896056	-0.780115	1.608710
7	6	0	-2.758565	-1.694312	2.208809
8	6	0	-2.194851	-3.333085	0.534283
9	1	0	-0.800591	-2.684824	-0.980326
10	1	0	-1.781997	0.216792	2.035759
11	1	0	-3.315200	-1.406142	3.099385
12	1	0	-2.312149	-4.328832	0.109420
13	1	0	-3.583799	-3.682474	2.146006
14	6	0	-0.388702	1.613879	0.381983
15	6	0	-1.150894	4.068937	1.485471
16	6	0	0.250012	2.103179	1.524457
17	6	0	-1.408953	2.370692	-0.203439
18	6	0	-1.794714	3.586523	0.348068
19	6	0	-0.127846	3.327985	2.069351
20	1	0	1.047076	1.524296	1.992390
21	1	0	-1.893160	1.996221	-1.107752
22	1	0	-2.592338	4.164591	-0.115966
23	1	0	0.380021	3.702267	2.957034
24	1	0	-1.443502	5.026305	1.914000
25	6	0	1.600594	-0.443852	0.413868
26	6	0	4.094443	-0.958404	1.570933
27	6	0	1.690950	-1.167930	1.605706
28	6	0	2.773586	0.012261	-0.195586
29	6	0	4.013196	-0.235697	0.382895
30	6	0	2.933493	-1.426381	2.178669

31	1	0	0.784369	-1.531263	2.090614
32	1	0	2.701078	0.559112	-1.138172
33	1	0	4.919814	0.125883	-0.100028
34	1	0	2.993664	-1.994630	3.105799
35	1	0	5.065256	-1.159928	2.020997

Zero-point correction=	0.273948	(Hartree/Particle)
Thermal correction to Energy=	0.291047	
Thermal correction to Enthalpy=	0.291991	
Thermal correction to Gibbs Free Energy=	0.226118	
Sum of electronic and zero-point Energies=	-1162.201443	
Sum of electronic and thermal Energies=	-1162.184343	
Sum of electronic and thermal Enthalpies=	-1162.183399	
Sum of electronic and thermal Free Energies=	-1162.249273	

1b-Pd



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.289248	1.202191	-2.311050
2	6	0	-1.590478	0.591995	-1.731960
3	6	0	-2.299876	-0.104685	-0.535975
4	1	0	-1.012129	-0.056285	-2.392834
5	6	0	-1.506104	0.785535	0.437085
6	6	0	-0.825006	1.370374	-0.661024
7	6	0	-1.823209	1.183005	1.817607
8	6	0	-2.400726	1.929409	4.478954
9	6	0	-2.925583	0.632231	2.500647
10	6	0	-1.018093	2.118582	2.500347
11	6	0	-1.307445	2.487716	3.810935
12	6	0	-3.204982	1.002071	3.816217
13	1	0	-3.586264	-0.065672	1.999895
14	1	0	-0.158019	2.548484	1.999035
15	1	0	-0.672602	3.212201	4.314254
16	1	0	-4.061785	0.563180	4.320124
17	1	0	-2.622024	2.215404	5.503503
18	53	0	-0.143382	3.380180	-1.000188
19	8	0	-2.083702	-1.518717	-0.565747
20	8	0	-3.692325	0.161474	-0.420372
21	16	0	-4.721084	-0.712307	-1.472664
22	8	0	-4.714280	-0.101085	-2.823570
23	6	0	-6.181209	0.070989	-0.561435
24	9	0	-6.182441	1.395404	-0.663796
25	9	0	-7.287522	-0.419453	-1.137461
26	9	0	-6.164679	-0.290618	0.724556
27	16	0	-1.939988	-2.317745	0.925163
28	8	0	-3.249488	-2.872607	1.341543
29	6	0	-1.078323	-3.735710	0.017724
30	9	0	-1.878600	-4.308987	-0.872893
31	9	0	-0.730955	-4.634062	0.950383
32	9	0	0.033316	-3.296824	-0.588114

33	46	0	0.628346	0.134370	0.272455
34	15	0	2.945300	-0.238495	-0.041285
35	6	0	3.994347	1.249190	0.258325
36	6	0	5.523046	3.534168	0.831969
37	6	0	5.152212	1.533712	-0.481267
38	6	0	3.607166	2.129150	1.281595
39	6	0	4.370743	3.259366	1.572157
40	6	0	5.909653	2.671924	-0.195516
41	1	0	5.461583	0.871639	-1.284231
42	1	0	2.699331	1.927266	1.844443
43	1	0	4.059170	3.931176	2.367380
44	1	0	6.801451	2.884361	-0.779203
45	1	0	6.112767	4.420431	1.050255
46	6	0	3.677030	-1.524749	1.067539
47	6	0	4.676475	-3.542837	2.749628
48	6	0	4.915138	-1.369183	1.708523
49	6	0	2.943550	-2.703593	1.285277
50	6	0	3.442983	-3.707321	2.114467
51	6	0	5.409063	-2.372908	2.545576
52	1	0	5.494387	-0.463570	1.559112
53	1	0	1.982216	-2.839160	0.798657
54	1	0	2.864174	-4.613741	2.270301
55	1	0	6.367902	-2.236769	3.038783
56	1	0	5.061468	-4.320916	3.403180
57	6	0	3.413322	-0.793220	-1.737147
58	6	0	4.055334	-1.546213	-4.365070
59	6	0	4.458150	-1.697066	-1.982462
60	6	0	2.689442	-0.276930	-2.824196
61	6	0	3.013337	-0.645912	-4.129754
62	6	0	4.774553	-2.071725	-3.290300
63	1	0	5.021442	-2.114222	-1.153218
64	1	0	1.868533	0.411545	-2.641212
65	1	0	2.446056	-0.237653	-4.961781
66	1	0	5.582483	-2.776777	-3.467207
67	1	0	4.301357	-1.841261	-5.381566

Zero-point correction=	0.461030	(Hartree/Particle)
Thermal correction to Energy=	0.505680	
Thermal correction to Enthalpy=	0.506624	
Thermal correction to Gibbs Free Energy=	0.370123	
Sum of electronic and zero-point Energies=	-3331.607553	
Sum of electronic and thermal Energies=	-3331.562903	
Sum of electronic and thermal Enthalpies=	-3331.561959	
Sum of electronic and thermal Free Energies=	-3331.698460	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.458599	(Hartree/Particle)
Thermal correction to Energy=	0.501540	
Thermal correction to Enthalpy=	0.502484	
Thermal correction to Gibbs Free Energy=	0.378161	
Sum of electronic and zero-point Energies=	-3330.355691	
Sum of electronic and thermal Energies=	-3330.312750	
Sum of electronic and thermal Enthalpies=	-3330.311806	
Sum of electronic and thermal Free Energies=	-3330.436130	

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.453866	(Hartree/Particle)
Thermal correction to Energy=	0.496506	

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Thermal correction to Enthalpy=                 0.497450
Thermal correction to Gibbs Free Energy=        0.375236
Sum of electronic and zero-point Energies=          -3332.209552
Sum of electronic and thermal Energies=             -3332.166913
Sum of electronic and thermal Enthalpies=           -3332.165968
Sum of electronic and thermal Free Energies=        -3332.288183
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M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.291270	-1.390436	-2.356015
2	6	0	1.594977	-0.759353	-1.787186
3	6	0	2.293560	-0.056539	-0.605025
4	1	0	1.019647	-0.114035	-2.460541
5	6	0	1.526535	-0.946368	0.367967
6	6	0	0.827513	-1.515134	-0.716401
7	6	0	1.832082	-1.311397	1.749490
8	6	0	2.374867	-1.972264	4.425158
9	6	0	2.883911	-0.692128	2.442138
10	6	0	1.058389	-2.270806	2.425069
11	6	0	1.331941	-2.598085	3.745231
12	6	0	3.146472	-1.020242	3.767309
13	1	0	3.520455	0.033886	1.938864
14	1	0	0.229914	-2.755034	1.909225
15	1	0	0.721739	-3.345526	4.249427
16	1	0	3.966814	-0.526940	4.285630
17	1	0	2.584348	-2.226686	5.462526
18	53	0	-0.017910	-3.430963	-1.050670
19	8	0	2.039270	1.338171	-0.635103
20	8	0	3.684264	-0.271744	-0.481059
21	16	0	4.647402	0.586371	-1.561356
22	8	0	4.962131	-0.268757	-2.719914
23	6	0	6.076301	0.323963	-0.386167
24	9	0	6.320737	-0.958195	-0.211745
25	9	0	7.131159	0.902556	-0.943727
26	9	0	5.821082	0.905017	0.774194
27	16	0	1.747400	2.086469	0.831114
28	8	0	3.004139	2.679429	1.324343
29	6	0	0.938992	3.488678	-0.114481
30	9	0	1.821914	4.098305	-0.877059
31	9	0	0.477005	4.338405	0.797425
32	9	0	-0.074007	3.056314	-0.848102
33	46	0	-0.555607	-0.211333	0.296536
34	15	0	-2.832687	0.296512	0.025644
35	6	0	-3.964452	-1.121304	0.259480
36	6	0	-5.644653	-3.296361	0.754430
37	6	0	-5.181471	-1.240104	-0.418401
38	6	0	-3.593630	-2.106379	1.179879
39	6	0	-4.432773	-3.186210	1.431011
40	6	0	-6.016934	-2.324596	-0.170848
41	1	0	-5.476179	-0.481066	-1.144168
42	1	0	-2.635286	-2.019617	1.697278
43	1	0	-4.136160	-3.947945	2.149937
44	1	0	-6.962434	-2.411936	-0.703554
45	1	0	-6.299135	-4.145205	0.944994
46	6	0	-3.494249	1.585414	1.147767
47	6	0	-4.370477	3.660959	2.802973
48	6	0	-4.764906	1.535403	1.726059
49	6	0	-2.666885	2.681046	1.414682

50	6	0	-3.102293	3.718067	2.229679
51	6	0	-5.197189	2.569891	2.552415
52	1	0	-5.418952	0.685057	1.533035
53	1	0	-1.673302	2.719306	0.968340
54	1	0	-2.445943	4.565115	2.422891
55	1	0	-6.187064	2.521063	3.003152
56	1	0	-4.712923	4.466726	3.449923
57	6	0	-3.248837	0.918412	-1.645581
58	6	0	-3.823030	1.723078	-4.258035
59	6	0	-4.166279	1.945269	-1.879519
60	6	0	-2.616525	0.303078	-2.731425
61	6	0	-2.908107	0.697239	-4.031656
62	6	0	-4.448360	2.346843	-3.183015
63	1	0	-4.662524	2.434710	-1.041017
64	1	0	-1.888563	-0.489675	-2.545511
65	1	0	-2.413940	0.209116	-4.869949
66	1	0	-5.162073	3.150315	-3.357570
67	1	0	-4.045472	2.039212	-5.275796

Zero-point correction=	0.462781	(Hartree/Particle)
Thermal correction to Energy=	0.506063	
Thermal correction to Enthalpy=	0.507007	
Thermal correction to Gibbs Free Energy=	0.379256	
Sum of electronic and zero-point Energies=	-3330.358024	
Sum of electronic and thermal Energies=	-3330.314742	
Sum of electronic and thermal Enthalpies=	-3330.313798	
Sum of electronic and thermal Free Energies=	-3330.441549	

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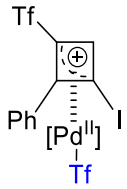


B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.279001	3.097596	-2.054852
2	6	0	-0.956817	2.131512	-1.641952
3	6	0	-1.820117	1.702774	-0.446200
4	1	0	-0.772076	1.423057	-2.449179
5	6	0	-0.929565	2.223794	0.520660
6	6	0	0.110932	2.263890	-0.517654
7	6	0	-1.048874	2.572589	1.933734
8	6	0	-1.319317	3.251960	4.643239
9	6	0	-2.319439	2.601037	2.539018
10	6	0	0.083863	2.888181	2.706031
11	6	0	-0.054491	3.224865	4.050313
12	6	0	-2.449229	2.938799	3.883755
13	1	0	-3.197758	2.354548	1.951858
14	1	0	1.069234	2.860569	2.253663
15	1	0	0.827978	3.464503	4.636999
16	1	0	-3.435028	2.955920	4.339869
17	1	0	-1.423563	3.514248	5.692473
18	53	0	1.754936	3.610938	-0.691449

19	8	0	-3.078923	1.285154	-0.318068
20	16	0	-3.546344	-0.190055	-1.261447
21	8	0	-2.608293	-0.358971	-2.389132
22	6	0	-4.942023	0.841335	-2.030115
23	9	0	-4.464487	1.866672	-2.734464
24	9	0	-5.631128	0.030327	-2.841368
25	9	0	-5.751534	1.290532	-1.067117
26	46	0	-0.019127	0.228498	-0.004875
27	15	0	2.003214	-0.981203	-0.230485
28	6	0	2.469799	-1.848463	1.327991
29	6	0	3.058576	-3.270686	3.676234
30	6	0	3.781299	-2.281455	1.588436
31	6	0	1.461465	-2.125382	2.264640
32	6	0	1.755012	-2.839551	3.427638
33	6	0	4.071487	-2.986564	2.756782
34	1	0	4.580713	-2.056233	0.889119
35	1	0	0.445637	-1.790779	2.085091
36	1	0	0.957273	-3.055681	4.132359
37	1	0	5.090049	-3.313785	2.948083
38	1	0	3.287354	-3.823100	4.583694
39	6	0	1.828425	-2.305752	-1.500168
40	6	0	1.488755	-4.309760	-3.433673
41	6	0	2.796771	-3.311502	-1.659164
42	6	0	0.689657	-2.318177	-2.319279
43	6	0	0.520707	-3.318259	-3.280358
44	6	0	2.627503	-4.304618	-2.621976
45	1	0	3.679067	-3.325875	-1.026650
46	1	0	-0.081551	-1.562498	-2.198297
47	1	0	-0.376740	-3.323351	-3.891410
48	1	0	3.381114	-5.079473	-2.734478
49	1	0	1.355299	-5.091528	-4.176544
50	6	0	3.521265	-0.065434	-0.719233
51	6	0	5.768135	1.450714	-1.460128
52	6	0	3.961227	-0.047987	-2.051545
53	6	0	4.211656	0.701702	0.234009
54	6	0	5.332095	1.445984	-0.133370
55	6	0	5.076901	0.706841	-2.417573
56	1	0	3.438906	-0.630333	-2.804016
57	1	0	3.880803	0.710034	1.268799
58	1	0	5.861612	2.025894	0.617761
59	1	0	5.407667	0.707147	-3.452645
60	1	0	6.640107	2.032699	-1.745926
61	8	0	-1.465642	-1.266801	0.569272
62	16	0	-1.610017	-2.817773	0.304203
63	8	0	-2.633709	-3.079624	-0.761323
64	6	0	-2.567180	-3.141185	1.904146
65	9	0	-3.669618	-2.387387	1.997662
66	9	0	-2.925239	-4.434571	1.968009
67	9	0	-1.777286	-2.877373	2.969173

Zero-point correction=	0.460086	(Hartree/Particle)
Thermal correction to Energy=	0.505088	
Thermal correction to Enthalpy=	0.506032	
Thermal correction to Gibbs Free Energy=	0.371835	
Sum of electronic and zero-point Energies=	-3331.597614	
Sum of electronic and thermal Energies=	-3331.552612	
Sum of electronic and thermal Enthalpies=	-3331.551668	
Sum of electronic and thermal Free Energies=	-3331.685865	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.456926 (Hartree/Particle)
Thermal correction to Energy=	0.499687
Thermal correction to Enthalpy=	0.500631
Thermal correction to Gibbs Free Energy=	0.377743
Sum of electronic and zero-point Energies=	-3330.344253
Sum of electronic and thermal Energies=	-3330.301492
Sum of electronic and thermal Enthalpies=	-3330.300547
Sum of electronic and thermal Free Energies=	-3330.423436

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.452342 (Hartree/Particle)
Thermal correction to Energy=	0.494690
Thermal correction to Enthalpy=	0.495634
Thermal correction to Gibbs Free Energy=	0.375693
Sum of electronic and zero-point Energies=	-3332.207031
Sum of electronic and thermal Energies=	-3332.164683
Sum of electronic and thermal Enthalpies=	-3332.163739
Sum of electronic and thermal Free Energies=	-3332.283680

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.241270	-3.206127	-1.900807
2	6	0	0.928970	-2.216494	-1.531986
3	6	0	1.715978	-1.772153	-0.298179
4	1	0	0.811464	-1.522194	-2.369228
5	6	0	0.748960	-2.244837	0.616994
6	6	0	-0.202122	-2.277401	-0.481975
7	6	0	0.731053	-2.489274	2.048611
8	6	0	0.730662	-2.926515	4.804072
9	6	0	1.940469	-2.565795	2.751014
10	6	0	-0.479635	-2.630681	2.740114
11	6	0	-0.475428	-2.848784	4.110726
12	6	0	1.936372	-2.783966	4.122164
13	1	0	2.880691	-2.450133	2.214253
14	1	0	-1.423754	-2.551907	2.200940
15	1	0	-1.419310	-2.954396	4.642121
16	1	0	2.879734	-2.840813	4.661708
17	1	0	0.730035	-3.095871	5.879240
18	53	0	-1.950611	-3.421278	-0.731102
19	8	0	2.971089	-1.382951	-0.077852
20	16	0	3.596080	-0.100340	-1.105218
21	8	0	2.697223	0.094188	-2.250450
22	6	0	4.791314	-1.357234	-1.825808
23	9	0	4.126834	-2.347276	-2.397678
24	9	0	5.511014	-0.727248	-2.742243
25	9	0	5.590214	-1.836279	-0.887556
26	46	0	0.061921	-0.227903	-0.019334
27	15	0	-1.878496	1.076403	-0.285298
28	6	0	-2.276847	2.031434	1.223454
29	6	0	-2.773543	3.534410	3.524101
30	6	0	-3.536180	2.605767	1.434249
31	6	0	-1.275352	2.204194	2.183740
32	6	0	-1.523289	2.957854	3.327354
33	6	0	-3.781248	3.354549	2.578977
34	1	0	-4.336924	2.447797	0.711405
35	1	0	-0.295140	1.748858	2.033866

36	1	0	-0.734665	3.090294	4.065473
37	1	0	-4.763700	3.796779	2.735703
38	1	0	-2.968839	4.120952	4.420237
39	6	0	-1.651064	2.304262	-1.620861
40	6	0	-1.179879	4.193739	-3.621754
41	6	0	-2.602128	3.294366	-1.894522
42	6	0	-0.467666	2.267190	-2.364289
43	6	0	-0.230716	3.213338	-3.358106
44	6	0	-2.367728	4.231370	-2.892499
45	1	0	-3.530555	3.335505	-1.324791
46	1	0	0.286284	1.501749	-2.165027
47	1	0	0.703499	3.183362	-3.914814
48	1	0	-3.111580	4.999165	-3.098148
49	1	0	-0.995537	4.937173	-4.395380
50	6	0	-3.426430	0.196522	-0.674922
51	6	0	-5.675564	-1.363480	-1.235307
52	6	0	-3.888907	0.073809	-1.987580
53	6	0	-4.091711	-0.482286	0.352456
54	6	0	-5.215513	-1.250165	0.074371
55	6	0	-5.008959	-0.704724	-2.263983
56	1	0	-3.374614	0.590275	-2.798088
57	1	0	-3.726423	-0.405864	1.378075
58	1	0	-5.731318	-1.766123	0.882580
59	1	0	-5.364823	-0.791755	-3.289107
60	1	0	-6.554530	-1.967086	-1.454981
61	8	0	1.636309	1.197654	0.479700
62	16	0	1.707009	2.733261	0.196240
63	8	0	2.673546	3.029104	-0.901367
64	6	0	2.745797	3.093867	1.706355
65	9	0	3.866184	2.380993	1.702470
66	9	0	3.066601	4.385789	1.737588
67	9	0	2.061090	2.808203	2.816698

Zero-point correction=	0.461931	(Hartree/Particle)
Thermal correction to Energy=	0.505352	
Thermal correction to Enthalpy=	0.506297	
Thermal correction to Gibbs Free Energy=	0.380835	
Sum of electronic and zero-point Energies=	-3330.346454	
Sum of electronic and thermal Energies=	-3330.303033	
Sum of electronic and thermal Enthalpies=	-3330.302089	
Sum of electronic and thermal Free Energies=	-3330.427551	

$TS_{1Pd\text{-}I}$

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Imaginary frequency: -176.2407 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.893561	-1.350456	-2.184912
2	6	0	1.351495	-0.669630	-1.521382
3	6	0	2.157083	-0.308521	-0.269981
4	1	0	0.935244	0.160126	-2.090370
5	6	0	1.267774	-1.008249	0.636022
6	6	0	0.432950	-1.363126	-0.488261

7	6	0	1.462397	-1.392602	2.034818
8	6	0	1.877287	-2.070786	4.734066
9	6	0	2.378486	-0.668507	2.824342
10	6	0	0.753567	-2.456779	2.623612
11	6	0	0.963731	-2.790249	3.960020
12	6	0	2.580582	-1.009229	4.159559
13	1	0	2.920204	0.164980	2.390060
14	1	0	0.043654	-3.024935	2.032353
15	1	0	0.412151	-3.618432	4.397148
16	1	0	3.289873	-0.439995	4.754250
17	1	0	2.038693	-2.334276	5.775747
18	53	0	-0.482325	-3.255146	-0.973630
19	8	0	3.450196	-0.223114	-0.107983
20	16	0	4.549068	0.360977	-1.446618
21	8	0	4.088996	-0.150710	-2.750505
22	6	0	5.718632	-1.018982	-0.860935
23	9	0	5.194087	-2.231900	-1.018327
24	9	0	6.817799	-0.911624	-1.623008
25	9	0	6.056704	-0.828169	0.416391
26	46	0	-0.724527	0.102902	0.416120
27	15	0	-2.974889	0.506008	-0.073465
28	6	0	-3.573918	1.954453	0.901580
29	6	0	-4.348674	4.207133	2.388193
30	6	0	-4.859617	2.030205	1.458396
31	6	0	-2.677989	3.018270	1.106130
32	6	0	-3.065690	4.139343	1.839843
33	6	0	-5.242447	3.151649	2.197584
34	1	0	-5.560203	1.212446	1.319858
35	1	0	-1.673161	2.965783	0.691852
36	1	0	-2.362477	4.953710	1.990548
37	1	0	-6.239892	3.197675	2.626632
38	1	0	-4.648201	5.076493	2.967205
39	6	0	-3.357902	0.939482	-1.823764
40	6	0	-3.875673	1.517040	-4.522751
41	6	0	-4.275994	1.941516	-2.172959
42	6	0	-2.697709	0.234758	-2.843634
43	6	0	-2.960053	0.517897	-4.183769
44	6	0	-4.530797	2.227957	-3.516081
45	1	0	-4.787104	2.504756	-1.398251
46	1	0	-1.975479	-0.534731	-2.585983
47	1	0	-2.441913	-0.035228	-4.962330
48	1	0	-5.239507	3.010605	-3.773396
49	1	0	-4.072309	1.744394	-5.566948
50	6	0	-4.156423	-0.845535	0.339877
51	6	0	-5.901005	-2.911353	1.094670
52	6	0	-5.325945	-1.091577	-0.395404
53	6	0	-3.865898	-1.654430	1.450019
54	6	0	-4.736902	-2.675084	1.829854
55	6	0	-6.191484	-2.121063	-0.018841
56	1	0	-5.559642	-0.485646	-1.265618
57	1	0	-2.947654	-1.486497	2.007370
58	1	0	-4.500372	-3.293117	2.691741
59	1	0	-7.091831	-2.305539	-0.598835
60	1	0	-6.574923	-3.713214	1.384068
61	8	0	1.465542	1.656123	0.081089
62	16	0	2.135453	2.887386	-0.601085
63	8	0	3.023903	2.430294	-1.740464
64	6	0	3.388317	3.323417	0.754383
65	9	0	4.178443	2.283354	1.095374
66	9	0	4.174511	4.328393	0.340454
67	9	0	2.727966	3.723408	1.853068

Zero-point correction=	0.459204 (Hartree/Particle)
Thermal correction to Energy=	0.503788
Thermal correction to Enthalpy=	0.504732
Thermal correction to Gibbs Free Energy=	0.370096
Sum of electronic and zero-point Energies=	-3331.583179
Sum of electronic and thermal Energies=	-3331.538596
Sum of electronic and thermal Enthalpies=	-3331.537651
Sum of electronic and thermal Free Energies=	-3331.672288

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Imaginary frequency: -141.8222 cm^{-1}

Zero-point correction=	0.456409 (Hartree/Particle)
Thermal correction to Energy=	0.500382
Thermal correction to Enthalpy=	0.501327
Thermal correction to Gibbs Free Energy=	0.373990
Sum of electronic and zero-point Energies=	-3330.327133
Sum of electronic and thermal Energies=	-3330.283160
Sum of electronic and thermal Enthalpies=	-3330.282216
Sum of electronic and thermal Free Energies=	-3330.409552

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Imaginary frequency: -105.2490 cm^{-1}

Zero-point correction=	0.452006 (Hartree/Particle)
Thermal correction to Energy=	0.495553
Thermal correction to Enthalpy=	0.496497
Thermal correction to Gibbs Free Energy=	0.372274
Sum of electronic and zero-point Energies=	-3332.185376
Sum of electronic and thermal Energies=	-3332.141829
Sum of electronic and thermal Enthalpies=	-3332.140885
Sum of electronic and thermal Free Energies=	-3332.265107

CuI

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.000000	0.000000	-1.575947
2	53	0	0.000000	0.000000	0.862311

Zero-point correction=	0.000550 (Hartree/Particle)
Thermal correction to Energy=	0.003409
Thermal correction to Enthalpy=	0.004353
Thermal correction to Gibbs Free Energy=	-0.024805
Sum of electronic and zero-point Energies=	-207.579255
Sum of electronic and thermal Energies=	-207.576396
Sum of electronic and thermal Enthalpies=	-207.575452

Sum of electronic and thermal Free Energies= -207.604610

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction= 0.000766 (Hartree/Particle)
Thermal correction to Energy= 0.003503
Thermal correction to Enthalpy= 0.004448
Thermal correction to Gibbs Free Energy= -0.024308
Sum of electronic and zero-point Energies= -207.585531
Sum of electronic and thermal Energies= -207.582794
Sum of electronic and thermal Enthalpies= -207.581850
Sum of electronic and thermal Free Energies= -207.610605

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction= 0.000537 (Hartree/Particle)
Thermal correction to Energy= 0.003404
Thermal correction to Enthalpy= 0.004348
Thermal correction to Gibbs Free Energy= -0.024830
Sum of electronic and zero-point Energies= -208.830622
Sum of electronic and thermal Energies= -208.827755
Sum of electronic and thermal Enthalpies= -208.826811
Sum of electronic and thermal Free Energies= -208.855989

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.000000	0.000000	-1.568497
2	53	0	0.000000	0.000000	0.858234

Zero-point correction= 0.000556 (Hartree/Particle)
Thermal correction to Energy= 0.003411
Thermal correction to Enthalpy= 0.004356
Thermal correction to Gibbs Free Energy= -0.024783
Sum of electronic and zero-point Energies= -207.590968
Sum of electronic and thermal Energies= -207.588113
Sum of electronic and thermal Enthalpies= -207.587169
Sum of electronic and thermal Free Energies= -207.616308

Et_3N

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	-0.021598
2	6	0	-0.331142	1.365602	-0.446808
3	1	0	-1.418738	1.479971	-0.395979
4	1	0	-0.054918	1.534891	-1.506808
5	6	0	1.348217	-0.396023	-0.446808
6	1	0	1.991062	0.488678	-0.395979
7	1	0	1.356714	-0.719885	-1.506808
8	6	0	0.304254	2.439615	0.439338
9	1	0	1.398992	2.404028	0.413345

10	1	0	-0.010878	2.307491	1.479600
11	1	0	0.000000	3.438605	0.105058
12	6	0	1.960642	-1.483299	0.439338
13	1	0	2.977919	-1.719302	0.105058
14	1	0	1.382454	-2.413577	0.413345
15	1	0	2.003785	-1.144325	1.479600
16	6	0	-1.017075	-0.969579	-0.446808
17	1	0	-0.572323	-1.968649	-0.395979
18	1	0	-1.301795	-0.815006	-1.506808
19	6	0	-2.264896	-0.956316	0.439338
20	1	0	-1.992907	-1.163166	1.479600
21	1	0	-2.977919	-1.719302	0.105058
22	1	0	-2.781446	0.009548	0.413345

Zero-point correction=	0.207002 (Hartree/Particle)
Thermal correction to Energy=	0.216434
Thermal correction to Enthalpy=	0.217378
Thermal correction to Gibbs Free Energy=	0.174056
Sum of electronic and zero-point Energies=	-292.203882
Sum of electronic and thermal Energies=	-292.194450
Sum of electronic and thermal Enthalpies=	-292.193506
Sum of electronic and thermal Free Energies=	-292.236828

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.203614 (Hartree/Particle)
Thermal correction to Energy=	0.212978
Thermal correction to Enthalpy=	0.213922
Thermal correction to Gibbs Free Energy=	0.171186
Sum of electronic and zero-point Energies=	-291.959290
Sum of electronic and thermal Energies=	-291.949927
Sum of electronic and thermal Enthalpies=	-291.948983
Sum of electronic and thermal Free Energies=	-291.991719

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.202725 (Hartree/Particle)
Thermal correction to Energy=	0.212179
Thermal correction to Enthalpy=	0.213124
Thermal correction to Gibbs Free Energy=	0.170120
Sum of electronic and zero-point Energies=	-292.058027
Sum of electronic and thermal Energies=	-292.048573
Sum of electronic and thermal Enthalpies=	-292.047629
Sum of electronic and thermal Free Energies=	-292.090632

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.037325
2	6	0	-0.341191	1.345059	-0.418575
3	1	0	-1.430391	1.464884	-0.343301
4	1	0	-0.096003	1.465131	-1.497195
5	6	0	1.335451	-0.377049	-0.418575
6	1	0	1.983822	0.506313	-0.343301
7	1	0	1.316842	-0.649424	-1.497195

8	6	0	0.317751	2.437487	0.402338
9	1	0	1.413068	2.405345	0.339480
10	1	0	0.040393	2.336468	1.458734
11	1	0	0.000000	3.427822	0.052612
12	6	0	1.952051	-1.493924	0.402338
13	1	0	2.968581	-1.713911	0.052612
14	1	0	1.376556	-2.426425	0.339480
15	1	0	2.003244	-1.203216	1.458734
16	6	0	-0.994260	-0.968010	-0.418575
17	1	0	-0.553431	-1.971196	-0.343301
18	1	0	-1.220839	-0.815707	-1.497195
19	6	0	-2.269801	-0.943564	0.402338
20	1	0	-2.043637	-1.133252	1.458734
21	1	0	-2.968581	-1.713911	0.052612
22	1	0	-2.789624	0.021080	0.339480

Zero-point correction= 0.205993 (Hartree/Particle)
Thermal correction to Energy= 0.215204
Thermal correction to Enthalpy= 0.216148
Thermal correction to Gibbs Free Energy= 0.173623
Sum of electronic and zero-point Energies= -291.962306
Sum of electronic and thermal Energies= -291.953095
Sum of electronic and thermal Enthalpies= -291.952151
Sum of electronic and thermal Free Energies= -291.994676

Phenylacetilene

Ph—≡—H

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	2.150485	0.428530
2	6	0	0.000000	1.213515	-0.119767
3	6	0	-0.000000	-1.208987	-1.512740
4	6	0	0.000000	0.000000	0.594243
5	6	0	0.000000	1.208987	-1.512740
6	6	0	0.000000	-0.000000	-2.213215
7	6	0	-0.000000	-1.213515	-0.119767
8	1	0	0.000000	2.151524	-2.053473
9	1	0	0.000000	-0.000000	-3.299822
10	1	0	-0.000000	-2.150485	0.428530
11	1	0	-0.000000	-2.151524	-2.053473
12	6	0	0.000000	0.000000	2.024330
13	1	0	0.000000	0.000000	4.300660
14	6	0	0.000000	0.000000	3.234497

Zero-point correction= 0.109557 (Hartree/Particle)

```
Thermal correction to Energy=                  0.116033
Thermal correction to Enthalpy=                0.116977
Thermal correction to Gibbs Free Energy=       0.079780
Sum of electronic and zero-point Energies=          -308.277380
Sum of electronic and thermal Energies=             -308.270904
Sum of electronic and thermal Enthalpies=           -308.269960
Sum of electronic and thermal Free Energies=        -308.307157
```

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

```
Zero-point correction=                         0.108883 (Hartree/Particle)
Thermal correction to Energy=                  0.115377
Thermal correction to Enthalpy=                0.116321
Thermal correction to Gibbs Free Energy=       0.079131
Sum of electronic and zero-point Energies=          -308.028056
Sum of electronic and thermal Energies=             -308.021561
Sum of electronic and thermal Enthalpies=           -308.020617
Sum of electronic and thermal Free Energies=        -308.057808
```

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

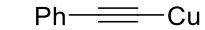
```
Zero-point correction=                         0.108311 (Hartree/Particle)
Thermal correction to Energy=                  0.114629
Thermal correction to Enthalpy=                0.115573
Thermal correction to Gibbs Free Energy=       0.078775
Sum of electronic and zero-point Energies=          -308.118986
Sum of electronic and thermal Energies=             -308.112669
Sum of electronic and thermal Enthalpies=           -308.111724
Sum of electronic and thermal Free Energies=        -308.148523
```

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.000000	2.147566	0.432846
2	6	0	-0.000000	1.209624	-0.119765
3	6	0	0.000000	-1.205605	-1.508130
4	6	0	0.000000	0.000000	0.589191
5	6	0	0.000000	1.205605	-1.508130
6	6	0	-0.000000	-0.000000	-2.205631
7	6	0	-0.000000	-1.209624	-0.119765
8	1	0	-0.000000	2.149677	-2.050151
9	1	0	-0.000000	-0.000000	-3.294097
10	1	0	-0.000000	-2.147566	0.432846
11	1	0	-0.000000	-2.149677	-2.050151
12	6	0	0.000000	0.000000	2.017200
13	1	0	0.000000	0.000000	4.296477
14	6	0	0.000000	0.000000	3.227069

```
Zero-point correction=                         0.109149 (Hartree/Particle)
Thermal correction to Energy=                  0.115609
Thermal correction to Enthalpy=                0.116553
Thermal correction to Gibbs Free Energy=       0.079399
Sum of electronic and zero-point Energies=          -308.027962
Sum of electronic and thermal Energies=             -308.021502
Sum of electronic and thermal Enthalpies=           -308.020558
Sum of electronic and thermal Free Energies=        -308.057712
```

(Phenylethynyl)copper



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.000239	1.320504	2.149188
2	6	0	-0.000158	1.868716	1.211971
3	6	0	-0.000158	3.261518	-1.207919
4	6	0	-0.000089	1.148413	0.000000
5	6	0	-0.000158	3.261518	1.207919
6	6	0	-0.000127	3.964118	0.000000
7	6	0	-0.000158	1.868716	-1.211971
8	1	0	-0.000196	3.801342	2.151390
9	1	0	-0.000128	5.050833	0.000000
10	1	0	-0.000239	1.320504	-2.149188
11	1	0	-0.000196	3.801342	-2.151390
12	6	0	-0.000242	-0.279522	-0.000000
13	29	0	0.000257	-3.338771	-0.000000
14	6	0	0.000011	-1.505171	-0.000000

Zero-point correction=	0.100295 (Hartree/Particle)
Thermal correction to Energy=	0.108237
Thermal correction to Enthalpy=	0.109182
Thermal correction to Gibbs Free Energy=	0.065787
Sum of electronic and zero-point Energies=	-503.834184
Sum of electronic and thermal Energies=	-503.826241
Sum of electronic and thermal Enthalpies=	-503.825297
Sum of electronic and thermal Free Energies=	-503.868692

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.099731 (Hartree/Particle)
Thermal correction to Energy=	0.107626
Thermal correction to Enthalpy=	0.108570
Thermal correction to Gibbs Free Energy=	0.065574
Sum of electronic and zero-point Energies=	-503.630959
Sum of electronic and thermal Energies=	-503.623064
Sum of electronic and thermal Enthalpies=	-503.622120
Sum of electronic and thermal Free Energies=	-503.665116

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.098851 (Hartree/Particle)
Thermal correction to Energy=	0.106667
Thermal correction to Enthalpy=	0.107612
Thermal correction to Gibbs Free Energy=	0.064912
Sum of electronic and zero-point Energies=	-504.922053
Sum of electronic and thermal Energies=	-504.914236
Sum of electronic and thermal Enthalpies=	-504.913292
Sum of electronic and thermal Free Energies=	-504.955992

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000053	-1.315605	2.146124
2	6	0	0.000043	-1.867654	1.207512
3	6	0	0.000043	-3.256051	-1.204310
4	6	0	0.000030	-1.151546	-0.000000
5	6	0	0.000043	-3.256051	1.204310
6	6	0	0.000034	-3.956086	-0.000000
7	6	0	0.000043	-1.867654	-1.207512
8	1	0	0.000048	-3.797095	2.149450
9	1	0	0.000031	-5.044724	-0.000000
10	1	0	0.000053	-1.315605	-2.146124
11	1	0	0.000048	-3.797095	-2.149450
12	6	0	0.000067	0.275474	0.000000
13	29	0	-0.000067	3.335770	0.000000
14	6	0	-0.000019	1.501702	0.000000

Zero-point correction= 0.099907 (Hartree/Particle)
Thermal correction to Energy= 0.107812
Thermal correction to Enthalpy= 0.108756
Thermal correction to Gibbs Free Energy= 0.065623
Sum of electronic and zero-point Energies= -503.630941
Sum of electronic and thermal Energies= -503.623036
Sum of electronic and thermal Enthalpies= -503.622092
Sum of electronic and thermal Free Energies= -503.665224

PPh_3

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.000268	0.000230	-1.207652
2	6	0	0.423428	-1.615299	-0.403794
3	6	0	1.168769	-4.116835	0.652467
4	6	0	1.406727	-2.398712	-1.032389
5	6	0	-0.188933	-2.113521	0.756896
6	6	0	0.180185	-3.355670	1.278801
7	6	0	1.783621	-3.633960	-0.505062
8	1	0	1.876346	-2.038498	-1.944973
9	1	0	-0.959910	-1.531716	1.253074
10	1	0	-0.306083	-3.727714	2.177166
11	1	0	2.548742	-4.223717	-1.003333
12	1	0	1.453786	-5.083401	1.059636
13	6	0	-1.611007	0.440681	-0.403382
14	6	0	-4.149564	1.047385	0.652632
15	6	0	-1.735610	1.216785	0.759353
16	6	0	-2.781334	-0.016041	-1.033840
17	6	0	-4.039415	0.275844	-0.506565
18	6	0	-2.995680	1.519086	1.281173
19	1	0	-0.845510	1.589544	1.257099
20	1	0	-2.704134	-0.601072	-1.947533
21	1	0	-4.932953	-0.089448	-1.006196
22	1	0	-3.074421	2.123805	2.181200
23	1	0	-5.129014	1.284562	1.059691
24	6	0	1.186903	1.174596	-0.403159
25	6	0	2.981582	3.069975	0.653178

26	6	0	1.921772	0.894363	0.759378
27	6	0	1.376920	2.416359	-1.033614
28	6	0	2.258630	3.360092	-0.506235
29	6	0	2.813333	1.834653	1.281433
30	1	0	1.800949	-0.063002	1.257206
31	1	0	0.832266	2.642092	-1.947656
32	1	0	2.389168	4.316453	-1.006045
33	1	0	3.376352	1.600255	2.181427
34	1	0	3.676474	3.799723	1.060408

Zero-point correction= 0.274418 (Hartree/Particle)
Thermal correction to Energy= 0.290316
Thermal correction to Enthalpy= 0.291260
Thermal correction to Gibbs Free Energy= 0.228059
Sum of electronic and zero-point Energies= -1036.007284
Sum of electronic and thermal Energies= -1035.991386
Sum of electronic and thermal Enthalpies= -1035.990442
Sum of electronic and thermal Free Energies= -1036.053642

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction= 0.271965 (Hartree/Particle)
Thermal correction to Energy= 0.287931
Thermal correction to Enthalpy= 0.288875
Thermal correction to Gibbs Free Energy= 0.226930
Sum of electronic and zero-point Energies= -1035.421634
Sum of electronic and thermal Energies= -1035.405669
Sum of electronic and thermal Enthalpies= -1035.404724
Sum of electronic and thermal Free Energies= -1035.466669

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction= 0.269881 (Hartree/Particle)
Thermal correction to Energy= 0.285567
Thermal correction to Enthalpy= 0.286512
Thermal correction to Gibbs Free Energy= 0.226370
Sum of electronic and zero-point Energies= -1035.642455
Sum of electronic and thermal Energies= -1035.626769
Sum of electronic and thermal Enthalpies= -1035.625824
Sum of electronic and thermal Free Energies= -1035.685966

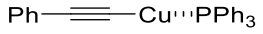
M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.012504	-0.003963	-1.266102
2	6	0	1.652149	-0.086604	-0.431836
3	6	0	4.203422	-0.068926	0.721908
4	6	0	2.715984	0.566700	-1.063025
5	6	0	1.885129	-0.737515	0.783445
6	6	0	3.154047	-0.729683	1.354996
7	6	0	3.982787	0.582279	-0.488551
8	1	0	2.546852	1.066036	-2.018573
9	1	0	1.066127	-1.253209	1.286073
10	1	0	3.323629	-1.240537	2.301867
11	1	0	4.800862	1.096545	-0.990641
12	1	0	5.195487	-0.065444	1.170714
13	6	0	-0.888875	-1.379975	-0.434319

14	6	0	-2.161062	-3.597575	0.710335
15	6	0	-1.687787	-1.230503	0.703214
16	6	0	-0.742474	-2.654697	-0.993286
17	6	0	-1.366936	-3.757843	-0.422234
18	6	0	-2.321335	-2.333239	1.269895
19	1	0	-1.813875	-0.244014	1.150733
20	1	0	-0.131572	-2.780179	-1.888906
21	1	0	-1.241138	-4.743785	-0.867247
22	1	0	-2.941663	-2.203713	2.155613
23	1	0	-2.657937	-4.458228	1.155415
24	6	0	-0.747104	1.463921	-0.452277
25	6	0	-2.065338	3.671692	0.661526
26	6	0	-0.178393	2.165489	0.613720
27	6	0	-1.981129	1.890711	-0.958483
28	6	0	-2.641238	2.979294	-0.401185
29	6	0	-0.833461	3.264857	1.164039
30	1	0	0.782840	1.850282	1.019732
31	1	0	-2.431054	1.357039	-1.797874
32	1	0	-3.603224	3.294963	-0.802129
33	1	0	-0.377624	3.803318	1.993837
34	1	0	-2.575597	4.530075	1.095624

Zero-point correction=	0.272705	(Hartree/Particle)
Thermal correction to Energy=	0.288648	
Thermal correction to Enthalpy=	0.289592	
Thermal correction to Gibbs Free Energy=	0.227164	
Sum of electronic and zero-point Energies=	-1035.421986	
Sum of electronic and thermal Energies=	-1035.406043	
Sum of electronic and thermal Enthalpies=	-1035.405099	
Sum of electronic and thermal Free Energies=	-1035.467527	

(Phenylethynyl)copper(triphenylphosphine)



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.860009	-0.020807	0.022889
2	15	0	-1.397541	-0.004174	0.004947
3	6	0	-2.118014	-1.051561	-1.323404
4	6	0	-3.123170	-2.744495	-3.321189
5	6	0	-3.320385	-0.740964	-1.976745
6	6	0	-1.418011	-2.212093	-1.691521
7	6	0	-1.922070	-3.056635	-2.680699
8	6	0	-3.818885	-1.585611	-2.970336
9	1	0	-3.861508	0.164655	-1.718911
10	1	0	-0.473226	-2.449572	-1.208389
11	1	0	-1.370790	-3.950805	-2.957720
12	1	0	-4.748851	-1.334574	-3.473315
13	1	0	-3.511435	-3.397708	-4.097843
14	6	0	-2.151220	-0.611242	1.568298
15	6	0	-3.204681	-1.473501	4.020981
16	6	0	-3.383133	-1.281734	1.614339
17	6	0	-1.447068	-0.389336	2.762994
18	6	0	-1.974583	-0.813435	3.982806
19	6	0	-3.905632	-1.709045	2.836341
20	1	0	-3.928779	-1.481072	0.696761

21	1	0	-0.480853	0.108864	2.736603
22	1	0	-1.419386	-0.637452	4.899842
23	1	0	-4.858409	-2.231007	2.861207
24	1	0	-3.611687	-1.811453	4.970066
25	6	0	-2.100574	1.674343	-0.259331
26	6	0	-3.072977	4.259247	-0.751991
27	6	0	-3.299157	2.105091	0.329335
28	6	0	-1.388023	2.557402	-1.087339
29	6	0	-1.875997	3.840009	-1.336925
30	6	0	-3.780988	3.392142	0.082533
31	1	0	-3.850531	1.441990	0.989252
32	1	0	-0.446258	2.242570	-1.530522
33	1	0	-1.315286	4.513997	-1.978448
34	1	0	-4.707940	3.717665	0.546898
35	1	0	-3.448275	5.261613	-0.939170
36	1	0	5.558525	2.136766	0.041945
37	6	0	6.110941	1.201884	0.027875
38	6	0	7.515458	-1.208467	-0.007944
39	6	0	5.391512	-0.012004	0.016255
40	6	0	7.503758	1.205281	0.021488
41	6	0	8.214051	0.001858	0.003513
42	6	0	6.122655	-1.218740	-0.001674
43	1	0	8.038403	2.152084	0.030618
44	1	0	9.300925	0.007205	-0.001522
45	1	0	5.579385	-2.159022	-0.010697
46	1	0	8.059268	-2.149968	-0.021976
47	6	0	3.964645	-0.018574	0.021668
48	6	0	2.734808	-0.022950	0.025229

Zero-point correction= 0.376466 (Hartree/Particle)
Thermal correction to Energy= 0.402024
Thermal correction to Enthalpy= 0.402968
Thermal correction to Gibbs Free Energy= 0.314196
Sum of electronic and zero-point Energies= -1539.902467
Sum of electronic and thermal Energies= -1539.876909
Sum of electronic and thermal Enthalpies= -1539.875965
Sum of electronic and thermal Free Energies= -1539.964737

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction= 0.373739 (Hartree/Particle)
Thermal correction to Energy= 0.399118
Thermal correction to Enthalpy= 0.400062
Thermal correction to Gibbs Free Energy= 0.315559
Sum of electronic and zero-point Energies= -1539.115958
Sum of electronic and thermal Energies= -1539.090579
Sum of electronic and thermal Enthalpies= -1539.089635
Sum of electronic and thermal Free Energies= -1539.174138

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction= 0.370534 (Hartree/Particle)
Thermal correction to Energy= 0.395583
Thermal correction to Enthalpy= 0.396528
Thermal correction to Gibbs Free Energy= 0.314278
Sum of electronic and zero-point Energies= -1540.619404
Sum of electronic and thermal Energies= -1540.594355
Sum of electronic and thermal Enthalpies= -1540.593411
Sum of electronic and thermal Free Energies= -1540.675661

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.850372	-0.012349	-0.041239
2	15	0	1.377812	-0.000854	-0.012546
3	6	0	2.070517	-0.213167	1.661573
4	6	0	3.053791	-0.660924	4.233015
5	6	0	3.240630	0.421850	2.085598
6	6	0	1.392450	-1.068097	2.536759
7	6	0	1.886509	-1.295052	3.816202
8	6	0	3.728704	0.197325	3.369244
9	1	0	3.769318	1.097226	1.412448
10	1	0	0.469991	-1.553276	2.213030
11	1	0	1.352789	-1.960250	4.492213
12	1	0	4.638573	0.697338	3.696476
13	1	0	3.436597	-0.831294	5.237694
14	6	0	2.126765	-1.330087	-1.011327
15	6	0	3.205569	-3.311301	-2.650139
16	6	0	3.329395	-1.950884	-0.662489
17	6	0	1.463907	-1.714886	-2.181047
18	6	0	2.005314	-2.699109	-3.000448
19	6	0	3.865690	-2.938638	-1.482226
20	1	0	3.845780	-1.664014	0.254095
21	1	0	0.516730	-1.241967	-2.446099
22	1	0	1.483305	-2.994956	-3.908413
23	1	0	4.800954	-3.422242	-1.205848
24	1	0	3.625875	-4.086953	-3.287810
25	6	0	2.109617	1.547069	-0.639636
26	6	0	3.148162	3.991250	-1.491999
27	6	0	3.340040	1.594017	-1.301396
28	6	0	1.400394	2.731327	-0.415741
29	6	0	1.920547	3.949966	-0.836423
30	6	0	3.855279	2.814769	-1.725344
31	1	0	3.893847	0.673951	-1.491099
32	1	0	0.432560	2.694397	0.087325
33	1	0	1.362626	4.867492	-0.659645
34	1	0	4.811687	2.846646	-2.244247
35	1	0	3.552049	4.943816	-1.830396
36	1	0	-5.539787	2.142350	-0.029173
37	6	0	-6.094261	1.205043	-0.019817
38	6	0	-7.489273	-1.201233	0.004320
39	6	0	-5.378173	-0.003445	-0.021971
40	6	0	-7.482625	1.206127	-0.005645
41	6	0	-8.187173	0.004416	0.006559
42	6	0	-6.100916	-1.207807	-0.009901
43	1	0	-8.020606	2.153270	-0.003953
44	1	0	-9.275867	0.007520	0.017996
45	1	0	-5.551633	-2.148206	-0.011465
46	1	0	-8.032524	-2.145309	0.013876
47	6	0	-3.951820	-0.007535	-0.034540
48	6	0	-2.722149	-0.011761	-0.043657

Zero-point correction=	0.374364	(Hartree/Particle)
Thermal correction to Energy=	0.399973	
Thermal correction to Enthalpy=	0.400917	
Thermal correction to Gibbs Free Energy=	0.313013	
Sum of electronic and zero-point Energies=	-1539.116580	
Sum of electronic and thermal Energies=	-1539.090971	
Sum of electronic and thermal Enthalpies=	-1539.090027	

Sum of electronic and thermal Free Energies= -1539.177932

Et_3NH^+

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.689292	-0.001957	-0.002335
2	6	0	2.132239	-1.350687	0.554298
3	1	0	2.090365	-1.268623	1.641563
4	1	0	3.179172	-1.466355	0.260772
5	6	0	2.128420	0.187654	-1.450249
6	1	0	2.075343	-0.793927	-1.923727
7	1	0	3.178456	0.489702	-1.407315
8	6	0	1.260796	-2.501738	0.068968
9	1	0	1.294562	-2.637746	-1.015995
10	1	0	0.216763	-2.375805	0.378056
11	1	0	1.625284	-3.427859	0.523381
12	6	0	1.263642	1.192742	-2.199606
13	1	0	1.625583	1.260824	-3.229859
14	1	0	1.307835	2.199179	-1.773078
15	1	0	0.216552	0.871477	-2.242230
16	6	0	2.139089	1.154380	0.883904
17	1	0	2.091604	2.055072	0.269864
18	1	0	3.188152	0.958565	1.122107
19	6	0	1.278277	1.309102	2.130800
20	1	0	0.231274	1.510115	1.876198
21	1	0	1.645284	2.168123	2.700486
22	1	0	1.320683	0.439061	2.792677
23	1	0	0.662199	0.000379	0.001551

Zero-point correction= 0.222484 (Hartree/Particle)
Thermal correction to Energy= 0.231978
Thermal correction to Enthalpy= 0.232922
Thermal correction to Gibbs Free Energy= 0.188530
Sum of electronic and zero-point Energies= -292.579138
Sum of electronic and thermal Energies= -292.569644
Sum of electronic and thermal Enthalpies= -292.568700
Sum of electronic and thermal Free Energies= -292.613092

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction= 0.220240 (Hartree/Particle)
Thermal correction to Energy= 0.229974
Thermal correction to Enthalpy= 0.230918
Thermal correction to Gibbs Free Energy= 0.185461
Sum of electronic and zero-point Energies= -292.376631
Sum of electronic and thermal Energies= -292.366897
Sum of electronic and thermal Enthalpies= -292.365953
Sum of electronic and thermal Free Energies= -292.411409

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction= 0.218167 (Hartree/Particle)
Thermal correction to Energy= 0.227504
Thermal correction to Enthalpy= 0.228448

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Thermal correction to Gibbs Free Energy=         0.184875
Sum of electronic and zero-point Energies=           -292.474925
Sum of electronic and thermal Energies=              -292.465589
Sum of electronic and thermal Enthalpies=            -292.464644
Sum of electronic and thermal Free Energies=         -292.508218
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M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000145	-0.001793	-0.005026
2	6	0	0.988175	-1.054830	0.443847
3	1	0	0.471837	-2.018182	0.387379
4	1	0	1.187334	-0.839522	1.500914
5	6	0	0.418395	1.378838	0.447580
6	1	0	1.511016	1.412747	0.396008
7	1	0	0.127452	1.444055	1.502928
8	6	0	2.240939	-1.063001	-0.398035
9	1	0	2.806903	-0.126906	-0.336183
10	1	0	2.016161	-1.269342	-1.451958
11	1	0	2.899333	-1.862614	-0.043423
12	6	0	-0.194601	2.468303	-0.397918
13	1	0	0.155708	3.438828	-0.031873
14	1	0	-1.289352	2.482271	-0.354521
15	1	0	0.114896	2.383862	-1.446908
16	6	0	-1.403670	-0.331796	0.451881
17	1	0	-1.977584	0.599466	0.415903
18	1	0	-1.309068	-0.629394	1.503469
19	6	0	-2.048962	-1.396452	-0.401371
20	1	0	-2.139145	-1.074369	-1.446275
21	1	0	-3.061858	-1.581173	-0.029389
22	1	0	-1.514945	-2.353003	-0.373011
23	1	0	-0.001362	-0.000549	-1.033785

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Zero-point correction=                           0.220461 (Hartree/Particle)
Thermal correction to Energy=                    0.229224
Thermal correction to Enthalpy=                  0.230169
Thermal correction to Gibbs Free Energy=         0.187521
Sum of electronic and zero-point Energies=           -292.377189
Sum of electronic and thermal Energies=              -292.368426
Sum of electronic and thermal Enthalpies=            -292.367482
Sum of electronic and thermal Free Energies=         -292.410130
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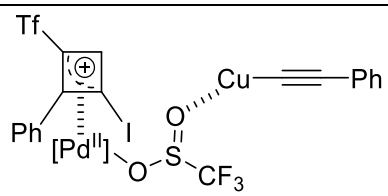
I-Cu



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.678578	-2.057601	1.759026

2	6	0	-2.471023	-1.422579	0.890430
3	6	0	-2.618756	-2.135393	-0.434011
4	1	0	-2.969914	-0.460695	1.010664
5	6	0	-1.284919	-2.225758	-0.736635
6	6	0	-0.965139	-1.389097	0.472912
7	6	0	-0.487002	-2.899809	-1.756934
8	6	0	1.042746	-4.199813	-3.723284
9	6	0	-1.109343	-3.710058	-2.728341
10	6	0	0.912509	-2.758927	-1.785350
11	6	0	1.668864	-3.402883	-2.763742
12	6	0	-0.347964	-4.350600	-3.701390
13	1	0	-2.186732	-3.838273	-2.711106
14	1	0	1.424878	-2.146777	-1.051105
15	1	0	2.746305	-3.268046	-2.765707
16	1	0	-0.840226	-4.972367	-4.444346
17	1	0	1.632906	-4.702090	-4.484867
18	53	0	0.464208	-2.196218	1.935693
19	8	0	-3.691291	-2.668899	-1.077488
20	16	0	-5.096482	-1.667279	-1.345966
21	8	0	-4.794642	-0.244944	-1.069917
22	6	0	-5.988926	-2.296023	0.207935
23	9	0	-7.219205	-1.771658	0.179483
24	9	0	-6.071090	-3.624867	0.156314
25	9	0	-5.376713	-1.920618	1.329930
26	46	0	-0.498668	0.264677	-0.589957
27	15	0	-0.478625	1.826229	1.135852
28	6	0	1.131563	1.990932	1.985130
29	6	0	3.633361	2.274275	3.212030
30	6	0	1.251585	2.704590	3.193046
31	6	0	2.271959	1.414197	1.409271
32	6	0	3.518680	1.557382	2.021271
33	6	0	2.499458	2.846845	3.797657
34	1	0	0.374474	3.140305	3.662633
35	1	0	2.204439	0.837537	0.492061
36	1	0	4.382716	1.089668	1.559915
37	1	0	2.585057	3.399483	4.729420
38	1	0	4.602747	2.381365	3.691312
39	6	0	-0.901302	3.464876	0.415587
40	6	0	-1.674256	5.944423	-0.642513
41	6	0	-0.221768	4.635230	0.784654
42	6	0	-1.955700	3.545900	-0.509879
43	6	0	-2.345841	4.781535	-1.025013
44	6	0	-0.608869	5.867268	0.255386
45	1	0	0.611712	4.589207	1.476846
46	1	0	-2.456509	2.643065	-0.845272
47	1	0	-3.162794	4.830444	-1.739400
48	1	0	-0.072071	6.766501	0.544793
49	1	0	-1.971932	6.905356	-1.053190
50	6	0	-1.712503	1.588206	2.486183
51	6	0	-3.616543	1.099686	4.497168
52	6	0	-2.994732	2.157102	2.409576
53	6	0	-1.397564	0.771460	3.585948
54	6	0	-2.343639	0.532687	4.583204
55	6	0	-3.937770	1.912888	3.408917
56	1	0	-3.258483	2.802755	1.579113
57	1	0	-0.413380	0.325240	3.669103
58	1	0	-2.081100	-0.097623	5.428340
59	1	0	-4.922489	2.366331	3.336672
60	1	0	-4.351563	0.912802	5.275251
61	8	0	-0.575526	1.527858	-2.385618
62	16	0	0.386364	1.863495	-3.540676

63	8	0	1.524154	0.839075	-3.681781
64	6	0	1.338917	3.314427	-2.779115
65	9	0	2.348699	3.652149	-3.590907
66	9	0	0.516768	4.365447	-2.652310
67	9	0	1.841165	3.010221	-1.571060
68	1	0	4.162145	-3.266914	1.265779
69	6	0	5.172706	-2.882349	1.367620
70	6	0	7.767239	-1.885430	1.613289
71	6	0	5.562880	-1.781783	0.574572
72	6	0	6.064584	-3.468172	2.262961
73	6	0	7.365631	-2.974112	2.392077
74	6	0	6.880525	-1.295177	0.715401
75	1	0	5.743377	-4.316385	2.862850
76	1	0	8.059755	-3.434050	3.090639
77	1	0	7.194356	-0.452613	0.106039
78	1	0	8.778267	-1.495511	1.703922
79	6	0	4.650472	-1.176645	-0.342554
80	29	0	2.689972	0.110576	-2.355506
81	6	0	3.861930	-0.652150	-1.128381

Zero-point correction=	0.562509 (Hartree/Particle)
Thermal correction to Energy=	0.616880
Thermal correction to Enthalpy=	0.617824
Thermal correction to Gibbs Free Energy=	0.459525
Sum of electronic and zero-point Energies=	-3835.506071
Sum of electronic and thermal Energies=	-3835.451700
Sum of electronic and thermal Enthalpies=	-3835.450756
Sum of electronic and thermal Free Energies=	-3835.609055

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.558882 (Hartree/Particle)
Thermal correction to Energy=	0.610286
Thermal correction to Enthalpy=	0.611231
Thermal correction to Gibbs Free Energy=	0.466358
Sum of electronic and zero-point Energies=	-3834.049504
Sum of electronic and thermal Energies=	-3833.998100
Sum of electronic and thermal Enthalpies=	-3833.997155
Sum of electronic and thermal Free Energies=	-3834.142028

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.552629 (Hartree/Particle)
Thermal correction to Energy=	0.603719
Thermal correction to Enthalpy=	0.604663
Thermal correction to Gibbs Free Energy=	0.463550
Sum of electronic and zero-point Energies=	-3837.186324
Sum of electronic and thermal Energies=	-3837.135234
Sum of electronic and thermal Enthalpies=	-3837.134290
Sum of electronic and thermal Free Energies=	-3837.275403

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

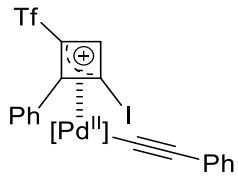
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.832996	-2.786813	1.549466
2	6	0	-1.828401	-1.963641	0.818633
3	6	0	-1.991251	-2.419232	-0.602527

4	1	0	-2.472567	-1.156791	1.175952
5	6	0	-0.687253	-2.252378	-0.986123
6	6	0	-0.413990	-1.581850	0.316966
7	6	0	0.107198	-2.583818	-2.157893
8	6	0	1.629799	-3.216924	-4.415261
9	6	0	-0.484643	-3.232592	-3.252285
10	6	0	1.470247	-2.264877	-2.206349
11	6	0	2.223978	-2.577734	-3.331637
12	6	0	0.274389	-3.543236	-4.371564
13	1	0	-1.541365	-3.493801	-3.215730
14	1	0	1.952836	-1.759849	-1.369898
15	1	0	3.280192	-2.312113	-3.350372
16	1	0	-0.193318	-4.045794	-5.216468
17	1	0	2.220591	-3.463807	-5.295633
18	53	0	1.280450	-2.127905	1.530837
19	8	0	-3.048103	-2.917151	-1.279983
20	16	0	-4.501425	-1.999974	-1.255597
21	8	0	-4.222765	-0.644572	-0.754942
22	6	0	-5.207285	-2.887139	0.249035
23	9	0	-6.479305	-2.522278	0.317968
24	9	0	-5.126820	-4.192802	0.085297
25	9	0	-4.589493	-2.526357	1.357509
26	46	0	-0.481438	0.220641	-0.622928
27	15	0	-0.705525	1.567628	1.263543
28	6	0	0.830066	2.014378	2.122576
29	6	0	3.223307	2.641356	3.406619
30	6	0	0.811527	2.599020	3.397401
31	6	0	2.051200	1.744558	1.503906
32	6	0	3.245335	2.054576	2.146450
33	6	0	2.006207	2.915530	4.030994
34	1	0	-0.137930	2.799230	3.895500
35	1	0	2.086161	1.279077	0.517954
36	1	0	4.184961	1.821576	1.647850
37	1	0	1.989054	3.371281	5.019379
38	1	0	4.156654	2.882211	3.912846
39	6	0	-1.562297	3.110772	0.797415
40	6	0	-2.987132	5.410053	0.110573
41	6	0	-1.156913	4.358476	1.278331
42	6	0	-2.670848	3.027047	-0.054695
43	6	0	-3.387976	4.171033	-0.382428
44	6	0	-1.869114	5.502727	0.932827
45	1	0	-0.280044	4.440553	1.918853
46	1	0	-2.961988	2.065650	-0.479561
47	1	0	-4.251202	4.096080	-1.041017
48	1	0	-1.543971	6.471453	1.308081
49	1	0	-3.542910	6.307376	-0.156224
50	6	0	-1.763508	0.813563	2.552379
51	6	0	-3.370721	-0.680532	4.290136
52	6	0	-3.158615	0.902212	2.480709
53	6	0	-1.183800	-0.018973	3.516969
54	6	0	-1.983983	-0.759410	4.380413
55	6	0	-3.955028	0.157350	3.343905
56	1	0	-3.631459	1.548318	1.742663
57	1	0	-0.099986	-0.098884	3.591044
58	1	0	-1.518253	-1.404928	5.122953
59	1	0	-5.038670	0.232861	3.273620
60	1	0	-3.996310	-1.267646	4.960085
61	8	0	-1.055497	1.655844	-2.220501
62	16	0	-0.202974	2.320553	-3.292914
63	8	0	1.082747	1.535961	-3.567675
64	6	0	0.505688	3.738094	-2.289903

65	9	0	1.424347	4.375703	-3.005078
66	9	0	-0.471840	4.581429	-1.986136
67	9	0	1.068658	3.308682	-1.162994
68	1	0	4.277526	-3.049664	-0.007431
69	6	0	5.072327	-2.570920	0.564900
70	6	0	7.109202	-1.326074	1.991139
71	6	0	5.253248	-1.182741	0.432857
72	6	0	5.893126	-3.317934	1.399029
73	6	0	6.914075	-2.699370	2.117929
74	6	0	6.290478	-0.573969	1.158271
75	1	0	5.738320	-4.392569	1.486751
76	1	0	7.558010	-3.286867	2.770489
77	1	0	6.449887	0.498476	1.049796
78	1	0	7.909785	-0.835935	2.543812
79	6	0	4.392176	-0.430956	-0.419991
80	29	0	2.322889	0.888043	-2.281890
81	6	0	3.614152	0.175849	-1.154845

Zero-point correction=	0.565072 (Hartree/Particle)
Thermal correction to Energy=	0.617369
Thermal correction to Enthalpy=	0.618313
Thermal correction to Gibbs Free Energy=	0.473183
Sum of electronic and zero-point Energies=	-3834.055901
Sum of electronic and thermal Energies=	-3834.003605
Sum of electronic and thermal Enthalpies=	-3834.002660
Sum of electronic and thermal Free Energies=	-3834.147790

II



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.301856	-3.252526	-2.358294
2	6	0	0.169349	-2.258343	-1.911587
3	6	0	1.055844	-2.055523	-0.659490
4	1	0	0.169619	-1.495541	-2.693973
5	6	0	-0.007780	-2.480710	0.221112
6	6	0	-0.936250	-2.219575	-0.837510
7	6	0	-0.035504	-2.975174	1.594490
8	6	0	-0.044072	-3.967678	4.220933
9	6	0	1.176726	-3.240304	2.262382
10	6	0	-1.250018	-3.214173	2.263992
11	6	0	-1.250584	-3.705173	3.566908
12	6	0	1.166717	-3.734323	3.564223
13	1	0	2.118712	-3.060711	1.756225
14	1	0	-2.190013	-3.011020	1.763364
15	1	0	-2.195256	-3.883955	4.072966
16	1	0	2.107721	-3.937021	4.067939
17	1	0	-0.047808	-4.351905	5.237349
18	53	0	-2.935691	-2.829083	-1.156002
19	8	0	2.389051	-2.347841	-0.508431

20	16	0	3.488958	-1.300043	-1.331328
21	8	0	3.356250	-1.490381	-2.793625
22	6	0	4.859126	-2.497434	-0.799598
23	9	0	4.698665	-3.707837	-1.326151
24	9	0	6.012757	-1.974349	-1.235728
25	9	0	4.900115	-2.584326	0.535899
26	46	0	-0.036445	-0.232425	-0.200759
27	15	0	-1.646844	1.547385	0.042032
28	6	0	-1.684684	2.331956	1.713708
29	6	0	-1.661485	3.554197	4.244491
30	6	0	-2.824494	2.999368	2.196418
31	6	0	-0.534196	2.283404	2.517141
32	6	0	-0.526226	2.893752	3.772957
33	6	0	-2.810717	3.606160	3.452908
34	1	0	-3.729750	3.036250	1.598773
35	1	0	0.356186	1.782505	2.150790
36	1	0	0.372350	2.848832	4.382255
37	1	0	-3.700127	4.116913	3.812620
38	1	0	-1.652919	4.024793	5.224149
39	6	0	-1.291022	2.924708	-1.132079
40	6	0	-0.750307	4.950627	-2.998414
41	6	0	-1.753613	4.232049	-0.916618
42	6	0	-0.548250	2.647332	-2.288819
43	6	0	-0.284619	3.653653	-3.220190
44	6	0	-1.482695	5.238283	-1.844032
45	1	0	-2.315272	4.470039	-0.018733
46	1	0	-0.159797	1.645921	-2.448770
47	1	0	0.294118	3.424362	-4.110731
48	1	0	-1.840562	6.248182	-1.662218
49	1	0	-0.538137	5.736493	-3.718486
50	6	0	-3.422212	1.149600	-0.274819
51	6	0	-6.102549	0.434205	-0.742052
52	6	0	-4.054286	1.495512	-1.478330
53	6	0	-4.147543	0.420961	0.683601
54	6	0	-5.479173	0.076843	0.455965
55	6	0	-5.384069	1.136706	-1.709742
56	1	0	-3.513878	2.054808	-2.235235
57	1	0	-3.676141	0.134173	1.619826
58	1	0	-6.028428	-0.475360	1.213987
59	1	0	-5.858832	1.416623	-2.646370
60	1	0	-7.139911	0.163853	-0.919954
61	6	0	1.514705	1.020667	0.097887
62	6	0	2.469230	1.777651	0.252833
63	6	0	3.576474	2.663939	0.420544
64	6	0	5.766466	4.413823	0.740763
65	6	0	4.637103	2.345189	1.294865
66	6	0	3.640285	3.881864	-0.289537
67	6	0	4.723468	4.742585	-0.129691
68	6	0	5.716480	3.211997	1.451737
69	1	0	4.597420	1.411636	1.848878
70	1	0	2.828798	4.136528	-0.964748
71	1	0	4.754291	5.675775	-0.686727
72	1	0	6.523151	2.948064	2.131247
73	1	0	6.610072	5.087828	0.863841

Zero-point correction= 0.537265 (Hartree/Particle)
Thermal correction to Energy= 0.581700
Thermal correction to Enthalpy= 0.582645
Thermal correction to Gibbs Free Energy= 0.446673
Sum of electronic and zero-point Energies= -2753.099971
Sum of electronic and thermal Energies= -2753.055536

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Sum of electronic and thermal Enthalpies=           -2753.054592
Sum of electronic and thermal Free Energies=        -2753.190563
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M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

```
Zero-point correction=                           0.533875 (Hartree/Particle)
Thermal correction to Energy=                    0.577760
Thermal correction to Enthalpy=                  0.578704
Thermal correction to Gibbs Free Energy=         0.451550
Sum of electronic and zero-point Energies=          -2751.782298
Sum of electronic and thermal Energies=             -2751.738414
Sum of electronic and thermal Enthalpies=           -2751.737470
Sum of electronic and thermal Free Energies=        -2751.864624
```

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

```
Zero-point correction=                           0.529304 (Hartree/Particle)
Thermal correction to Energy=                    0.572648
Thermal correction to Enthalpy=                  0.573592
Thermal correction to Gibbs Free Energy=         0.450039
Sum of electronic and zero-point Energies=          -2753.558574
Sum of electronic and thermal Energies=             -2753.515230
Sum of electronic and thermal Enthalpies=           -2753.514285
Sum of electronic and thermal Free Energies=        -2753.637839
```

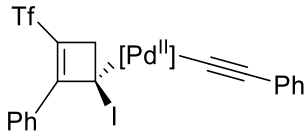
M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.001265	-3.370463	-2.350202
2	6	0	0.034931	-2.366023	-1.901848
3	6	0	0.797563	-2.326301	-0.565754
4	1	0	0.273075	-1.619745	-2.670119
5	6	0	-0.427767	-2.498021	0.190789
6	6	0	-1.141501	-2.094782	-0.963055
7	6	0	-0.723827	-2.853228	1.567962
8	6	0	-1.252247	-3.518683	4.227634
9	6	0	0.324239	-3.207260	2.429815
10	6	0	-2.038800	-2.838513	2.053152
11	6	0	-2.297776	-3.166571	3.376692
12	6	0	0.056342	-3.538986	3.750892
13	1	0	1.346728	-3.219196	2.055523
14	1	0	-2.857707	-2.553469	1.393425
15	1	0	-3.321851	-3.148057	3.745845
16	1	0	0.874765	-3.813024	4.413740
17	1	0	-1.458222	-3.776600	5.264956
18	53	0	-3.159273	-2.076406	-1.520748
19	8	0	2.002971	-2.922421	-0.280160
20	16	0	3.342225	-2.050276	-0.828097
21	8	0	3.398093	-2.131461	-2.296725
22	6	0	4.394321	-3.491358	-0.257558
23	9	0	4.072420	-4.605816	-0.883649
24	9	0	5.651849	-3.177227	-0.543523
25	9	0	4.273775	-3.654458	1.052517
26	46	0	0.110137	-0.341466	-0.187472
27	15	0	-1.217707	1.624436	0.089762
28	6	0	-0.928361	2.716006	1.531735
29	6	0	-0.479267	4.418648	3.702638
30	6	0	-1.907116	3.640096	1.923596

31	6	0	0.271354	2.648206	2.244331
32	6	0	0.493195	3.500120	3.323247
33	6	0	-1.681105	4.487919	3.000869
34	1	0	-2.852524	3.696644	1.382547
35	1	0	1.037063	1.936978	1.937570
36	1	0	1.434093	3.441258	3.867708
37	1	0	-2.447481	5.202568	3.296310
38	1	0	-0.303872	5.082233	4.547858
39	6	0	-1.046183	2.691458	-1.381349
40	6	0	-0.770512	4.182568	-3.727346
41	6	0	-0.905934	4.078900	-1.319462
42	6	0	-1.031470	2.055909	-2.628864
43	6	0	-0.906011	2.797792	-3.796152
44	6	0	-0.765526	4.819468	-2.490707
45	1	0	-0.898094	4.584140	-0.353860
46	1	0	-1.111990	0.967519	-2.681014
47	1	0	-0.898388	2.293583	-4.760734
48	1	0	-0.649746	5.900423	-2.433425
49	1	0	-0.659390	4.764344	-4.640681
50	6	0	-3.009877	1.285609	0.239577
51	6	0	-5.703745	0.647398	0.611943
52	6	0	-3.968762	1.738258	-0.665949
53	6	0	-3.408994	0.501826	1.329237
54	6	0	-4.747828	0.188412	1.517704
55	6	0	-5.312759	1.418235	-0.477524
56	1	0	-3.669391	2.347505	-1.518838
57	1	0	-2.658883	0.133176	2.033453
58	1	0	-5.046329	-0.419513	2.371261
59	1	0	-6.056226	1.779152	-1.186469
60	1	0	-6.754347	0.401195	0.756646
61	6	0	1.795644	0.766149	-0.029905
62	6	0	2.721826	1.571660	0.015763
63	6	0	3.743631	2.562153	0.115207
64	6	0	5.726477	4.535496	0.346585
65	6	0	5.100556	2.210645	0.192628
66	6	0	3.400350	3.924523	0.153433
67	6	0	4.383355	4.898225	0.269141
68	6	0	6.079849	3.188631	0.306675
69	1	0	5.372876	1.156205	0.162578
70	1	0	2.347526	4.200422	0.085314
71	1	0	4.100509	5.949690	0.297097
72	1	0	7.127958	2.898270	0.364390
73	1	0	6.495788	5.300650	0.437991

Zero-point correction=	0.536582	(Hartree/Particle)
Thermal correction to Energy=	0.579247	
Thermal correction to Enthalpy=	0.580191	
Thermal correction to Gibbs Free Energy=	0.455294	
Sum of electronic and zero-point Energies=	-2751.786962	
Sum of electronic and thermal Energies=	-2751.744297	
Sum of electronic and thermal Enthalpies=	-2751.743353	
Sum of electronic and thermal Free Energies=	-2751.868250	

IIa



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.520814	4.041174	0.494016
2	6	0	-0.560331	3.066051	-0.002673
3	6	0	-1.926818	2.681858	-0.509213
4	1	0	0.292635	2.958889	-0.674640
5	6	0	-2.194254	1.728494	0.424302
6	6	0	-0.800212	1.868244	0.971848
7	6	0	-3.310088	0.858457	0.780070
8	6	0	-5.441188	-0.837387	1.482824
9	6	0	-4.609387	1.104721	0.300303
10	6	0	-3.104209	-0.243978	1.628082
11	6	0	-4.158253	-1.089773	1.970529
12	6	0	-5.662225	0.264568	0.650309
13	1	0	-4.787600	1.961532	-0.341452
14	1	0	-2.113901	-0.424934	2.045970
15	1	0	-3.977448	-1.939488	2.622667
16	1	0	-6.660872	0.469941	0.274311
17	1	0	-6.265855	-1.491256	1.752818
18	53	0	-0.643141	2.363761	3.148959
19	8	0	-2.625619	3.148854	-1.602030
20	16	0	-2.736745	2.199911	-3.031621
21	8	0	-2.933029	0.762348	-2.722662
22	6	0	-0.892897	2.287759	-3.495917
23	9	0	-0.180070	1.416254	-2.784871
24	9	0	-0.812553	1.968439	-4.794965
25	9	0	-0.417849	3.520706	-3.318286
26	46	0	0.026332	0.041476	0.571802
27	15	0	0.628715	-2.247770	-0.068864
28	6	0	1.798200	-2.514004	-1.463331
29	6	0	3.673063	-2.892734	-3.513333
30	6	0	1.550239	-3.440719	-2.487589
31	6	0	2.989966	-1.770655	-1.479386
32	6	0	3.922411	-1.965496	-2.498611
33	6	0	2.485638	-3.626800	-3.507745
34	1	0	0.627354	-4.012620	-2.493403
35	1	0	3.173417	-1.027502	-0.709599
36	1	0	4.840603	-1.384404	-2.501292
37	1	0	2.283492	-4.344966	-4.298052
38	1	0	4.398887	-3.038652	-4.309003
39	6	0	1.272961	-3.315360	1.282459
40	6	0	2.200904	-4.884045	3.414765
41	6	0	1.920277	-4.537126	1.036046
42	6	0	1.111609	-2.881871	2.607362
43	6	0	1.569491	-3.665223	3.668180
44	6	0	2.378226	-5.317226	2.098168
45	1	0	2.075705	-4.872590	0.014712
46	1	0	0.644397	-1.920295	2.804993
47	1	0	1.443161	-3.316140	4.689229
48	1	0	2.879820	-6.260102	1.897287
49	1	0	2.564056	-5.490845	4.239875
50	6	0	-0.950865	-3.016102	-0.621974
51	6	0	-3.437130	-3.995555	-1.479674
52	6	0	-1.396895	-4.278807	-0.203974
53	6	0	-1.768943	-2.246567	-1.469856
54	6	0	-3.002520	-2.735567	-1.897619
55	6	0	-2.634016	-4.763969	-0.634261
56	1	0	-0.783454	-4.881623	0.458395

57	1	0	-1.451570	-1.259366	-1.796900
58	1	0	-3.622252	-2.118930	-2.541569
59	1	0	-2.970381	-5.743500	-0.304486
60	1	0	-4.401981	-4.374917	-1.805567
61	6	0	1.760372	0.916619	0.442883
62	6	0	2.842337	1.478723	0.337647
63	6	0	4.119371	2.106495	0.203393
64	6	0	6.638663	3.343191	-0.067191
65	6	0	4.761591	2.687199	1.316353
66	6	0	4.767684	2.160874	-1.048306
67	6	0	6.012225	2.773271	-1.178637
68	6	0	6.006821	3.296406	1.178431
69	1	0	4.268374	2.652821	2.282992
70	1	0	4.278216	1.720396	-1.912348
71	1	0	6.495054	2.807075	-2.152240
72	1	0	6.486356	3.738612	2.048094
73	1	0	7.609487	3.820448	-0.170952

Zero-point correction=	0.537304	(Hartree/Particle)
Thermal correction to Energy=	0.580717	
Thermal correction to Enthalpy=	0.581661	
Thermal correction to Gibbs Free Energy=	0.451234	
Sum of electronic and zero-point Energies=	-2753.101701	
Sum of electronic and thermal Energies=	-2753.058289	
Sum of electronic and thermal Enthalpies=	-2753.057345	
Sum of electronic and thermal Free Energies=	-2753.187771	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.533710	(Hartree/Particle)
Thermal correction to Energy=	0.575885	
Thermal correction to Enthalpy=	0.576829	
Thermal correction to Gibbs Free Energy=	0.454046	
Sum of electronic and zero-point Energies=	-2751.781348	
Sum of electronic and thermal Energies=	-2751.739173	
Sum of electronic and thermal Enthalpies=	-2751.738229	
Sum of electronic and thermal Free Energies=	-2751.861012	

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.529000	(Hartree/Particle)
Thermal correction to Energy=	0.570723	
Thermal correction to Enthalpy=	0.571667	
Thermal correction to Gibbs Free Energy=	0.448629	
Sum of electronic and zero-point Energies=	-2753.552891	
Sum of electronic and thermal Energies=	-2753.511168	
Sum of electronic and thermal Enthalpies=	-2753.510224	
Sum of electronic and thermal Free Energies=	-2753.633262	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

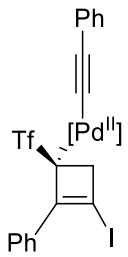
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.858084	-4.005983	-1.200805
2	6	0	0.597585	-3.164618	-0.545528
3	6	0	-0.667580	-3.333759	0.244206
4	1	0	1.491655	-2.827534	-0.008435
5	6	0	-1.409006	-2.424822	-0.434434

6	6	0	-0.208977	-2.039246	-1.234196
7	6	0	-2.710712	-1.782306	-0.363799
8	6	0	-5.090750	-0.330856	-0.075193
9	6	0	-3.767151	-2.298548	0.394949
10	6	0	-2.888582	-0.548724	-1.008039
11	6	0	-4.058945	0.184535	-0.851093
12	6	0	-4.945878	-1.579162	0.531165
13	1	0	-3.651327	-3.261337	0.889594
14	1	0	-2.117743	-0.170259	-1.697325
15	1	0	-4.157994	1.157714	-1.330088
16	1	0	-5.758762	-1.989112	1.127973
17	1	0	-6.011566	0.234739	0.054191
18	53	0	-0.356128	-2.194428	-3.430176
19	8	0	-0.894972	-4.097405	1.364782
20	16	0	-0.983140	-3.382236	2.884228
21	8	0	-1.740453	-2.118685	2.828239
22	6	0	0.802479	-2.773373	2.951756
23	9	0	0.948306	-1.650885	2.276224
24	9	0	1.060843	-2.549191	4.233865
25	9	0	1.630885	-3.694559	2.492322
26	46	0	-0.112700	-0.053682	-0.731182
27	15	0	-0.316208	2.190657	0.137626
28	6	0	1.001431	2.845170	1.215847
29	6	0	3.081763	3.880994	2.759699
30	6	0	0.738271	3.385262	2.477384
31	6	0	2.315428	2.820075	0.733731
32	6	0	3.349084	3.342970	1.502412
33	6	0	1.778733	3.898682	3.246890
34	1	0	-0.282063	3.405178	2.860374
35	1	0	2.529042	2.367967	-0.235381
36	1	0	4.368604	3.320267	1.120226
37	1	0	1.568491	4.316061	4.230262
38	1	0	3.893579	4.284123	3.362960
39	6	0	-0.602185	3.517281	-1.084592
40	6	0	-1.140370	5.476042	-2.999579
41	6	0	-0.389943	4.868122	-0.789702
42	6	0	-1.075600	3.157654	-2.349752
43	6	0	-1.348889	4.133870	-3.302385
44	6	0	-0.659225	5.842492	-1.744877
45	1	0	-0.010596	5.156976	0.191264
46	1	0	-1.210562	2.102728	-2.598240
47	1	0	-1.711707	3.843590	-4.286645
48	1	0	-0.487890	6.891799	-1.510829
49	1	0	-1.343657	6.240376	-3.747668
50	6	0	-1.819890	2.165851	1.178150
51	6	0	-4.130351	1.917970	2.726783
52	6	0	-2.779595	3.180771	1.174050
53	6	0	-2.026621	1.026113	1.966415
54	6	0	-3.177377	0.901993	2.734718
55	6	0	-3.929589	3.055776	1.950042
56	1	0	-2.633651	4.068478	0.558394
57	1	0	-1.296217	0.213924	1.966101
58	1	0	-3.328389	-0.004934	3.318695
59	1	0	-4.674065	3.850388	1.942339
60	1	0	-5.036923	1.820255	3.322152
61	6	0	1.833855	-0.236312	-0.668548
62	6	0	3.054160	-0.306566	-0.596570
63	6	0	4.476188	-0.317420	-0.476680
64	6	0	7.271237	-0.312796	-0.223851
65	6	0	5.291479	-0.760154	-1.530324
66	6	0	5.088865	0.128150	0.706553

67	6	0	6.472375	0.127452	0.829233
68	6	0	6.674481	-0.754835	-1.402355
69	1	0	4.821631	-1.106192	-2.449755
70	1	0	4.456769	0.475939	1.523696
71	1	0	6.931376	0.473719	1.754448
72	1	0	7.292540	-1.099076	-2.230437
73	1	0	8.355630	-0.311736	-0.126201

Zero-point correction=	0.538306 (Hartree/Particle)
Thermal correction to Energy=	0.581134
Thermal correction to Enthalpy=	0.582078
Thermal correction to Gibbs Free Energy=	0.456603
Sum of electronic and zero-point Energies=	-2751.784765
Sum of electronic and thermal Energies=	-2751.741938
Sum of electronic and thermal Enthalpies=	-2751.740994
Sum of electronic and thermal Free Energies=	-2751.866468

IIb



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.306327	-0.199047	-1.622413
2	6	0	1.493359	-0.675449	-0.385343
3	1	0	2.627846	-0.977694	-2.314838
4	1	0	1.844722	0.625007	-2.173633
5	6	0	3.301605	0.195112	-0.560416
6	6	0	2.625484	-0.281564	0.513335
7	6	0	2.798184	-0.372228	1.958819
8	6	0	3.100102	-0.571672	4.749297
9	6	0	4.068120	-0.255546	2.553351
10	6	0	1.684705	-0.598591	2.788201
11	6	0	1.835114	-0.693842	4.169819
12	6	0	4.214359	-0.353358	3.935231
13	1	0	4.940836	-0.096439	1.929198
14	1	0	0.697357	-0.676191	2.341237
15	1	0	0.962198	-0.860365	4.795468
16	1	0	5.202854	-0.261773	4.377351
17	1	0	3.217289	-0.647040	5.827060
18	46	0	-0.485593	-0.300764	-0.141365
19	15	0	-2.914665	-0.404376	0.067822
20	6	0	-3.832692	0.432615	-1.287037
21	6	0	-5.158381	1.669169	-3.427555
22	6	0	-5.137615	0.923714	-1.124901
23	6	0	-3.194898	0.579691	-2.528707
24	6	0	-3.857811	1.189485	-3.594528
25	6	0	-5.795731	1.537740	-2.191573
26	1	0	-5.636768	0.836248	-0.164368

27	1	0	-2.173333	0.231371	-2.652941
28	1	0	-3.352249	1.300374	-4.549746
29	1	0	-6.804527	1.917946	-2.054521
30	1	0	-5.671154	2.151827	-4.255241
31	6	0	-3.489771	-2.157358	0.027972
32	6	0	-4.217323	-4.872230	0.013308
33	6	0	-4.521336	-2.612868	-0.805459
34	6	0	-2.821621	-3.083136	0.849516
35	6	0	-3.187312	-4.428453	0.847364
36	6	0	-4.880018	-3.963405	-0.812200
37	1	0	-5.043885	-1.915264	-1.452042
38	1	0	-2.013872	-2.748741	1.497143
39	1	0	-2.664683	-5.130442	1.491463
40	1	0	-5.679387	-4.302784	-1.465479
41	1	0	-4.497800	-5.921939	0.005115
42	6	0	-3.627063	0.277032	1.622681
43	6	0	-4.663325	1.411829	3.968317
44	6	0	-4.704613	-0.328870	2.287736
45	6	0	-3.067437	1.454625	2.147004
46	6	0	-3.589596	2.017989	3.311940
47	6	0	-5.218672	0.237815	3.455741
48	1	0	-5.139668	-1.244411	1.898365
49	1	0	-2.225986	1.923188	1.643431
50	1	0	-3.150435	2.929026	3.709151
51	1	0	-6.051649	-0.240235	3.964509
52	1	0	-5.063233	1.850443	4.878726
53	53	0	5.046201	1.381584	-0.797131
54	8	0	1.003491	-2.078909	-0.234443
55	16	0	1.075611	-3.357796	-1.349022
56	8	0	1.130833	-2.889974	-2.754134
57	6	0	2.863762	-3.848798	-0.927796
58	9	0	3.091585	-5.016645	-1.544962
59	9	0	3.756424	-2.952987	-1.345452
60	9	0	2.977205	-4.021433	0.389763
61	6	0	-0.363303	1.648201	-0.207930
62	6	0	-0.294427	2.868989	-0.277482
63	6	0	-0.226058	4.294386	-0.359270
64	6	0	-0.094486	7.105976	-0.520987
65	6	0	-1.288927	5.037091	-0.914439
66	6	0	0.904670	4.992992	0.112249
67	6	0	0.965657	6.382407	0.031587
68	6	0	-1.220241	6.426148	-0.993693
69	1	0	-2.162493	4.507052	-1.282561
70	1	0	1.728998	4.429484	0.538793
71	1	0	1.845938	6.903056	0.400252
72	1	0	-2.049013	6.981163	-1.426389
73	1	0	-0.043361	8.189807	-0.583693

Zero-point correction= 0.536869 (Hartree/Particle)
Thermal correction to Energy= 0.581380
Thermal correction to Enthalpy= 0.582324
Thermal correction to Gibbs Free Energy= 0.445142
Sum of electronic and zero-point Energies= -2753.099492
Sum of electronic and thermal Energies= -2753.054981
Sum of electronic and thermal Enthalpies= -2753.054037
Sum of electronic and thermal Free Energies= -2753.191219

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction= 0.533093 (Hartree/Particle)
Thermal correction to Energy= 0.576344

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Thermal correction to Enthalpy=                 0.577288
Thermal correction to Gibbs Free Energy=        0.450527
Sum of electronic and zero-point Energies=          -2751.769464
Sum of electronic and thermal Energies=             -2751.726213
Sum of electronic and thermal Enthalpies=           -2751.725269
Sum of electronic and thermal Free Energies=        -2751.852030
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M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

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Zero-point correction=                          0.528696 (Hartree/Particle)
Thermal correction to Energy=                   0.572234
Thermal correction to Enthalpy=                 0.573178
Thermal correction to Gibbs Free Energy=        0.448138
Sum of electronic and zero-point Energies=          -2753.543473
Sum of electronic and thermal Energies=             -2753.499935
Sum of electronic and thermal Enthalpies=           -2753.498991
Sum of electronic and thermal Free Energies=        -2753.624031
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M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.385739	-0.870275	-1.552300
2	6	0	1.310151	-1.110867	-0.475908
3	1	0	2.716337	-1.744688	-2.118919
4	1	0	2.154838	-0.046392	-2.239229
5	6	0	3.213432	-0.509295	-0.352168
6	6	0	2.288283	-0.785468	0.594313
7	6	0	2.157016	-0.706762	2.038269
8	6	0	1.895701	-0.516313	4.821504
9	6	0	3.289125	-0.725146	2.863716
10	6	0	0.890959	-0.608176	2.633160
11	6	0	0.762827	-0.507448	4.012134
12	6	0	3.157485	-0.629987	4.242973
13	1	0	4.277542	-0.827226	2.417263
14	1	0	-0.001379	-0.580864	2.002347
15	1	0	-0.228193	-0.416666	4.454832
16	1	0	4.046829	-0.645522	4.870691
17	1	0	1.795555	-0.437602	5.902747
18	46	0	-0.536244	-0.283199	-0.452448
19	15	0	-2.860983	0.187664	-0.033765
20	6	0	-3.798360	1.277531	-1.151108
21	6	0	-5.195121	2.884554	-2.949213
22	6	0	-4.963710	1.936297	-0.745017
23	6	0	-3.331912	1.438414	-2.458379
24	6	0	-4.032697	2.237654	-3.356369
25	6	0	-5.660205	2.735552	-1.644072
26	1	0	-5.323842	1.824811	0.278796
27	1	0	-2.409404	0.942924	-2.763320
28	1	0	-3.662509	2.363249	-4.372119
29	1	0	-6.565800	3.248733	-1.325260
30	1	0	-5.739782	3.515583	-3.649494
31	6	0	-3.809517	-1.374184	0.058839
32	6	0	-5.088094	-3.852122	0.245753
33	6	0	-5.071308	-1.558088	-0.508481
34	6	0	-3.192035	-2.445473	0.718909
35	6	0	-3.829735	-3.675602	0.818092
36	6	0	-5.705040	-2.795446	-0.415700
37	1	0	-5.561070	-0.734717	-1.028064
38	1	0	-2.204871	-2.308064	1.170052

39	1	0	-3.342510	-4.499115	1.337339
40	1	0	-6.687616	-2.932265	-0.864275
41	1	0	-5.586426	-4.817495	0.314683
42	6	0	-3.054843	0.932236	1.626068
43	6	0	-3.234195	2.147877	4.132366
44	6	0	-4.003550	0.493864	2.554030
45	6	0	-2.193399	1.984529	1.962491
46	6	0	-2.289867	2.591530	3.209260
47	6	0	-4.088866	1.099617	3.804722
48	1	0	-4.677791	-0.324552	2.301051
49	1	0	-1.438026	2.316183	1.245833
50	1	0	-1.617809	3.408998	3.464323
51	1	0	-4.827334	0.750082	4.524505
52	1	0	-3.302852	2.619170	5.111506
53	53	0	5.076726	0.470392	-0.311961
54	8	0	0.596896	-2.369942	-0.289861
55	16	0	0.232520	-3.434228	-1.536912
56	8	0	0.568993	-2.862921	-2.851361
57	6	0	1.690650	-4.545300	-1.116202
58	9	0	1.731953	-5.503930	-2.028164
59	9	0	2.837706	-3.891314	-1.110645
60	9	0	1.475609	-5.074542	0.077046
61	6	0	0.163093	1.543852	-0.692413
62	6	0	0.645969	2.667123	-0.782481
63	6	0	1.187132	3.985189	-0.866665
64	6	0	2.246359	6.581254	-1.015621
65	6	0	1.414307	4.597634	-2.109572
66	6	0	1.500375	4.701005	0.300307
67	6	0	2.024669	5.984324	0.223451
68	6	0	1.938884	5.881614	-2.179968
69	1	0	1.171532	4.048078	-3.017936
70	1	0	1.327500	4.230389	1.267548
71	1	0	2.263620	6.524211	1.138859
72	1	0	2.108043	6.340955	-3.153078
73	1	0	2.657872	7.587670	-1.073737

Zero-point correction=	0.536524 (Hartree/Particle)
Thermal correction to Energy=	0.580227
Thermal correction to Enthalpy=	0.581171
Thermal correction to Gibbs Free Energy=	0.451572
Sum of electronic and zero-point Energies=	-2751.771237
Sum of electronic and thermal Energies=	-2751.727534
Sum of electronic and thermal Enthalpies=	-2751.726590
Sum of electronic and thermal Free Energies=	-2751.856190

$TS_{IIb\text{-}VI}$

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Imaginary frequency: -276.9142 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.156198	-2.210023	0.812786
2	6	0	1.396737	-0.631841	0.645273
3	1	0	1.156097	-2.512968	1.863940
4	1	0	0.303666	-2.671560	0.297102
5	6	0	2.472050	-2.290750	0.098749
6	6	0	2.712586	-0.971104	-0.036435

7	6	0	3.818747	-0.151643	-0.533361
8	6	0	6.000861	1.366518	-1.439772
9	6	0	4.515890	-0.525339	-1.694537
10	6	0	4.227857	0.997505	0.166457
11	6	0	5.312203	1.746305	-0.285438
12	6	0	5.598183	0.229934	-2.143549
13	1	0	4.198991	-1.401951	-2.250246
14	1	0	3.698129	1.295302	1.064427
15	1	0	5.617501	2.632609	0.263723
16	1	0	6.124062	-0.068571	-3.046517
17	1	0	6.844025	1.955420	-1.790816
18	46	0	-0.720196	-0.438891	-0.025568
19	15	0	-3.071387	-0.224014	-0.392976
20	6	0	-3.691685	1.489828	-0.122499
21	6	0	-4.553681	4.139149	0.207579
22	6	0	-4.967166	1.761612	0.396347
23	6	0	-2.846816	2.559211	-0.462592
24	6	0	-3.280809	3.875871	-0.303651
25	6	0	-5.393856	3.081035	0.560238
26	1	0	-5.624064	0.944662	0.679690
27	1	0	-1.845949	2.358112	-0.834988
28	1	0	-2.618313	4.694896	-0.570118
29	1	0	-6.381744	3.280584	0.967023
30	1	0	-4.887007	5.165270	0.338305
31	6	0	-3.631386	-0.657438	-2.094982
32	6	0	-4.406265	-1.423034	-4.683958
33	6	0	-4.702898	-0.016429	-2.735392
34	6	0	-2.945840	-1.677553	-2.773897
35	6	0	-3.335120	-2.063108	-4.056532
36	6	0	-5.086054	-0.398350	-4.022801
37	1	0	-5.234172	0.786632	-2.233708
38	1	0	-2.096777	-2.161566	-2.297331
39	1	0	-2.794272	-2.853831	-4.569325
40	1	0	-5.914634	0.109127	-4.509660
41	1	0	-4.704162	-1.715738	-5.687168
42	6	0	-4.101643	-1.270638	0.724234
43	6	0	-5.578098	-2.842449	2.522006
44	6	0	-5.269154	-1.925077	0.302698
45	6	0	-3.674943	-1.420939	2.055931
46	6	0	-4.414922	-2.196864	2.948443
47	6	0	-6.001487	-2.707315	1.198768
48	1	0	-5.605320	-1.829866	-0.725262
49	1	0	-2.762113	-0.938232	2.398410
50	1	0	-4.074200	-2.303314	3.974627
51	1	0	-6.902192	-3.212242	0.859548
52	1	0	-6.148223	-3.453698	3.216516
53	53	0	3.529217	-4.036700	-0.472213
54	8	0	1.617752	0.040952	1.880470
55	16	0	0.256342	0.731043	2.611752
56	8	0	-0.466883	-0.272494	3.439038
57	6	0	1.440986	1.582774	3.819680
58	9	0	0.682101	2.288060	4.669925
59	9	0	2.189548	0.726984	4.507799
60	9	0	2.232079	2.433731	3.145530
61	6	0	0.674483	0.852923	-0.523811
62	6	0	1.212895	1.876083	-0.940004
63	6	0	1.778780	3.100260	-1.397731
64	6	0	2.879326	5.538609	-2.278479
65	6	0	1.976648	3.346274	-2.772338
66	6	0	2.147790	4.101384	-0.472896
67	6	0	2.690519	5.305563	-0.913193

68	6	0	2.521557	4.553317	-3.202859
69	1	0	1.697429	2.580566	-3.489601
70	1	0	2.008658	3.913565	0.587923
71	1	0	2.968823	6.065868	-0.187779
72	1	0	2.667352	4.726714	-4.265995
73	1	0	3.302916	6.479616	-2.618968

Zero-point correction=	0.536357 (Hartree/Particle)
Thermal correction to Energy=	0.580119
Thermal correction to Enthalpy=	0.581063
Thermal correction to Gibbs Free Energy=	0.448207
Sum of electronic and zero-point Energies=	-2753.078195
Sum of electronic and thermal Energies=	-2753.034433
Sum of electronic and thermal Enthalpies=	-2753.033489
Sum of electronic and thermal Free Energies=	-2753.166345

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Imaginary frequency: -259.4744 cm^{-1}

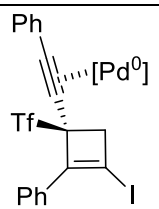
Zero-point correction=	0.532115 (Hartree/Particle)
Thermal correction to Energy=	0.573045
Thermal correction to Enthalpy=	0.573989
Thermal correction to Gibbs Free Energy=	0.454257
Sum of electronic and zero-point Energies=	-2751.761621
Sum of electronic and thermal Energies=	-2751.720691
Sum of electronic and thermal Enthalpies=	-2751.719747
Sum of electronic and thermal Free Energies=	-2751.839479

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Imaginary frequency: -263.5779 cm^{-1}

Zero-point correction=	0.527503 (Hartree/Particle)
Thermal correction to Energy=	0.569681
Thermal correction to Enthalpy=	0.570625
Thermal correction to Gibbs Free Energy=	0.448731
Sum of electronic and zero-point Energies=	-2753.532896
Sum of electronic and thermal Energies=	-2753.490717
Sum of electronic and thermal Enthalpies=	-2753.489773
Sum of electronic and thermal Free Energies=	-2753.611668

VI



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.926007	-0.490485	-1.891054
2	6	0	2.221253	-0.589536	-0.485261
3	1	0	2.886174	-1.428495	-2.453059
4	1	0	2.601071	0.344182	-2.519709
5	6	0	4.167492	-0.269246	-1.067737
6	6	0	3.604838	-0.380504	0.154210
7	6	0	3.978618	-0.313192	1.560796
8	6	0	4.645963	-0.181499	4.290302
9	6	0	5.240301	0.160000	1.969272
10	6	0	3.058259	-0.720542	2.545601
11	6	0	3.392602	-0.654357	3.896469
12	6	0	5.567395	0.223675	3.321182
13	1	0	5.961174	0.483913	1.227014
14	1	0	2.091101	-1.110212	2.248931
15	1	0	2.671840	-0.976416	4.643072
16	1	0	6.544704	0.593783	3.619038
17	1	0	4.904206	-0.129802	5.344545
18	46	0	-0.842533	-0.000283	-0.223209
19	15	0	-3.218602	0.138657	-0.178326
20	6	0	-3.942173	-0.777202	1.255893
21	6	0	-4.915673	-2.120836	3.526277
22	6	0	-5.114680	-1.543819	1.182269
23	6	0	-3.258956	-0.701645	2.481975
24	6	0	-3.746379	-1.361108	3.610297
25	6	0	-5.594986	-2.213206	2.310587
26	1	0	-5.651582	-1.627780	0.242586
27	1	0	-2.336434	-0.129391	2.545150
28	1	0	-3.207047	-1.290402	4.551128
29	1	0	-6.500764	-2.809316	2.236115
30	1	0	-5.290698	-2.643923	4.401922
31	6	0	-4.006068	1.810541	-0.065655
32	6	0	-5.121770	4.391257	-0.016561
33	6	0	-5.031100	2.126234	0.837781
34	6	0	-3.540683	2.808941	-0.938202
35	6	0	-4.099864	4.086147	-0.920105
36	6	0	-5.581854	3.410910	0.863039
37	1	0	-5.402317	1.371816	1.524325
38	1	0	-2.729950	2.584904	-1.627257
39	1	0	-3.730579	4.845252	-1.604491
40	1	0	-6.373177	3.641653	1.571582
41	1	0	-5.552488	5.388824	0.003766
42	6	0	-4.060227	-0.585033	-1.658539
43	6	0	-5.273929	-1.755708	-3.908115
44	6	0	-5.358343	-0.211902	-2.045882
45	6	0	-3.375160	-1.542038	-2.423416
46	6	0	-3.980769	-2.127014	-3.537147
47	6	0	-5.960426	-0.794980	-3.161791
48	1	0	-5.897757	0.541724	-1.479779
49	1	0	-2.360801	-1.825987	-2.160090
50	1	0	-3.434155	-2.865506	-4.117023
51	1	0	-6.964336	-0.494485	-3.450405
52	1	0	-5.742610	-2.206064	-4.779135
53	53	0	6.123571	0.119445	-1.771436
54	8	0	1.741778	-1.926676	-0.191027
55	16	0	0.128997	-2.250368	-0.581388
56	8	0	0.056871	-2.988294	-1.868357
57	6	0	0.101284	-3.582672	0.763868
58	9	0	-1.098463	-4.171871	0.699979
59	9	0	1.050676	-4.496493	0.591914
60	9	0	0.237792	-3.005480	1.965232
61	6	0	1.200802	0.447426	-0.218592

62	6	0	0.726525	1.596148	-0.015190
63	6	0	0.768166	3.014629	0.233801
64	6	0	0.911806	5.777887	0.720883
65	6	0	-0.375657	3.730413	0.626223
66	6	0	1.989348	3.705790	0.088553
67	6	0	2.055528	5.075303	0.329739
68	6	0	-0.300805	5.100520	0.868761
69	1	0	-1.315055	3.199441	0.733335
70	1	0	2.877504	3.157267	-0.210758
71	1	0	3.002589	5.595645	0.213948
72	1	0	-1.194556	5.639636	1.171126
73	1	0	0.966943	6.846815	0.908717

Zero-point correction=	0.539067 (Hartree/Particle)
Thermal correction to Energy=	0.582707
Thermal correction to Enthalpy=	0.583651
Thermal correction to Gibbs Free Energy=	0.450915
Sum of electronic and zero-point Energies=	-2753.151769
Sum of electronic and thermal Energies=	-2753.108129
Sum of electronic and thermal Enthalpies=	-2753.107184
Sum of electronic and thermal Free Energies=	-2753.239921

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.535038 (Hartree/Particle)
Thermal correction to Energy=	0.577456
Thermal correction to Enthalpy=	0.578400
Thermal correction to Gibbs Free Energy=	0.455312
Sum of electronic and zero-point Energies=	-2751.834660
Sum of electronic and thermal Energies=	-2751.792242
Sum of electronic and thermal Enthalpies=	-2751.791298
Sum of electronic and thermal Free Energies=	-2751.914387

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.530555 (Hartree/Particle)
Thermal correction to Energy=	0.573295
Thermal correction to Enthalpy=	0.574239
Thermal correction to Gibbs Free Energy=	0.451596
Sum of electronic and zero-point Energies=	-2753.603394
Sum of electronic and thermal Energies=	-2753.560654
Sum of electronic and thermal Enthalpies=	-2753.559710
Sum of electronic and thermal Free Energies=	-2753.682353

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.002354	-0.669801	-1.861469
2	6	0	2.249966	-0.639160	-0.495167
3	1	0	2.977103	-1.658305	-2.337909
4	1	0	2.707849	0.105560	-2.580061
5	6	0	4.207257	-0.382522	-1.014911
6	6	0	3.590646	-0.402088	0.182182
7	6	0	3.875139	-0.214149	1.589484
8	6	0	4.344524	0.165228	4.319822
9	6	0	5.135897	0.199215	2.041915
10	6	0	2.854795	-0.439222	2.525013

11	6	0	3.090568	-0.249755	3.880029
12	6	0	5.365262	0.386775	3.397734
13	1	0	5.934995	0.379688	1.324512
14	1	0	1.878905	-0.779307	2.180286
15	1	0	2.291659	-0.427559	4.597583
16	1	0	6.346797	0.711876	3.738220
17	1	0	4.527832	0.315944	5.382312
18	46	0	-0.780486	0.015023	-0.366460
19	15	0	-3.143545	0.153643	-0.198733
20	6	0	-3.764642	-1.051575	1.037533
21	6	0	-4.562651	-2.891692	2.985858
22	6	0	-5.019464	-1.663109	0.959017
23	6	0	-2.917370	-1.371799	2.102721
24	6	0	-3.312147	-2.287106	3.072723
25	6	0	-5.414964	-2.577988	1.929825
26	1	0	-5.687123	-1.429853	0.129011
27	1	0	-1.929974	-0.907947	2.155769
28	1	0	-2.634449	-2.536805	3.887746
29	1	0	-6.391411	-3.054259	1.856953
30	1	0	-4.872802	-3.615269	3.737957
31	6	0	-3.945969	1.731772	0.281397
32	6	0	-5.077969	4.213630	0.899913
33	6	0	-4.849965	1.850620	1.338640
34	6	0	-3.611615	2.870798	-0.461546
35	6	0	-4.178927	4.102468	-0.159578
36	6	0	-5.409275	3.089047	1.647896
37	1	0	-5.121405	0.972946	1.925230
38	1	0	-2.892432	2.787764	-1.279757
39	1	0	-3.914643	4.979116	-0.749164
40	1	0	-6.110790	3.171606	2.476558
41	1	0	-5.518546	5.179373	1.142034
42	6	0	-4.057657	-0.298721	-1.725726
43	6	0	-5.394054	-1.133574	-4.036498
44	6	0	-5.320823	0.214683	-2.037400
45	6	0	-3.468347	-1.226476	-2.590661
46	6	0	-4.135428	-1.646974	-3.736062
47	6	0	-5.983926	-0.200880	-3.187901
48	1	0	-5.789301	0.945163	-1.376899
49	1	0	-2.473844	-1.617076	-2.366768
50	1	0	-3.666129	-2.370682	-4.400051
51	1	0	-6.966038	0.206874	-3.422112
52	1	0	-5.914060	-1.456189	-4.936990
53	53	0	6.173091	-0.000482	-1.643100
54	8	0	1.710221	-1.916521	-0.108204
55	16	0	0.154882	-2.230313	-0.622549
56	8	0	0.203423	-3.106778	-1.809230
57	6	0	-0.073288	-3.394761	0.821785
58	9	0	-1.285581	-3.914873	0.701884
59	9	0	0.822155	-4.361081	0.816626
60	9	0	-0.000226	-2.714803	1.958349
61	6	0	1.276220	0.456016	-0.346017
62	6	0	0.804082	1.603438	-0.168432
63	6	0	0.750917	3.020917	0.045524
64	6	0	0.697220	5.783973	0.455275
65	6	0	-0.393508	3.636696	0.565656
66	6	0	1.873453	3.805159	-0.263764
67	6	0	1.841166	5.177976	-0.061093
68	6	0	-0.416911	5.009567	0.770533
69	1	0	-1.258942	3.018535	0.803366
70	1	0	2.764902	3.321501	-0.662978
71	1	0	2.714666	5.779455	-0.307034

72	1	0	-1.314229	5.475031	1.175887
73	1	0	0.675361	6.861097	0.611786

Zero-point correction=	0.539018 (Hartree/Particle)
Thermal correction to Energy=	0.581730
Thermal correction to Enthalpy=	0.582674
Thermal correction to Gibbs Free Energy=	0.456945
Sum of electronic and zero-point Energies=	-2751.836182
Sum of electronic and thermal Energies=	-2751.793470
Sum of electronic and thermal Enthalpies=	-2751.792526
Sum of electronic and thermal Free Energies=	-2751.918256

CuTf

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.571496	-0.237898	-0.000120
2	16	0	0.244821	1.107554	0.000526
3	8	0	-0.591429	0.660211	-1.225140
4	8	0	-0.591653	0.658897	1.225499
5	9	0	1.009889	-1.457420	-0.001153
6	9	0	2.338349	-0.112943	-1.089617
7	9	0	2.337686	-0.114477	1.090131
8	29	0	-1.898440	-0.402854	-0.000166

Zero-point correction=	0.022918 (Hartree/Particle)
Thermal correction to Energy=	0.031392
Thermal correction to Enthalpy=	0.032336
Thermal correction to Gibbs Free Energy=	-0.012632
Sum of electronic and zero-point Energies=	-1082.341154
Sum of electronic and thermal Energies=	-1082.332680
Sum of electronic and thermal Enthalpies=	-1082.331735
Sum of electronic and thermal Free Energies=	-1082.376703

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.022759 (Hartree/Particle)
Thermal correction to Energy=	0.031370
Thermal correction to Enthalpy=	0.032314
Thermal correction to Gibbs Free Energy=	-0.013564
Sum of electronic and zero-point Energies=	-1082.193149
Sum of electronic and thermal Energies=	-1082.184539
Sum of electronic and thermal Enthalpies=	-1082.183594
Sum of electronic and thermal Free Energies=	-1082.229472

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.022186 (Hartree/Particle)
Thermal correction to Energy=	0.030764
Thermal correction to Enthalpy=	0.031708
Thermal correction to Gibbs Free Energy=	-0.013647
Sum of electronic and zero-point Energies=	-1083.561011
Sum of electronic and thermal Energies=	-1083.552433
Sum of electronic and thermal Enthalpies=	-1083.551489
Sum of electronic and thermal Free Energies=	-1083.596844

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.542717	0.243586	-0.000002
2	16	0	-0.261415	-1.116590	0.000629
3	8	0	0.561705	-0.667448	-1.214772
4	8	0	0.562042	-0.665807	1.215247
5	9	0	-0.948545	1.433464	-0.000826
6	9	0	-2.304790	0.142754	-1.080667
7	9	0	-2.304417	0.144068	1.081032
8	29	0	1.878232	0.399565	-0.000335

Zero-point correction= 0.023483 (Hartree/Particle)
Thermal correction to Energy= 0.032000
Thermal correction to Enthalpy= 0.032945
Thermal correction to Gibbs Free Energy= -0.012258
Sum of electronic and zero-point Energies= -1082.193559
Sum of electronic and thermal Energies= -1082.185042
Sum of electronic and thermal Enthalpies= -1082.184098
Sum of electronic and thermal Free Energies= -1082.229300

[Cu]Tf = (Triflyl)copper(triphenylphosphine)

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-1.012058	0.409697	-0.907440
2	15	0	1.020037	-0.008096	-0.099373
3	6	0	2.294931	-0.409342	-1.361360
4	6	0	4.192783	-0.915448	-3.364605
5	6	0	3.363679	-1.285640	-1.120081
6	6	0	2.180149	0.199193	-2.621998
7	6	0	3.127514	-0.047484	-3.615201
8	6	0	4.306806	-1.535646	-2.118989
9	1	0	3.454741	-1.782327	-0.158926
10	1	0	1.342072	0.861092	-2.827592
11	1	0	3.027048	0.429316	-4.586167
12	1	0	5.128475	-2.219351	-1.923617
13	1	0	4.926422	-1.114932	-4.140845
14	6	0	1.661611	1.448300	0.818992
15	6	0	2.521042	3.681916	2.274949
16	6	0	3.027943	1.759591	0.895163
17	6	0	0.725311	2.273709	1.465840
18	6	0	1.159548	3.381607	2.194977
19	6	0	3.453490	2.872613	1.622158
20	1	0	3.758011	1.143034	0.378820
21	1	0	-0.338754	2.059349	1.392888
22	1	0	0.429450	4.014637	2.691284
23	1	0	4.512816	3.109508	1.673582
24	1	0	2.854691	4.549941	2.837161
25	6	0	1.035917	-1.401119	1.098729
26	6	0	0.986882	-3.583717	2.858622
27	6	0	1.946441	-1.472850	2.164716

28	6	0	0.090175	-2.425557	0.934620
29	6	0	0.070282	-3.513563	1.807801
30	6	0	1.921462	-2.561311	3.037802
31	1	0	2.663518	-0.672607	2.322587
32	1	0	-0.642546	-2.363724	0.134128
33	1	0	-0.668964	-4.298069	1.673372
34	1	0	2.627491	-2.606128	3.862570
35	1	0	0.965896	-4.427017	3.543456
36	8	0	-2.705120	0.814808	-1.777101
37	16	0	-3.619202	1.262125	-0.588491
38	8	0	-2.708201	1.522693	0.597750
39	6	0	-4.316781	-0.445723	-0.152119
40	9	0	-3.326680	-1.335791	0.064091
41	9	0	-5.061981	-0.366554	0.960402
42	9	0	-5.086068	-0.903617	-1.150691

Zero-point correction=	0.299171 (Hartree/Particle)
Thermal correction to Energy=	0.325465
Thermal correction to Enthalpy=	0.326409
Thermal correction to Gibbs Free Energy=	0.235374
Sum of electronic and zero-point Energies=	-2118.415315
Sum of electronic and thermal Energies=	-2118.389021
Sum of electronic and thermal Enthalpies=	-2118.388077
Sum of electronic and thermal Free Energies=	-2118.479112

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.297660 (Hartree/Particle)
Thermal correction to Energy=	0.323479
Thermal correction to Enthalpy=	0.324423
Thermal correction to Gibbs Free Energy=	0.238617
Sum of electronic and zero-point Energies=	-2117.686084
Sum of electronic and thermal Energies=	-2117.660265
Sum of electronic and thermal Enthalpies=	-2117.659321
Sum of electronic and thermal Free Energies=	-2117.745127

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.294790 (Hartree/Particle)
Thermal correction to Energy=	0.320359
Thermal correction to Enthalpy=	0.321303
Thermal correction to Gibbs Free Energy=	0.237043
Sum of electronic and zero-point Energies=	-2119.270218
Sum of electronic and thermal Energies=	-2119.244648
Sum of electronic and thermal Enthalpies=	-2119.243704
Sum of electronic and thermal Free Energies=	-2119.327965

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.968938	0.398495	1.022424
2	15	0	-0.988433	0.002222	0.108378
3	6	0	-2.334347	-0.396270	1.271570
4	6	0	-4.375997	-0.878165	3.108153
5	6	0	-3.313994	-1.352914	0.994815
6	6	0	-2.379711	0.312386	2.476648
7	6	0	-3.400885	0.076151	3.388801

8	6	0	-4.331123	-1.591817	1.914245
9	1	0	-3.279981	-1.917044	0.062461
10	1	0	-1.606763	1.050333	2.699027
11	1	0	-3.430519	0.631159	4.324486
12	1	0	-5.090187	-2.341363	1.697834
13	1	0	-5.170790	-1.069534	3.826846
14	6	0	-1.570355	1.445965	-0.836307
15	6	0	-2.356117	3.663670	-2.326340
16	6	0	-2.929184	1.718851	-1.022415
17	6	0	-0.605150	2.292423	-1.393480
18	6	0	-1.002568	3.396579	-2.140366
19	6	0	-3.318572	2.826149	-1.767916
20	1	0	-3.683013	1.067468	-0.578365
21	1	0	0.457599	2.091716	-1.237041
22	1	0	-0.250487	4.055700	-2.569557
23	1	0	-4.376780	3.038533	-1.909791
24	1	0	-2.663151	4.533241	-2.904963
25	6	0	-0.923422	-1.388704	-1.065537
26	6	0	-0.787044	-3.604482	-2.749937
27	6	0	-1.703440	-1.436218	-2.224072
28	6	0	-0.068815	-2.452758	-0.760965
29	6	0	-0.005408	-3.560273	-1.598802
30	6	0	-1.632410	-2.543390	-3.063200
31	1	0	-2.362313	-0.604183	-2.473816
32	1	0	0.555732	-2.407215	0.133156
33	1	0	0.662093	-4.385135	-1.357594
34	1	0	-2.237487	-2.575288	-3.967467
35	1	0	-0.732548	-4.467698	-3.410836
36	8	0	2.662330	0.781212	1.832394
37	16	0	3.617424	1.242650	0.695643
38	8	0	2.788127	1.659614	-0.485212
39	6	0	4.153598	-0.469047	0.150460
40	9	0	3.098368	-1.224339	-0.160144
41	9	0	4.931900	-0.375272	-0.922124
42	9	0	4.832301	-1.072411	1.121131

Zero-point correction=	0.298953	(Hartree/Particle)
Thermal correction to Energy=	0.324880	
Thermal correction to Enthalpy=	0.325825	
Thermal correction to Gibbs Free Energy=	0.237150	
Sum of electronic and zero-point Energies=	-2117.687121	
Sum of electronic and thermal Energies=	-2117.661193	
Sum of electronic and thermal Enthalpies=	-2117.660249	
Sum of electronic and thermal Free Energies=	-2117.748924	

TS_{I-II}

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Imaginary frequency: -24.5272 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.559745	-1.085293	-2.192761
2	6	0	2.250847	-0.870654	-1.164150
3	6	0	2.512235	-1.979850	-0.189781
4	1	0	2.590687	0.125835	-0.887308
5	6	0	1.219430	-2.372180	-0.000424

6	6	0	0.751806	-1.215053	-0.854989
7	6	0	0.601721	-3.498547	0.698811
8	6	0	-0.529509	-5.705374	2.030822
9	6	0	1.368332	-4.269141	1.597736
10	6	0	-0.739402	-3.858786	0.476907
11	6	0	-1.295684	-4.954169	1.139151
12	6	0	0.805879	-5.357299	2.257577
13	1	0	2.406961	-4.012185	1.773779
14	1	0	-1.352054	-3.281521	-0.202970
15	1	0	-2.334695	-5.212831	0.955479
16	1	0	1.410731	-5.936553	2.950032
17	1	0	-0.966760	-6.556596	2.545762
18	53	0	-0.413076	-1.717074	-2.691244
19	8	0	3.674240	-2.534163	0.277109
20	16	0	4.860978	-1.508108	1.002813
21	8	0	4.290315	-0.180090	1.332769
22	6	0	5.831026	-1.233626	-0.607804
23	9	0	5.177237	-0.454806	-1.468501
24	9	0	6.978243	-0.637061	-0.259185
25	9	0	6.098400	-2.410926	-1.170646
26	46	0	-0.195186	0.059560	0.402136
27	15	0	0.397730	2.119754	-0.614496
28	6	0	-1.141795	2.907529	-1.233002
29	6	0	-3.498360	4.086045	-2.188890
30	6	0	-1.086227	4.077327	-2.012752
31	6	0	-2.387882	2.330170	-0.945920
32	6	0	-3.559680	2.918913	-1.427556
33	6	0	-2.260252	4.665766	-2.480263
34	1	0	-0.126969	4.520752	-2.263385
35	1	0	-2.451380	1.412892	-0.367756
36	1	0	-4.515453	2.448304	-1.217330
37	1	0	-2.207082	5.570034	-3.080551
38	1	0	-4.411586	4.539546	-2.564800
39	6	0	1.107095	3.213086	0.682605
40	6	0	2.265192	4.805864	2.680151
41	6	0	0.618008	4.502139	0.931025
42	6	0	2.172767	2.720883	1.455790
43	6	0	2.753473	3.518498	2.441246
44	6	0	1.196085	5.292160	1.927269
45	1	0	-0.220070	4.888767	0.361323
46	1	0	2.549020	1.713193	1.299273
47	1	0	3.578455	3.126040	3.029112
48	1	0	0.803404	6.287590	2.116101
49	1	0	2.710938	5.422600	3.455845
50	6	0	1.552650	2.278090	-2.042669
51	6	0	3.272982	2.420877	-4.259348
52	6	0	2.840818	2.820533	-1.910300
53	6	0	1.136583	1.808601	-3.301118
54	6	0	1.991682	1.881850	-4.399661
55	6	0	3.693418	2.889853	-3.014168
56	1	0	3.179656	3.196827	-0.951098
57	1	0	0.144963	1.386231	-3.425280
58	1	0	1.654789	1.515307	-5.365310
59	1	0	4.685442	3.317762	-2.897601
60	1	0	3.938034	2.477098	-5.116822
61	8	0	-0.838404	1.357477	2.152693
62	16	0	-0.519024	0.818273	3.562845
63	8	0	-0.707383	-0.725229	3.575784
64	6	0	-2.113496	1.344016	4.438243
65	9	0	-2.058490	0.946933	5.717710
66	9	0	-2.222391	2.678136	4.402063

67	9	0	-3.192726	0.801248	3.862272
68	1	0	-6.091487	0.028208	-0.083072
69	6	0	-5.983652	-0.491721	-1.030715
70	6	0	-5.698475	-1.857105	-3.447578
71	6	0	-4.811267	-1.243098	-1.264049
72	6	0	-6.990564	-0.427832	-1.991232
73	6	0	-6.853030	-1.108367	-3.204351
74	6	0	-4.688268	-1.928048	-2.490842
75	1	0	-7.888229	0.152019	-1.791223
76	1	0	-7.640040	-1.057987	-3.952148
77	1	0	-3.790933	-2.509169	-2.678349
78	1	0	-5.585329	-2.391159	-4.387751
79	6	0	-3.782794	-1.303074	-0.275774
80	29	0	-1.834559	-1.277166	2.106321
81	6	0	-2.916156	-1.341171	0.596641

Zero-point correction=	0.562326 (Hartree/Particle)
Thermal correction to Energy=	0.615921
Thermal correction to Enthalpy=	0.616865
Thermal correction to Gibbs Free Energy=	0.461523
Sum of electronic and zero-point Energies=	-3835.502028
Sum of electronic and thermal Energies=	-3835.448434
Sum of electronic and thermal Enthalpies=	-3835.447489
Sum of electronic and thermal Free Energies=	-3835.602831

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Imaginary frequency: -37.6042 cm^{-1}

Zero-point correction=	0.558261 (Hartree/Particle)
Thermal correction to Energy=	0.608930
Thermal correction to Enthalpy=	0.609874
Thermal correction to Gibbs Free Energy=	0.467365
Sum of electronic and zero-point Energies=	-3834.046749
Sum of electronic and thermal Energies=	-3833.996080
Sum of electronic and thermal Enthalpies=	-3833.995136
Sum of electronic and thermal Free Energies=	-3834.137645

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Imaginary frequency: -34.6298 cm^{-1}

Zero-point correction=	0.553387 (Hartree/Particle)
Thermal correction to Energy=	0.605177
Thermal correction to Enthalpy=	0.606122
Thermal correction to Gibbs Free Energy=	0.463091
Sum of electronic and zero-point Energies=	-3837.180122
Sum of electronic and thermal Energies=	-3837.128331
Sum of electronic and thermal Enthalpies=	-3837.127387
Sum of electronic and thermal Free Energies=	-3837.270418

TS_{II-III}

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Imaginary frequency: -310.5039 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	1	0	0.909751	-3.800378	-0.832631
2	6	0	0.836768	-2.709542	-0.887101
3	6	0	2.093508	-1.968241	-0.546354
4	1	0	0.308256	-2.418945	-1.798122
5	6	0	1.688769	-1.480084	0.658163
6	6	0	0.290588	-2.069010	0.437912
7	6	0	2.329866	-0.773698	1.769102
8	6	0	3.585643	0.562533	3.908523
9	6	0	3.728571	-0.601365	1.789997
10	6	0	1.577715	-0.283027	2.853473
11	6	0	2.201616	0.382319	3.909551
12	6	0	4.345435	0.063817	2.845908
13	1	0	4.333029	-1.000154	0.982409
14	1	0	0.502152	-0.437676	2.874856
15	1	0	1.602019	0.750048	4.737719
16	1	0	5.424939	0.188104	2.843123
17	1	0	4.071355	1.077745	4.732613
18	53	0	-0.238221	-3.535308	2.041046
19	8	0	3.242676	-1.840115	-1.286239
20	16	0	3.529357	-0.258536	-1.924430
21	8	0	2.917896	-0.118241	-3.266069
22	6	0	5.321371	-0.771665	-2.240276
23	9	0	5.406744	-1.837421	-3.025055
24	9	0	5.921230	0.268942	-2.831447
25	9	0	5.927375	-1.013944	-1.070846
26	46	0	-0.397461	0.029153	0.418494
27	15	0	-1.123672	2.264448	0.025142
28	6	0	-2.739781	2.400615	-0.847120
29	6	0	-5.245314	2.541380	-2.100589
30	6	0	-3.051890	3.478754	-1.691061
31	6	0	-3.690732	1.387927	-0.648032
32	6	0	-4.938772	1.462798	-1.269141
33	6	0	-4.299383	3.547311	-2.312784
34	1	0	-2.319790	4.260519	-1.870311
35	1	0	-3.442215	0.529749	-0.031573
36	1	0	-5.662991	0.668149	-1.113308
37	1	0	-4.529415	4.384173	-2.967002
38	1	0	-6.214159	2.594022	-2.590236
39	6	0	-1.313459	3.322289	1.527178
40	6	0	-1.495675	4.869080	3.867060
41	6	0	-2.432111	4.136219	1.756947
42	6	0	-0.290859	3.286054	2.490890
43	6	0	-0.377565	4.060078	3.646920
44	6	0	-2.521699	4.902152	2.922498
45	1	0	-3.236671	4.171002	1.029531
46	1	0	0.574672	2.645499	2.340021
47	1	0	0.423681	4.024296	4.380307
48	1	0	-3.396927	5.524475	3.089240
49	1	0	-1.567970	5.465188	4.772764
50	6	0	0.054691	3.207069	-1.038787
51	6	0	1.865616	4.527838	-2.732212
52	6	0	0.307295	4.578186	-0.878461
53	6	0	0.727811	2.505396	-2.053184
54	6	0	1.623591	3.161691	-2.897767
55	6	0	1.208503	5.232577	-1.721816
56	1	0	-0.193145	5.135113	-0.091959
57	1	0	0.554089	1.439813	-2.179942
58	1	0	2.135431	2.596967	-3.671453
59	1	0	1.397478	6.294254	-1.585752
60	1	0	2.568280	5.039872	-3.384297
61	6	0	-1.486941	-1.499901	-0.161901

62	6	0	-2.423592	-2.155476	-0.613816
63	6	0	-3.537615	-2.889517	-1.109075
64	6	0	-5.742866	-4.350798	-2.082538
65	6	0	-3.770970	-3.008009	-2.496594
66	6	0	-4.436464	-3.519481	-0.220300
67	6	0	-5.524182	-4.240017	-0.706322
68	6	0	-4.860795	-3.731893	-2.972881
69	1	0	-3.087587	-2.524444	-3.188335
70	1	0	-4.262027	-3.437151	0.848140
71	1	0	-6.204528	-4.719926	-0.007334
72	1	0	-5.023678	-3.812868	-4.044634
73	1	0	-6.592588	-4.914796	-2.457727

Zero-point correction= 0.536412 (Hartree/Particle)
Thermal correction to Energy= 0.580270
Thermal correction to Enthalpy= 0.581214
Thermal correction to Gibbs Free Energy= 0.447709
Sum of electronic and zero-point Energies= -2753.076142
Sum of electronic and thermal Energies= -2753.032285
Sum of electronic and thermal Enthalpies= -2753.031341
Sum of electronic and thermal Free Energies= -2753.164845

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Imaginary frequency: -278.7204 cm^{-1}

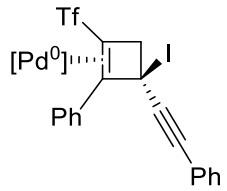
Zero-point correction= 0.532413 (Hartree/Particle)
Thermal correction to Energy= 0.574251
Thermal correction to Enthalpy= 0.575195
Thermal correction to Gibbs Free Energy= 0.453090
Sum of electronic and zero-point Energies= -2751.762049
Sum of electronic and thermal Energies= -2751.720211
Sum of electronic and thermal Enthalpies= -2751.719267
Sum of electronic and thermal Free Energies= -2751.841372

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Imaginary frequency: -273.8561 cm^{-1}

Zero-point correction= 0.527952 (Hartree/Particle)
Thermal correction to Energy= 0.570093
Thermal correction to Enthalpy= 0.571037
Thermal correction to Gibbs Free Energy= 0.449974
Sum of electronic and zero-point Energies= -2753.532397
Sum of electronic and thermal Energies= -2753.490256
Sum of electronic and thermal Enthalpies= -2753.489312
Sum of electronic and thermal Free Energies= -2753.610375

IIIa



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-2.023238	-0.340532	0.616691
2	6	0	-1.717526	-1.312279	-0.349657
3	6	0	-2.216577	-0.501919	-1.539856
4	1	0	-3.135790	-0.891779	-1.986531
5	1	0	-1.495308	-0.249564	-2.320407
6	6	0	-2.480961	0.623400	-0.472127
7	6	0	-2.207104	-0.313902	2.068318
8	6	0	-2.552745	-0.239377	4.856190
9	6	0	-2.473239	0.902180	2.723914
10	6	0	-2.120961	-1.495513	2.831540
11	6	0	-2.292189	-1.452972	4.212374
12	6	0	-2.643898	0.935458	4.106578
13	1	0	-2.546230	1.817450	2.145093
14	1	0	-1.923973	-2.439898	2.335192
15	1	0	-2.225926	-2.372060	4.788337
16	1	0	-2.852385	1.881872	4.598276
17	1	0	-2.687567	-0.211348	5.934096
18	6	0	-1.906243	1.924798	-0.625695
19	6	0	-1.416784	3.028511	-0.774101
20	53	0	-4.797376	0.920596	-0.332321
21	6	0	-0.831242	4.317346	-0.948854
22	6	0	0.323090	6.851630	-1.300760
23	6	0	-1.373095	5.226249	-1.879904
24	6	0	0.298379	4.697589	-0.196637
25	6	0	0.867849	5.955478	-0.377184
26	6	0	-0.798113	6.483174	-2.049402
27	1	0	-2.244437	4.935305	-2.458451
28	1	0	0.721816	4.000103	0.519123
29	1	0	1.742423	6.233117	0.204603
30	1	0	-1.225834	7.177175	-2.767827
31	1	0	0.770110	7.832615	-1.437404
32	8	0	-1.756902	-2.694693	-0.230353
33	16	0	-0.454240	-3.513694	-0.975955
34	8	0	0.306266	-4.262181	0.053057
35	6	0	-1.676777	-4.772873	-1.672787
36	9	0	-2.399914	-5.357820	-0.724671
37	9	0	-0.964277	-5.701392	-2.324480
38	9	0	-2.481116	-4.151780	-2.544145
39	46	0	0.193285	-0.381906	0.282412
40	15	0	2.531810	-0.181844	0.125793
41	6	0	3.067195	1.447889	0.819273
42	6	0	3.796077	3.901486	1.982965
43	6	0	4.007552	2.280335	0.195258
44	6	0	2.489709	1.865003	2.031353
45	6	0	2.856403	3.079180	2.612034
46	6	0	4.367076	3.500503	0.774198
47	1	0	4.458577	1.980790	-0.745658
48	1	0	1.747438	1.236485	2.518158
49	1	0	2.403851	3.385271	3.551412
50	1	0	5.095902	4.135892	0.277829
51	1	0	4.079791	4.849064	2.433288
52	6	0	3.603988	-1.393381	1.011610
53	6	0	5.173658	-3.316266	2.322251
54	6	0	4.864891	-1.051050	1.527837
55	6	0	3.134064	-2.706698	1.168879
56	6	0	3.919931	-3.662532	1.815541
57	6	0	5.643757	-2.008505	2.179436
58	1	0	5.236220	-0.035313	1.428839
59	1	0	2.153491	-2.986237	0.795246

60	1	0	3.542401	-4.674956	1.929240
61	1	0	6.615810	-1.730935	2.578767
62	1	0	5.780286	-4.059474	2.833080
63	6	0	3.176419	-0.159338	-1.604203
64	6	0	4.044134	-0.048274	-4.273996
65	6	0	4.401061	-0.731643	-1.978043
66	6	0	2.386915	0.461288	-2.587305
67	6	0	2.822360	0.524702	-3.910464
68	6	0	4.828927	-0.678034	-3.307203
69	1	0	5.020041	-1.224664	-1.235159
70	1	0	1.426998	0.889279	-2.307967
71	1	0	2.203481	1.012160	-4.659070
72	1	0	5.776979	-1.131212	-3.584784
73	1	0	4.378724	-0.009038	-5.307202

Zero-point correction=	0.538539 (Hartree/Particle)
Thermal correction to Energy=	0.582797
Thermal correction to Enthalpy=	0.583741
Thermal correction to Gibbs Free Energy=	0.448247
Sum of electronic and zero-point Energies=	-2753.145604
Sum of electronic and thermal Energies=	-2753.101347
Sum of electronic and thermal Enthalpies=	-2753.100402
Sum of electronic and thermal Free Energies=	-2753.235896

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.534962 (Hartree/Particle)
Thermal correction to Energy=	0.576953
Thermal correction to Enthalpy=	0.577897
Thermal correction to Gibbs Free Energy=	0.456025
Sum of electronic and zero-point Energies=	-2751.831556
Sum of electronic and thermal Energies=	-2751.789565
Sum of electronic and thermal Enthalpies=	-2751.788621
Sum of electronic and thermal Free Energies=	-2751.910493

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.530374 (Hartree/Particle)
Thermal correction to Energy=	0.573630
Thermal correction to Enthalpy=	0.574574
Thermal correction to Gibbs Free Energy=	0.450003
Sum of electronic and zero-point Energies=	-2753.601721
Sum of electronic and thermal Energies=	-2753.558464
Sum of electronic and thermal Enthalpies=	-2753.557520
Sum of electronic and thermal Free Energies=	-2753.682091

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

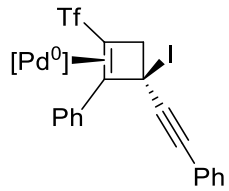
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.979440	0.807133	0.389714
2	6	0	-2.470327	-0.018517	-0.621098
3	6	0	-2.412128	1.018933	-1.717373
4	1	0	-3.391410	1.367488	-2.069787
5	1	0	-1.760028	0.812275	-2.574472
6	6	0	-1.789178	1.933962	-0.611876
7	6	0	-1.896045	0.800167	1.842548
8	6	0	-1.652651	0.770245	4.627085

9	6	0	-1.221633	1.833798	2.506279
10	6	0	-2.450399	-0.249801	2.590523
11	6	0	-2.324275	-0.261920	3.971945
12	6	0	-1.106711	1.818452	3.890825
13	1	0	-0.767428	2.638739	1.927987
14	1	0	-2.966792	-1.060291	2.077729
15	1	0	-2.753623	-1.082973	4.543082
16	1	0	-0.584983	2.629668	4.396682
17	1	0	-1.558104	0.756700	5.711449
18	6	0	-0.483149	2.492888	-0.799052
19	6	0	0.637390	2.942444	-0.933581
20	53	0	-3.233088	3.615363	-0.155176
21	6	0	1.989120	3.373614	-1.047039
22	6	0	4.670478	4.116342	-1.265045
23	6	0	2.445427	4.041832	-2.193346
24	6	0	2.891030	3.079639	-0.012044
25	6	0	4.223608	3.449846	-0.125787
26	6	0	3.780443	4.411256	-2.295859
27	1	0	1.742309	4.265273	-2.993817
28	1	0	2.528414	2.546628	0.867901
29	1	0	4.916469	3.209346	0.679213
30	1	0	4.129012	4.933381	-3.185186
31	1	0	5.716388	4.405696	-1.350804
32	8	0	-3.316523	-1.110836	-0.564608
33	16	0	-2.589829	-2.559516	-1.023461
34	8	0	-2.322845	-3.382578	0.171087
35	6	0	-4.276553	-3.174022	-1.558949
36	9	0	-5.147929	-3.125227	-0.571052
37	9	0	-4.119970	-4.434184	-1.944356
38	9	0	-4.711775	-2.457266	-2.583801
39	46	0	-0.341819	-0.580069	-0.239499
40	15	0	1.863746	-1.371826	0.051411
41	6	0	2.706522	-0.380493	1.349851
42	6	0	3.884544	1.125166	3.391386
43	6	0	4.071807	-0.080478	1.308915
44	6	0	1.935260	0.091699	2.417415
45	6	0	2.522097	0.839154	3.433598
46	6	0	4.657923	0.663228	2.328952
47	1	0	4.678375	-0.418400	0.467512
48	1	0	0.864242	-0.123372	2.445890
49	1	0	1.907343	1.200601	4.257038
50	1	0	5.723096	0.887876	2.290451
51	1	0	4.344315	1.711598	4.185228
52	6	0	2.114781	-3.102955	0.585296
53	6	0	2.403300	-5.779749	1.325550
54	6	0	3.312503	-3.553398	1.152924
55	6	0	1.058559	-4.000689	0.412069
56	6	0	1.204522	-5.335910	0.777748
57	6	0	3.456178	-4.886826	1.517682
58	1	0	4.134955	-2.856078	1.317624
59	1	0	0.107403	-3.643176	0.014797
60	1	0	0.373396	-6.025943	0.643745
61	1	0	4.390551	-5.231114	1.958084
62	1	0	2.516610	-6.823135	1.615498
63	6	0	2.973268	-1.143102	-1.388176
64	6	0	4.655294	-0.545517	-3.539426
65	6	0	3.886195	-2.092207	-1.850446
66	6	0	2.897568	0.100248	-2.026993
67	6	0	3.742623	0.405162	-3.085233
68	6	0	4.718710	-1.793306	-2.927550
69	1	0	3.952194	-3.068246	-1.370083

70	1	0	2.170244	0.835911	-1.678288
71	1	0	3.679955	1.385268	-3.557201
72	1	0	5.424395	-2.540927	-3.286578
73	1	0	5.313166	-0.314676	-4.375727

Zero-point correction=	0.537845	(Hartree/Particle)
Thermal correction to Energy=	0.581126	
Thermal correction to Enthalpy=	0.582070	
Thermal correction to Gibbs Free Energy=	0.455070	
Sum of electronic and zero-point Energies=	-2751.838842	
Sum of electronic and thermal Energies=	-2751.795562	
Sum of electronic and thermal Enthalpies=	-2751.794617	
Sum of electronic and thermal Free Energies=	-2751.921617	

IIIb



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.418468	-0.118692	-0.615874
2	6	0	0.752264	0.847957	0.190223
3	6	0	1.379891	0.381277	1.501255
4	1	0	0.709797	-0.013842	2.265452
5	1	0	2.079877	1.094183	1.954278
6	6	0	2.121383	-0.673908	0.607824
7	6	0	1.753569	-0.257998	-2.033618
8	6	0	2.410807	-0.545501	-4.757102
9	6	0	2.541987	-1.339328	-2.472979
10	6	0	1.298249	0.677890	-2.986754
11	6	0	1.628511	0.532172	-4.331473
12	6	0	2.864095	-1.478574	-3.821939
13	1	0	2.895050	-2.071894	-1.754661
14	1	0	0.693024	1.520433	-2.669302
15	1	0	1.275122	1.267134	-5.049685
16	1	0	3.470371	-2.321773	-4.142603
17	1	0	2.665467	-0.655490	-5.807741
18	6	0	3.551187	-0.632084	0.614696
19	6	0	4.764951	-0.562941	0.588922
20	53	0	1.513954	-2.864950	1.190222
21	6	0	6.187101	-0.484037	0.545227
22	6	0	8.987389	-0.330108	0.447857
23	6	0	6.941335	-0.432141	1.734645
24	6	0	6.858321	-0.457606	-0.694245
25	6	0	8.247754	-0.380706	-0.737073
26	6	0	8.330596	-0.356459	1.681247
27	1	0	6.425796	-0.455163	2.689738
28	1	0	6.276594	-0.497508	-1.610000
29	1	0	8.755766	-0.360390	-1.697296
30	1	0	8.903020	-0.318562	2.603984
31	1	0	10.071654	-0.270700	0.410191
32	8	0	0.337553	2.146997	-0.091377

33	16	0	1.580188	3.349178	-0.170256
34	8	0	1.446984	4.083303	-1.448461
35	6	0	0.648440	4.378992	1.108465
36	9	0	-0.607473	4.629252	0.737481
37	9	0	1.297954	5.537528	1.267801
38	9	0	0.649997	3.713371	2.270447
39	46	0	-0.781310	-0.527375	-0.392897
40	15	0	-3.088900	-0.378506	-0.013051
41	6	0	-4.083805	0.149804	-1.476411
42	6	0	-5.528852	0.867242	-3.776871
43	6	0	-5.243124	0.933804	-1.373414
44	6	0	-3.652240	-0.259555	-2.748424
45	6	0	-4.373463	0.090377	-3.889917
46	6	0	-5.959624	1.290152	-2.518210
47	1	0	-5.583599	1.274783	-0.400278
48	1	0	-2.740727	-0.845171	-2.842797
49	1	0	-4.026266	-0.233778	-4.867280
50	1	0	-6.852911	1.902184	-2.424681
51	1	0	-6.085768	1.148670	-4.666616
52	6	0	-3.876152	-1.963171	0.515301
53	6	0	-4.954540	-4.403491	1.393749
54	6	0	-5.188573	-2.325244	0.173642
55	6	0	-3.107365	-2.844937	1.293123
56	6	0	-3.646191	-4.053707	1.734765
57	6	0	-5.722518	-3.539311	0.610698
58	1	0	-5.792636	-1.663618	-0.439806
59	1	0	-2.081107	-2.585595	1.541651
60	1	0	-3.039098	-4.725999	2.334959
61	1	0	-6.738576	-3.810184	0.335719
62	1	0	-5.371349	-5.349272	1.729749
63	6	0	-3.564077	0.828143	1.301620
64	6	0	-4.196536	2.750622	3.249682
65	6	0	-4.572752	0.579389	2.244510
66	6	0	-2.870616	2.048849	1.351330
67	6	0	-3.189930	3.005088	2.314886
68	6	0	-4.884364	1.536729	3.213539
69	1	0	-5.112746	-0.362357	2.229615
70	1	0	-2.072600	2.245911	0.642195
71	1	0	-2.639518	3.941077	2.338454
72	1	0	-5.664520	1.329487	3.941433
73	1	0	-4.438955	3.492108	4.006427

Zero-point correction=	0.538075 (Hartree/Particle)
Thermal correction to Energy=	0.582321
Thermal correction to Enthalpy=	0.583265
Thermal correction to Gibbs Free Energy=	0.448169
Sum of electronic and zero-point Energies=	-2753.140946
Sum of electronic and thermal Energies=	-2753.096700
Sum of electronic and thermal Enthalpies=	-2753.095756
Sum of electronic and thermal Free Energies=	-2753.230852

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.533015 (Hartree/Particle)
Thermal correction to Energy=	0.573658
Thermal correction to Enthalpy=	0.574602
Thermal correction to Gibbs Free Energy=	0.456289
Sum of electronic and zero-point Energies=	-2751.826337
Sum of electronic and thermal Energies=	-2751.785693
Sum of electronic and thermal Enthalpies=	-2751.784749
Sum of electronic and thermal Free Energies=	-2751.903062

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.528657 (Hartree/Particle)
Thermal correction to Energy=	0.569583
Thermal correction to Enthalpy=	0.570527
Thermal correction to Gibbs Free Energy=	0.452972
Sum of electronic and zero-point Energies=	-2753.595799
Sum of electronic and thermal Energies=	-2753.554873
Sum of electronic and thermal Enthalpies=	-2753.553929
Sum of electronic and thermal Free Energies=	-2753.671484

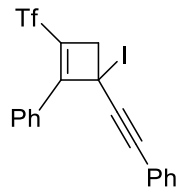
M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.416906	-0.137580	0.684362
2	6	0	-0.685411	0.791354	-0.091678
3	6	0	-1.191768	0.285373	-1.427189
4	1	0	-0.454602	-0.120577	-2.129119
5	1	0	-1.868351	0.971059	-1.959726
6	6	0	-1.999066	-0.743396	-0.573660
7	6	0	-1.896091	-0.192075	2.056497
8	6	0	-2.826395	-0.286978	4.699208
9	6	0	-2.832726	-1.159656	2.448575
10	6	0	-1.430946	0.728281	3.011848
11	6	0	-1.896270	0.678840	4.318126
12	6	0	-3.290732	-1.203779	3.760044
13	1	0	-3.205337	-1.877042	1.717951
14	1	0	-0.702389	1.484180	2.718480
15	1	0	-1.529682	1.401700	5.045034
16	1	0	-4.015883	-1.962759	4.049895
17	1	0	-3.187826	-0.323783	5.725364
18	6	0	-3.425758	-0.655023	-0.688953
19	6	0	-4.636418	-0.567742	-0.717313
20	53	0	-1.402141	-2.890783	-0.962960
21	6	0	-6.056825	-0.475058	-0.706869
22	6	0	-8.842780	-0.311997	-0.653406
23	6	0	-6.784878	-0.421922	-1.904141
24	6	0	-6.740593	-0.445130	0.518661
25	6	0	-8.125782	-0.363467	0.540232
26	6	0	-8.170220	-0.341204	-1.873167
27	1	0	-6.250183	-0.448138	-2.851978
28	1	0	-6.165026	-0.486212	1.442933
29	1	0	-8.650736	-0.340224	1.493480
30	1	0	-8.729978	-0.302347	-2.805874
31	1	0	-9.929211	-0.248766	-0.632577
32	8	0	-0.311182	2.096665	0.197952
33	16	0	-1.567661	3.225326	0.110201
34	8	0	-1.497317	4.074037	1.309614
35	6	0	-0.602220	4.181569	-1.173676
36	9	0	0.582249	4.532529	-0.708763
37	9	0	-1.291380	5.267142	-1.488651
38	9	0	-0.450025	3.427967	-2.255645
39	46	0	0.786000	-0.561965	0.632142
40	15	0	3.051550	-0.350243	0.080994
41	6	0	4.161452	0.359614	1.352277
42	6	0	5.828290	1.302099	3.385641
43	6	0	5.287681	1.126749	1.041058
44	6	0	3.873602	0.077934	2.691021

45	6	0	4.706583	0.541020	3.703567
46	6	0	6.116047	1.596577	2.055690
47	1	0	5.517559	1.357008	0.000113
48	1	0	2.982715	-0.504463	2.934789
49	1	0	4.474210	0.315817	4.743045
50	1	0	6.989734	2.196423	1.805822
51	1	0	6.477212	1.672909	4.177328
52	6	0	3.872506	-1.922874	-0.382040
53	6	0	5.004677	-4.335400	-1.224321
54	6	0	5.188425	-2.241712	-0.037641
55	6	0	3.126873	-2.828167	-1.145694
56	6	0	3.691715	-4.024717	-1.570663
57	6	0	5.749492	-3.445480	-0.456462
58	1	0	5.779702	-1.548095	0.560436
59	1	0	2.093894	-2.584687	-1.405005
60	1	0	3.102946	-4.719573	-2.167126
61	1	0	6.775047	-3.687348	-0.181777
62	1	0	5.446042	-5.275670	-1.550686
63	6	0	3.337992	0.711742	-1.387840
64	6	0	3.714286	2.426171	-3.564220
65	6	0	4.269405	0.397546	-2.381699
66	6	0	2.593686	1.892507	-1.496637
67	6	0	2.786240	2.746555	-2.576474
68	6	0	4.453873	1.251873	-3.465539
69	1	0	4.853790	-0.520132	-2.311487
70	1	0	1.859837	2.143143	-0.728256
71	1	0	2.199131	3.659834	-2.649286
72	1	0	5.179588	0.997039	-4.236284
73	1	0	3.858748	3.092003	-4.413467

Zero-point correction=	0.538675 (Hartree/Particle)
Thermal correction to Energy=	0.581756
Thermal correction to Enthalpy=	0.582700
Thermal correction to Gibbs Free Energy=	0.455069
Sum of electronic and zero-point Energies=	-2751.826361
Sum of electronic and thermal Energies=	-2751.783279
Sum of electronic and thermal Enthalpies=	-2751.782335
Sum of electronic and thermal Free Energies=	-2751.909966

III



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.423700	0.537307	-0.257376
2	6	0	1.341193	-0.405697	0.062380
3	6	0	0.547863	-1.105557	1.133864
4	1	0	0.919602	-1.019635	2.158953
5	1	0	0.251879	-2.140757	0.926422

6	6	0	-0.540846	-0.035860	0.747584
7	6	0	0.325304	1.634373	-1.206096
8	6	0	0.132692	3.752975	-3.040803
9	6	0	-0.845894	2.408519	-1.282863
10	6	0	1.400970	1.938216	-2.063767
11	6	0	1.301032	2.988040	-2.972163
12	6	0	-0.937758	3.459412	-2.193860
13	1	0	-1.679919	2.186561	-0.625305
14	1	0	2.310478	1.347414	-2.013953
15	1	0	2.137746	3.211857	-3.628400
16	1	0	-1.847731	4.051486	-2.239796
17	1	0	0.058902	4.573161	-3.749735
18	6	0	-1.827131	-0.490013	0.323202
19	6	0	-2.906790	-0.884624	-0.072621
20	53	0	-0.872838	1.401679	2.571619
21	6	0	-4.172310	-1.345549	-0.538527
22	6	0	-6.664128	-2.249175	-1.459133
23	6	0	-4.899792	-2.304113	0.195117
24	6	0	-4.713061	-0.846961	-1.740966
25	6	0	-5.949760	-1.298561	-2.193565
26	6	0	-6.136028	-2.749057	-0.265615
27	1	0	-4.485449	-2.687330	1.122395
28	1	0	-4.152902	-0.109251	-2.307055
29	1	0	-6.357957	-0.908293	-3.121742
30	1	0	-6.689565	-3.487396	0.307833
31	1	0	-7.629102	-2.598899	-1.815527
32	8	0	2.576563	-0.638424	-0.466249
33	16	0	3.424804	-1.993345	0.171101
34	8	0	3.282350	-3.159654	-0.723969
35	6	0	5.031632	-1.134679	-0.334567
36	9	0	5.050920	-0.832992	-1.627267
37	9	0	6.024256	-1.986270	-0.056962
38	9	0	5.179369	-0.030042	0.398994

Zero-point correction=	0.262729 (Hartree/Particle)
Thermal correction to Energy=	0.287116
Thermal correction to Enthalpy=	0.288060
Thermal correction to Gibbs Free Energy=	0.200101
Sum of electronic and zero-point Energies=	-1590.337463
Sum of electronic and thermal Energies=	-1590.313075
Sum of electronic and thermal Enthalpies=	-1590.312131
Sum of electronic and thermal Free Energies=	-1590.400091

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.261266 (Hartree/Particle)
Thermal correction to Energy=	0.285296
Thermal correction to Enthalpy=	0.286240
Thermal correction to Gibbs Free Energy=	0.203318
Sum of electronic and zero-point Energies=	-1589.583375
Sum of electronic and thermal Energies=	-1589.559346
Sum of electronic and thermal Enthalpies=	-1589.558401
Sum of electronic and thermal Free Energies=	-1589.641324

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.258899 (Hartree/Particle)
Thermal correction to Energy=	0.282561
Thermal correction to Enthalpy=	0.283505
Thermal correction to Gibbs Free Energy=	0.202930

```
Sum of electronic and zero-point Energies=          -1589.977836
Sum of electronic and thermal Energies=             -1589.954174
Sum of electronic and thermal Enthalpies=           -1589.953230
Sum of electronic and thermal Free Energies=        -1590.033805
```

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.412127	0.522869	-0.196513
2	6	0	1.372298	-0.352570	0.160859
3	6	0	0.625093	-1.024085	1.270660
4	1	0	1.011454	-0.884594	2.288695
5	1	0	0.370608	-2.081482	1.111237
6	6	0	-0.503389	-0.023540	0.859099
7	6	0	0.233129	1.539394	-1.210127
8	6	0	-0.111662	3.488915	-3.182773
9	6	0	-1.004034	2.176822	-1.366956
10	6	0	1.297404	1.891548	-2.053077
11	6	0	1.122746	2.859591	-3.031464
12	6	0	-1.172106	3.145429	-2.349156
13	1	0	-1.836672	1.904135	-0.718598
14	1	0	2.262132	1.399499	-1.932128
15	1	0	1.954985	3.127127	-3.680272
16	1	0	-2.137948	3.634496	-2.463973
17	1	0	-0.245776	4.248325	-3.951237
18	6	0	-1.768926	-0.553739	0.450117
19	6	0	-2.836756	-0.966711	0.046656
20	53	0	-0.869857	1.478566	2.526521
21	6	0	-4.085888	-1.418918	-0.464944
22	6	0	-6.536065	-2.271834	-1.495715
23	6	0	-4.837123	-2.391420	0.211039
24	6	0	-4.577030	-0.878765	-1.663862
25	6	0	-5.795476	-1.305266	-2.172521
26	6	0	-6.055191	-2.812331	-0.305226
27	1	0	-4.453951	-2.806175	1.141665
28	1	0	-3.988636	-0.123985	-2.183633
29	1	0	-6.170507	-0.882879	-3.102963
30	1	0	-6.633224	-3.567485	0.224147
31	1	0	-7.491210	-2.605669	-1.897224
32	8	0	2.594673	-0.584363	-0.380010
33	16	0	3.548268	-1.711270	0.455329
34	8	0	3.287763	-3.060858	-0.063324
35	6	0	5.012040	-1.100816	-0.539451
36	9	0	4.801038	-1.247991	-1.829684
37	9	0	6.044382	-1.843209	-0.170365
38	9	0	5.252608	0.165567	-0.253257

```
Zero-point correction=                           0.263087 (Hartree/Particle)
Thermal correction to Energy=                    0.286230
Thermal correction to Enthalpy=                  0.287174
Thermal correction to Gibbs Free Energy=         0.205132
Sum of electronic and zero-point Energies=          -1589.584507
Sum of electronic and thermal Energies=             -1589.561365
Sum of electronic and thermal Enthalpies=           -1589.560420
Sum of electronic and thermal Free Energies=        -1589.642462
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$TS_{III\text{-}IV}$

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Imaginary frequency: -86.6627 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.486460	0.281953	0.734794
2	6	0	-0.592891	1.014877	-0.132880
3	6	0	-1.345071	0.589854	-1.407114
4	1	0	-0.795056	0.025517	-2.160661
5	1	0	-1.917482	1.394781	-1.887322
6	6	0	-2.221449	-0.227774	-0.419483
7	6	0	-1.783078	0.257122	2.164671
8	6	0	-2.379411	0.198132	4.913745
9	6	0	-2.688356	-0.690221	2.682254
10	6	0	-1.175954	1.171456	3.050703
11	6	0	-1.478701	1.140792	4.409593
12	6	0	-2.978894	-0.716795	4.044663
13	1	0	-3.146929	-1.412044	2.014277
14	1	0	-0.476107	1.908895	2.671659
15	1	0	-1.009640	1.858690	5.077050
16	1	0	-3.673761	-1.458769	4.429125
17	1	0	-2.610902	0.176559	5.975186
18	6	0	-3.616849	-0.340653	-0.517211
19	6	0	-4.833474	-0.380737	-0.595321
20	53	0	-1.527244	-2.829009	-0.840046
21	6	0	-6.250192	-0.431366	-0.673458
22	6	0	-9.048890	-0.537710	-0.820016
23	6	0	-6.897667	-0.499685	-1.925205
24	6	0	-7.028474	-0.416768	0.503657
25	6	0	-8.416595	-0.469757	0.425173
26	6	0	-8.286588	-0.552870	-1.991891
27	1	0	-6.298827	-0.515515	-2.830340
28	1	0	-6.528946	-0.363410	1.465895
29	1	0	-9.008105	-0.458544	1.336325
30	1	0	-8.777122	-0.608139	-2.959632
31	1	0	-10.133073	-0.579542	-0.876970
32	8	0	0.022787	2.245443	0.058801
33	16	0	-1.012819	3.635202	0.060103
34	8	0	-0.690089	4.450754	1.251551
35	6	0	-0.019450	4.391908	-1.356675
36	9	0	1.275018	4.504751	-1.062660
37	9	0	-0.521359	5.604995	-1.612545
38	9	0	-0.167284	3.619830	-2.441561
39	46	0	0.608505	-0.631776	0.398854
40	15	0	2.896335	-0.584807	-0.022776
41	6	0	3.887626	0.259599	1.283471
42	6	0	5.338072	1.482562	3.353588
43	6	0	5.109999	0.896007	1.016012
44	6	0	3.396268	0.254726	2.598014
45	6	0	4.119891	0.856891	3.627701
46	6	0	5.829707	1.503459	2.046818
47	1	0	5.495668	0.926381	0.001185
48	1	0	2.435870	-0.210488	2.806997
49	1	0	3.726541	0.846637	4.640565
50	1	0	6.772595	1.997131	1.826674
51	1	0	5.897740	1.959928	4.153512
52	6	0	3.644376	-2.266840	-0.158341
53	6	0	4.664210	-4.869359	-0.422337

54	6	0	4.940127	-2.571122	0.287841
55	6	0	2.861711	-3.284786	-0.729370
56	6	0	3.373047	-4.576090	-0.865753
57	6	0	5.444638	-3.866128	0.156429
58	1	0	5.553894	-1.801172	0.744952
59	1	0	1.847384	-3.068551	-1.055947
60	1	0	2.755483	-5.353304	-1.307312
61	1	0	6.447609	-4.090717	0.509889
62	1	0	5.058444	-5.877414	-0.520009
63	6	0	3.399959	0.277014	-1.574546
64	6	0	4.068762	1.686399	-3.909654
65	6	0	4.233939	-0.304833	-2.539468
66	6	0	2.900566	1.571853	-1.794448
67	6	0	3.237865	2.272719	-2.950759
68	6	0	4.563468	0.398535	-3.701737
69	1	0	4.624991	-1.306068	-2.389376
70	1	0	2.245171	2.030446	-1.061376
71	1	0	2.840438	3.272366	-3.102325
72	1	0	5.207667	-0.065052	-4.444263
73	1	0	4.325517	2.229541	-4.815287

Zero-point correction= 0.537642 (Hartree/Particle)
Thermal correction to Energy= 0.581376
Thermal correction to Enthalpy= 0.582320
Thermal correction to Gibbs Free Energy= 0.449091
Sum of electronic and zero-point Energies= -2753.138475
Sum of electronic and thermal Energies= -2753.094741
Sum of electronic and thermal Enthalpies= -2753.093797
Sum of electronic and thermal Free Energies= -2753.227026

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Imaginary frequency: -143.1861 cm^{-1}

Zero-point correction= 0.534877 (Hartree/Particle)
Thermal correction to Energy= 0.577050
Thermal correction to Enthalpy= 0.577995
Thermal correction to Gibbs Free Energy= 0.455405
Sum of electronic and zero-point Energies= -2751.818465
Sum of electronic and thermal Energies= -2751.776291
Sum of electronic and thermal Enthalpies= -2751.775347
Sum of electronic and thermal Free Energies= -2751.897937

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Imaginary frequency: -157.6942 cm^{-1}

Zero-point correction= 0.529325 (Hartree/Particle)
Thermal correction to Energy= 0.571282
Thermal correction to Enthalpy= 0.572227
Thermal correction to Gibbs Free Energy= 0.451390
Sum of electronic and zero-point Energies= -2753.587955
Sum of electronic and thermal Energies= -2753.545998
Sum of electronic and thermal Enthalpies= -2753.545054
Sum of electronic and thermal Free Energies= -2753.665890

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

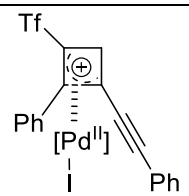
Imaginary frequency: -166.1870 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.489283	0.319089	0.682461
2	6	0	-0.488442	0.905085	-0.161256
3	6	0	-1.177572	0.445928	-1.445678
4	1	0	-0.613851	-0.191234	-2.134880
5	1	0	-1.679024	1.251411	-2.006084
6	6	0	-2.155940	-0.247137	-0.475187
7	6	0	-1.872014	0.432936	2.076982
8	6	0	-2.609577	0.661439	4.766028
9	6	0	-2.913279	-0.350619	2.595982
10	6	0	-1.198664	1.327680	2.925804
11	6	0	-1.571238	1.440164	4.257781
12	6	0	-3.275008	-0.234021	3.932141
13	1	0	-3.427593	-1.059537	1.947370
14	1	0	-0.388224	1.939591	2.528270
15	1	0	-1.048191	2.142468	4.904510
16	1	0	-4.080842	-0.851027	4.326449
17	1	0	-2.897923	0.751051	5.811826
18	6	0	-3.547025	-0.312776	-0.647226
19	6	0	-4.760843	-0.327016	-0.745106
20	53	0	-1.563619	-2.860218	-0.607473
21	6	0	-6.177783	-0.339366	-0.797770
22	6	0	-8.965803	-0.376444	-0.855773
23	6	0	-6.857846	-0.391009	-2.025059
24	6	0	-6.911594	-0.305217	0.399908
25	6	0	-8.297610	-0.325218	0.366501
26	6	0	-8.244792	-0.408451	-2.047849
27	1	0	-6.283970	-0.420042	-2.949318
28	1	0	-6.373623	-0.262882	1.346024
29	1	0	-8.862113	-0.300969	1.296546
30	1	0	-8.768541	-0.450115	-3.000910
31	1	0	-10.053791	-0.392163	-0.879567
32	8	0	0.205516	2.093542	-0.005535
33	16	0	-0.739161	3.498203	-0.104112
34	8	0	-0.401542	4.346668	1.048638
35	6	0	0.356472	4.136734	-1.479954
36	9	0	1.617744	4.186259	-1.105604
37	9	0	-0.058116	5.350817	-1.805543
38	9	0	0.230378	3.332341	-2.530760
39	46	0	0.546064	-0.770331	0.557731
40	15	0	2.806573	-0.651006	0.066444
41	6	0	3.694874	0.645532	1.002266
42	6	0	4.976590	2.613479	2.511932
43	6	0	4.899011	1.202919	0.557493
44	6	0	3.135939	1.091389	2.202176
45	6	0	3.776141	2.068506	2.957572
46	6	0	5.536804	2.181683	1.311742
47	1	0	5.334352	0.872621	-0.386953
48	1	0	2.181734	0.672786	2.530056
49	1	0	3.331103	2.413336	3.889215
50	1	0	6.471986	2.613281	0.958752
51	1	0	5.474313	3.385582	3.096264
52	6	0	3.754175	-2.192196	0.338322
53	6	0	5.081084	-4.629686	0.655833
54	6	0	5.056439	-2.224002	0.843302
55	6	0	3.119493	-3.393449	-0.000257
56	6	0	3.783709	-4.605398	0.150001
57	6	0	5.714161	-3.440266	1.004102

58	1	0	5.558670	-1.297124	1.119750
59	1	0	2.096466	-3.372737	-0.383185
60	1	0	3.282252	-5.533597	-0.118105
61	1	0	6.726641	-3.457338	1.404116
62	1	0	5.597090	-5.579741	0.784413
63	6	0	3.163819	-0.213734	-1.677072
64	6	0	3.602681	0.583507	-4.320361
65	6	0	3.974576	-0.979245	-2.516211
66	6	0	2.575713	0.955960	-2.173589
67	6	0	2.797374	1.355309	-3.484316
68	6	0	4.188476	-0.580347	-3.834716
69	1	0	4.442011	-1.890775	-2.144326
70	1	0	1.951596	1.565049	-1.519218
71	1	0	2.335622	2.270984	-3.850899
72	1	0	4.820083	-1.185649	-4.483058
73	1	0	3.773457	0.890502	-5.350835

Zero-point correction=	0.538138	(Hartree/Particle)
Thermal correction to Energy=	0.580928	
Thermal correction to Enthalpy=	0.581873	
Thermal correction to Gibbs Free Energy=	0.455165	
Sum of electronic and zero-point Energies=	-2751.820509	
Sum of electronic and thermal Energies=	-2751.777718	
Sum of electronic and thermal Enthalpies=	-2751.776774	
Sum of electronic and thermal Free Energies=	-2751.903482	

IV



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.007669	1.771823	0.182677
2	6	0	0.020443	1.701166	-0.838373
3	6	0	-1.039411	1.528928	-1.953709
4	1	0	-0.890124	0.753806	-2.711563
5	1	0	-1.325563	2.470376	-2.446566
6	6	0	-1.953399	1.223742	-0.741663
7	6	0	-1.061309	2.208205	1.573989
8	6	0	-1.176160	3.076122	4.239010
9	6	0	-2.231400	2.024629	2.333274
10	6	0	0.049586	2.838183	2.166784
11	6	0	-0.012090	3.267211	3.489748
12	6	0	-2.284302	2.455794	3.656147
13	1	0	-3.090468	1.539269	1.882098
14	1	0	0.948992	3.001046	1.584123
15	1	0	0.849287	3.755644	3.936938
16	1	0	-3.191879	2.306402	4.234414
17	1	0	-1.220411	3.412009	5.271498
18	6	0	-3.323979	0.961264	-0.707392
19	6	0	-4.520247	0.722492	-0.712376
20	6	0	-5.916818	0.461708	-0.721843

21	6	0	-8.678692	-0.042978	-0.744787
22	6	0	-6.614929	0.354088	-1.942990
23	6	0	-6.626736	0.309062	0.487491
24	6	0	-7.995510	0.058704	0.470471
25	6	0	-7.984009	0.104535	-1.948728
26	1	0	-6.070103	0.466392	-2.875100
27	1	0	-6.090597	0.381314	1.428476
28	1	0	-8.531544	-0.060169	1.408029
29	1	0	-8.511341	0.022727	-2.895182
30	1	0	-9.747299	-0.239184	-0.753565
31	8	0	1.227438	2.361113	-0.920066
32	16	0	1.105743	3.947071	-1.628253
33	8	0	0.228824	4.811959	-0.805155
34	6	0	2.875596	4.295511	-1.061330
35	9	0	3.054765	4.068225	0.239709
36	9	0	3.107887	5.589145	-1.314383
37	9	0	3.716887	3.549562	-1.777655
38	53	0	-1.881417	-2.557173	0.119167
39	46	0	-0.267560	-0.362360	-0.234088
40	15	0	1.805455	-1.468123	0.005836
41	6	0	3.324454	-0.501042	-0.410987
42	6	0	5.648789	0.987663	-0.937993
43	6	0	4.147152	-0.826890	-1.498083
44	6	0	3.670371	0.594476	0.397999
45	6	0	4.829028	1.324559	0.142707
46	6	0	5.300595	-0.082605	-1.760832
47	1	0	3.897974	-1.668157	-2.135993
48	1	0	3.038341	0.868189	1.238410
49	1	0	5.085264	2.165238	0.780993
50	1	0	5.930268	-0.350542	-2.605196
51	1	0	6.550679	1.560095	-1.137729
52	6	0	2.167529	-2.025727	1.728646
53	6	0	2.688034	-2.894792	4.349225
54	6	0	3.488365	-2.243391	2.160845
55	6	0	1.113143	-2.243553	2.628261
56	6	0	1.375459	-2.676540	3.929715
57	6	0	3.744376	-2.678208	3.461402
58	1	0	4.319612	-2.063824	1.486279
59	1	0	0.088695	-2.086911	2.307272
60	1	0	0.547488	-2.840559	4.613804
61	1	0	4.770077	-2.842609	3.780989
62	1	0	2.889222	-3.228742	5.363752
63	6	0	1.945975	-2.965707	-1.058048
64	6	0	2.166264	-5.164419	-2.787377
65	6	0	2.699114	-4.088416	-0.685438
66	6	0	1.295128	-2.962229	-2.300883
67	6	0	1.411841	-4.051616	-3.164079
68	6	0	2.805020	-5.182140	-1.546212
69	1	0	3.193524	-4.118080	0.280027
70	1	0	0.677680	-2.113702	-2.581370
71	1	0	0.897609	-4.037650	-4.121029
72	1	0	3.383263	-6.050593	-1.242215
73	1	0	2.246936	-6.019018	-3.453791

Zero-point correction=	0.538921 (Hartree/Particle)
Thermal correction to Energy=	0.583013
Thermal correction to Enthalpy=	0.583957
Thermal correction to Gibbs Free Energy=	0.450203
Sum of electronic and zero-point Energies=	-2753.173306
Sum of electronic and thermal Energies=	-2753.129214
Sum of electronic and thermal Enthalpies=	-2753.128270

```
 Sum of electronic and thermal Free Energies=        -2753.262024
```

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

```
 Zero-point correction=                           0.534501 (Hartree/Particle)
 Thermal correction to Energy=                    0.575787
 Thermal correction to Enthalpy=                  0.576731
 Thermal correction to Gibbs Free Energy=         0.457019
 Sum of electronic and zero-point Energies=          -2751.858640
 Sum of electronic and thermal Energies=             -2751.817354
 Sum of electronic and thermal Enthalpies=           -2751.816410
 Sum of electronic and thermal Free Energies=        -2751.936122
```

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

```
 Zero-point correction=                           0.529830 (Hartree/Particle)
 Thermal correction to Energy=                    0.572423
 Thermal correction to Enthalpy=                  0.573367
 Thermal correction to Gibbs Free Energy=         0.450642
 Sum of electronic and zero-point Energies=          -2753.628992
 Sum of electronic and thermal Energies=             -2753.586398
 Sum of electronic and thermal Enthalpies=           -2753.585454
 Sum of electronic and thermal Free Energies=        -2753.708179
```

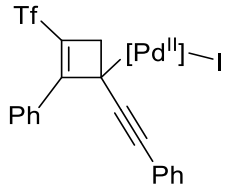
M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.908786	1.779224	0.115643
2	6	0	0.083987	1.780455	-0.927501
3	6	0	-0.987833	1.747349	-2.026341
4	1	0	-0.870317	1.032609	-2.850327
5	1	0	-1.254091	2.736530	-2.435999
6	6	0	-1.885577	1.355477	-0.836885
7	6	0	-0.891126	1.958709	1.556499
8	6	0	-0.817062	2.199152	4.331784
9	6	0	-2.001005	1.583268	2.324316
10	6	0	0.255515	2.457736	2.189254
11	6	0	0.287752	2.577752	3.571429
12	6	0	-1.959641	1.703439	3.706443
13	1	0	-2.883479	1.179087	1.827775
14	1	0	1.112965	2.756142	1.587001
15	1	0	1.179107	2.967436	4.059325
16	1	0	-2.821905	1.406460	4.300469
17	1	0	-0.787657	2.292129	5.416022
18	6	0	-3.264330	1.139462	-0.780258
19	6	0	-4.466479	0.947144	-0.738929
20	6	0	-5.870722	0.747766	-0.688430
21	6	0	-8.637467	0.377656	-0.588552
22	6	0	-6.624454	0.708932	-1.872396
23	6	0	-6.521777	0.594899	0.546483
24	6	0	-7.896195	0.411378	0.590662
25	6	0	-7.998483	0.525177	-1.817929
26	1	0	-6.116582	0.824278	-2.828208
27	1	0	-5.932490	0.616986	1.461818
28	1	0	-8.393037	0.291611	1.551706
29	1	0	-8.576077	0.496597	-2.740040
30	1	0	-9.715669	0.233725	-0.549160
31	8	0	1.321366	2.369096	-0.968200
32	16	0	1.259190	3.988921	-1.496909

33	8	0	0.479476	4.780341	-0.530961
34	6	0	3.039181	4.183784	-0.953265
35	9	0	3.220011	3.795640	0.296259
36	9	0	3.319703	5.473520	-1.052777
37	9	0	3.821735	3.494551	-1.763067
38	53	0	-1.916308	-2.448386	-0.011265
39	46	0	-0.299920	-0.292985	-0.452022
40	15	0	1.713622	-1.453592	-0.087439
41	6	0	3.301708	-0.699124	-0.606910
42	6	0	5.758439	0.473553	-1.247191
43	6	0	4.148003	-1.297811	-1.543310
44	6	0	3.691784	0.503554	-0.004577
45	6	0	4.918475	1.076429	-0.313276
46	6	0	5.367871	-0.708158	-1.865664
47	1	0	3.863575	-2.236440	-2.016687
48	1	0	3.038349	0.986750	0.724921
49	1	0	5.219272	2.002650	0.172351
50	1	0	6.019923	-1.185779	-2.595087
51	1	0	6.718029	0.926915	-1.489838
52	6	0	1.988621	-1.702010	1.703906
53	6	0	2.401009	-2.036187	4.444471
54	6	0	3.240420	-2.106221	2.186436
55	6	0	0.950855	-1.458859	2.607053
56	6	0	1.159220	-1.623979	3.973653
57	6	0	3.441893	-2.279434	3.550099
58	1	0	4.061965	-2.278003	1.489383
59	1	0	-0.025521	-1.146479	2.233508
60	1	0	0.345777	-1.423693	4.668601
61	1	0	4.415489	-2.599234	3.917619
62	1	0	2.562947	-2.165043	5.513511
63	6	0	1.743026	-3.104988	-0.865472
64	6	0	1.724022	-5.567562	-2.179257
65	6	0	2.104605	-4.266222	-0.182812
66	6	0	1.359841	-3.187710	-2.208543
67	6	0	1.361259	-4.410781	-2.865699
68	6	0	2.090239	-5.494009	-0.840072
69	1	0	2.387310	-4.219338	0.868112
70	1	0	1.045506	-2.285772	-2.737587
71	1	0	1.061556	-4.464503	-3.910663
72	1	0	2.363042	-6.397438	-0.297328
73	1	0	1.710742	-6.529586	-2.688640

Zero-point correction= 0.540039 (Hartree/Particle)
Thermal correction to Energy= 0.582931
Thermal correction to Enthalpy= 0.583875
Thermal correction to Gibbs Free Energy= 0.458427
Sum of electronic and zero-point Energies= -2751.860104
Sum of electronic and thermal Energies= -2751.817212
Sum of electronic and thermal Enthalpies= -2751.816268
Sum of electronic and thermal Free Energies= -2751.941716

IVa



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.691846	1.616044	0.442352
2	6	0	2.601527	1.320245	-0.521199
3	6	0	1.617962	1.114790	-1.648642
4	1	0	1.531166	0.091444	-2.029214
5	1	0	1.679991	1.822321	-2.484136
6	6	0	0.577648	1.482977	-0.544895
7	6	0	1.743524	1.962925	1.855568
8	6	0	1.835381	2.630803	4.586018
9	6	0	0.557806	2.101216	2.599853
10	6	0	2.978761	2.164479	2.503540
11	6	0	3.019805	2.495288	3.855299
12	6	0	0.606635	2.431791	3.953480
13	1	0	-0.399821	1.939657	2.114124
14	1	0	3.901515	2.067774	1.939441
15	1	0	3.979552	2.650898	4.340956
16	1	0	-0.318655	2.532163	4.514304
17	1	0	1.871423	2.889339	5.640798
18	6	0	-0.498874	2.361254	-0.726396
19	6	0	-1.680817	2.746544	-0.784790
20	6	0	-2.825067	3.600396	-0.882993
21	6	0	-5.009954	5.340395	-1.088516
22	6	0	-3.851586	3.341954	-1.810396
23	6	0	-2.912503	4.734369	-0.050247
24	6	0	-3.999366	5.597129	-0.157660
25	6	0	-4.932654	4.213465	-1.910724
26	1	0	-3.797417	2.453673	-2.429195
27	1	0	-2.121659	4.928358	0.667867
28	1	0	-4.058253	6.470728	0.485563
29	1	0	-5.722344	4.006421	-2.627232
30	1	0	-5.858682	6.014199	-1.168365
31	8	0	3.964483	1.269655	-0.458841
32	16	0	4.764183	0.837176	-1.917474
33	8	0	4.979302	2.029989	-2.763266
34	6	0	6.351280	0.649865	-0.901771
35	9	0	6.655685	1.765982	-0.251054
36	9	0	7.322478	0.360018	-1.774708
37	9	0	6.229395	-0.362740	-0.035800
38	53	0	-4.021687	-0.165424	-0.183578
39	46	0	-1.315800	0.349445	-0.284917
40	15	0	-0.622393	-1.849390	0.102268
41	6	0	-0.892278	-2.466051	1.820116
42	6	0	-1.370173	-3.403370	4.424500
43	6	0	-0.138488	-3.530877	2.346034
44	6	0	-1.883831	-1.875285	2.617526
45	6	0	-2.120080	-2.344703	3.911136
46	6	0	-0.378895	-3.996131	3.639060
47	1	0	0.644323	-3.991733	1.751847
48	1	0	-2.479088	-1.060698	2.218865
49	1	0	-2.893109	-1.877989	4.515272
50	1	0	0.211671	-4.819130	4.032751
51	1	0	-1.554058	-3.764668	5.432869
52	6	0	-1.452776	-3.056826	-1.015121
53	6	0	-2.625567	-4.849110	-2.827726
54	6	0	-1.684863	-4.389334	-0.645051
55	6	0	-1.827732	-2.628823	-2.297765
56	6	0	-2.401587	-3.522830	-3.201946

57	6	0	-2.271522	-5.278059	-1.547309
58	1	0	-1.422789	-4.735136	0.349615
59	1	0	-1.691135	-1.587915	-2.576239
60	1	0	-2.690836	-3.176752	-4.190348
61	1	0	-2.455921	-6.305586	-1.245397
62	1	0	-3.084591	-5.542742	-3.527086
63	6	0	1.173321	-2.197881	-0.171561
64	6	0	3.924536	-2.646262	-0.557702
65	6	0	1.633202	-2.887385	-1.305092
66	6	0	2.114457	-1.723839	0.759399
67	6	0	3.477121	-1.953634	0.570709
68	6	0	2.999513	-3.109075	-1.495181
69	1	0	0.925188	-3.265118	-2.035299
70	1	0	1.783217	-1.185688	1.642366
71	1	0	4.189536	-1.582107	1.300982
72	1	0	3.336536	-3.653829	-2.373188
73	1	0	4.986807	-2.824084	-0.701075

Zero-point correction=	0.539286	(Hartree/Particle)
Thermal correction to Energy=	0.583375	
Thermal correction to Enthalpy=	0.584319	
Thermal correction to Gibbs Free Energy=	0.451739	
Sum of electronic and zero-point Energies=	-2753.182808	
Sum of electronic and thermal Energies=	-2753.138719	
Sum of electronic and thermal Enthalpies=	-2753.137775	
Sum of electronic and thermal Free Energies=	-2753.270355	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.534183	(Hartree/Particle)
Thermal correction to Energy=	0.575874	
Thermal correction to Enthalpy=	0.576818	
Thermal correction to Gibbs Free Energy=	0.454315	
Sum of electronic and zero-point Energies=	-2751.872092	
Sum of electronic and thermal Energies=	-2751.830401	
Sum of electronic and thermal Enthalpies=	-2751.829457	
Sum of electronic and thermal Free Energies=	-2751.951960	

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.530416	(Hartree/Particle)
Thermal correction to Energy=	0.572921	
Thermal correction to Enthalpy=	0.573865	
Thermal correction to Gibbs Free Energy=	0.452289	
Sum of electronic and zero-point Energies=	-2753.642371	
Sum of electronic and thermal Energies=	-2753.599866	
Sum of electronic and thermal Enthalpies=	-2753.598921	
Sum of electronic and thermal Free Energies=	-2753.720498	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

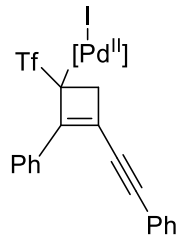
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.501442	-1.809021	0.420440
2	6	0	-2.426320	-1.591865	-0.545980
3	6	0	-1.462783	-1.456529	-1.689975
4	1	0	-1.394600	-0.455703	-2.144848
5	1	0	-1.526582	-2.216857	-2.479787

6	6	0	-0.419491	-1.720012	-0.581328
7	6	0	-1.517200	-1.967422	1.859689
8	6	0	-1.545477	-2.124366	4.652083
9	6	0	-0.317191	-1.974926	2.582212
10	6	0	-2.734356	-2.042815	2.554093
11	6	0	-2.743880	-2.122551	3.939707
12	6	0	-0.334285	-2.050549	3.970001
13	1	0	0.632334	-1.909583	2.048267
14	1	0	-3.671093	-2.036350	1.995835
15	1	0	-3.693021	-2.182602	4.469740
16	1	0	0.604771	-2.048525	4.521058
17	1	0	-1.557538	-2.182802	5.738890
18	6	0	0.757162	-2.459833	-0.708861
19	6	0	1.999371	-2.607619	-0.740762
20	6	0	3.265531	-3.269886	-0.816843
21	6	0	5.701532	-4.614596	-0.980383
22	6	0	4.254470	-2.827983	-1.706381
23	6	0	3.512029	-4.384477	-0.001475
24	6	0	4.726640	-5.050848	-0.086055
25	6	0	5.462678	-3.505412	-1.788338
26	1	0	4.065049	-1.944800	-2.313371
27	1	0	2.740325	-4.718878	0.690091
28	1	0	4.913847	-5.915259	0.548209
29	1	0	6.227296	-3.158243	-2.480484
30	1	0	6.653988	-5.137943	-1.044037
31	8	0	-3.777109	-1.552042	-0.491984
32	16	0	-4.508388	-0.794463	-1.829349
33	8	0	-4.566327	-1.746718	-2.948240
34	6	0	-6.160530	-1.033824	-0.971136
35	9	0	-6.432803	-2.317329	-0.883167
36	9	0	-7.056628	-0.437462	-1.745562
37	9	0	-6.185748	-0.481792	0.229391
38	53	0	3.892151	0.605149	-0.174462
39	46	0	1.346542	-0.396670	-0.326524
40	15	0	0.365535	1.688297	0.062959
41	6	0	0.620764	2.336617	1.752830
42	6	0	0.960924	3.263880	4.363550
43	6	0	-0.034107	3.498945	2.181325
44	6	0	1.434349	1.638790	2.647268
45	6	0	1.601829	2.101793	3.949572
46	6	0	0.142749	3.963887	3.478303
47	1	0	-0.691930	4.038225	1.498263
48	1	0	1.940253	0.732324	2.313513
49	1	0	2.236886	1.549635	4.639821
50	1	0	-0.365400	4.870396	3.802418
51	1	0	1.093491	3.626589	5.381517
52	6	0	1.024072	2.926077	-1.105399
53	6	0	2.045754	4.698096	-3.005175
54	6	0	1.561899	4.149051	-0.705660
55	6	0	1.019730	2.588018	-2.463743
56	6	0	1.516688	3.474462	-3.410172
57	6	0	2.073200	5.029551	-1.655107
58	1	0	1.602959	4.409861	0.350691
59	1	0	0.635522	1.614072	-2.775962
60	1	0	1.507133	3.203571	-4.464343
61	1	0	2.500531	5.977608	-1.333287
62	1	0	2.448158	5.388827	-3.744120
63	6	0	-1.457033	1.856651	-0.098477
64	6	0	-4.245551	2.104097	-0.178510
65	6	0	-2.076802	2.550719	-1.142524
66	6	0	-2.253194	1.269359	0.893052

67	6	0	-3.636844	1.393800	0.854937
68	6	0	-3.463390	2.676163	-1.177611
69	1	0	-1.476428	3.021153	-1.920184
70	1	0	-1.786668	0.733661	1.722119
71	1	0	-4.236639	0.936465	1.640462
72	1	0	-3.932157	3.235265	-1.985826
73	1	0	-5.329090	2.217563	-0.202046

Zero-point correction=	0.539589	(Hartree/Particle)
Thermal correction to Energy=	0.582383	
Thermal correction to Enthalpy=	0.583327	
Thermal correction to Gibbs Free Energy=	0.459582	
Sum of electronic and zero-point Energies=	-2751.874946	
Sum of electronic and thermal Energies=	-2751.832152	
Sum of electronic and thermal Enthalpies=	-2751.831208	
Sum of electronic and thermal Free Energies=	-2751.954954	

IVb



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.140450	0.656337	-1.435615
2	6	0	-1.139949	0.802425	-0.258259
3	1	0	-2.371341	1.575554	-1.976126
4	1	0	-1.899891	-0.141087	-2.143300
5	6	0	-3.126098	0.295494	-0.325019
6	6	0	-2.239806	0.531805	0.700692
7	6	0	-2.295884	0.487987	2.152523
8	6	0	-2.402744	0.422926	4.963952
9	6	0	-3.527313	0.348346	2.821984
10	6	0	-1.121280	0.596524	2.920473
11	6	0	-1.175328	0.561848	4.311832
12	6	0	-3.576799	0.315586	4.212646
13	1	0	-4.441479	0.267325	2.242410
14	1	0	-0.162859	0.689604	2.417208
15	1	0	-0.257169	0.639530	4.888021
16	1	0	-4.534961	0.206911	4.713989
17	1	0	-2.444652	0.396237	6.049496
18	46	0	0.688282	-0.097382	-0.205255
19	15	0	3.107821	-0.443397	-0.061718
20	6	0	3.904639	-1.424951	-1.396629
21	6	0	5.062500	-2.855224	-3.513010
22	6	0	5.130045	-2.086532	-1.219357
23	6	0	3.260370	-1.498137	-2.641007
24	6	0	3.840691	-2.204986	-3.695127
25	6	0	5.704565	-2.797388	-2.273748
26	1	0	5.631649	-2.053667	-0.256743
27	1	0	2.296146	-1.016947	-2.776092

28	1	0	3.329560	-2.258669	-4.652274
29	1	0	6.651097	-3.310309	-2.125071
30	1	0	5.509297	-3.413837	-4.331184
31	6	0	3.955306	1.199338	-0.120900
32	6	0	5.097316	3.769757	-0.165676
33	6	0	4.998535	1.499992	-1.007979
34	6	0	3.487907	2.208500	0.740813
35	6	0	4.058856	3.480352	0.724127
36	6	0	5.562517	2.778758	-1.030286
37	1	0	5.372346	0.737669	-1.683845
38	1	0	2.676555	1.995226	1.433401
39	1	0	3.691202	4.245819	1.402432
40	1	0	6.368509	2.996840	-1.725910
41	1	0	5.538308	4.762672	-0.184949
42	6	0	3.717602	-1.192207	1.508459
43	6	0	4.564595	-2.414347	3.888845
44	6	0	4.885453	-0.756537	2.154911
45	6	0	2.974445	-2.243623	2.070834
46	6	0	3.401245	-2.852024	3.251917
47	6	0	5.304775	-1.365698	3.339285
48	1	0	5.464575	0.062461	1.738970
49	1	0	2.063944	-2.582608	1.584116
50	1	0	2.817979	-3.664454	3.676624
51	1	0	6.209181	-1.018425	3.832054
52	1	0	4.891136	-2.885710	4.812086
53	53	0	-0.192623	-2.594041	-0.640497
54	8	0	-0.302598	1.974125	-0.014370
55	16	0	0.097767	3.193336	-1.158310
56	8	0	-0.190536	2.782803	-2.549989
57	6	0	-1.359288	4.302273	-0.645142
58	9	0	-1.274483	5.417930	-1.379834
59	9	0	-2.545741	3.731636	-0.845572
60	9	0	-1.220421	4.613043	0.645283
61	6	0	-4.444999	-0.159792	-0.408428
62	6	0	-5.597923	-0.541384	-0.533878
63	6	0	-6.937684	-0.993152	-0.676326
64	6	0	-9.586996	-1.881628	-0.964215
65	6	0	-7.526204	-1.091031	-1.955140
66	6	0	-7.701211	-1.350309	0.455231
67	6	0	-9.013428	-1.789736	0.307235
68	6	0	-8.839131	-1.531854	-2.092222
69	1	0	-6.940745	-0.819488	-2.827964
70	1	0	-7.250601	-1.281404	1.440469
71	1	0	-9.591004	-2.063171	1.186022
72	1	0	-9.281073	-1.603971	-3.082203
73	1	0	-10.611452	-2.225961	-1.075585

Zero-point correction= 0.538400 (Hartree/Particle)
Thermal correction to Energy= 0.582769
Thermal correction to Enthalpy= 0.583713
Thermal correction to Gibbs Free Energy= 0.447005
Sum of electronic and zero-point Energies= -2753.167631
Sum of electronic and thermal Energies= -2753.123262
Sum of electronic and thermal Enthalpies= -2753.122318
Sum of electronic and thermal Free Energies= -2753.259026

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction= 0.534992 (Hartree/Particle)
Thermal correction to Energy= 0.578848
Thermal correction to Enthalpy= 0.579792

```
Thermal correction to Gibbs Free Energy=         0.450479
Sum of electronic and zero-point Energies=          -2751.842966
Sum of electronic and thermal Energies=             -2751.799110
Sum of electronic and thermal Enthalpies=           -2751.798165
Sum of electronic and thermal Free Energies=        -2751.927478
```

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

```
Zero-point correction=                           0.530136 (Hartree/Particle)
Thermal correction to Energy=                    0.573541
Thermal correction to Enthalpy=                  0.574485
Thermal correction to Gibbs Free Energy=         0.448834
Sum of electronic and zero-point Energies=          -2753.613280
Sum of electronic and thermal Energies=             -2753.569875
Sum of electronic and thermal Enthalpies=           -2753.568931
Sum of electronic and thermal Free Energies=        -2753.694583
```

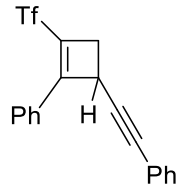
M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.183555	1.166185	-1.326538
2	6	0	-1.131633	1.005798	-0.216344
3	1	0	-2.448960	2.193698	-1.591289
4	1	0	-1.969848	0.593942	-2.237550
5	6	0	-3.100465	0.499367	-0.314394
6	6	0	-2.156692	0.441397	0.677570
7	6	0	-2.099418	-0.069564	2.030718
8	6	0	-1.978767	-1.100579	4.631852
9	6	0	-3.273877	-0.411925	2.715848
10	6	0	-0.865931	-0.246940	2.674489
11	6	0	-0.805673	-0.764094	3.961304
12	6	0	-3.210787	-0.921553	4.005094
13	1	0	-4.237688	-0.274196	2.225569
14	1	0	0.057068	0.002833	2.143815
15	1	0	0.162666	-0.909390	4.438329
16	1	0	-4.129598	-1.183864	4.527007
17	1	0	-1.933704	-1.505358	5.641451
18	46	0	0.655557	0.024306	-0.370859
19	15	0	2.976455	-0.530948	-0.065706
20	6	0	3.937266	-1.313403	-1.403051
21	6	0	5.396179	-2.346936	-3.543431
22	6	0	5.044843	-2.132203	-1.166990
23	6	0	3.559714	-1.024698	-2.718112
24	6	0	4.291581	-1.534520	-3.784636
25	6	0	5.769615	-2.648377	-2.236152
26	1	0	5.338852	-2.370614	-0.144623
27	1	0	2.679001	-0.407080	-2.901318
28	1	0	3.991409	-1.307028	-4.805790
29	1	0	6.628655	-3.289947	-2.047226
30	1	0	5.964053	-2.754412	-4.378185
31	6	0	3.887720	1.019386	0.294901
32	6	0	5.101910	3.464867	0.902133
33	6	0	5.067016	1.398915	-0.348171
34	6	0	3.321041	1.879494	1.245079
35	6	0	3.926825	3.091142	1.552269
36	6	0	5.668073	2.619403	-0.045911
37	1	0	5.518196	0.740704	-1.090591
38	1	0	2.399956	1.587193	1.756798

39	1	0	3.481024	3.747932	2.297595
40	1	0	6.585684	2.908030	-0.555922
41	1	0	5.574611	4.417491	1.134852
42	6	0	3.271076	-1.548593	1.425305
43	6	0	3.620782	-3.154759	3.683033
44	6	0	4.407924	-1.400165	2.227969
45	6	0	2.308284	-2.504409	1.767786
46	6	0	2.486117	-3.305872	2.891258
47	6	0	4.581426	-2.202056	3.350932
48	1	0	5.158157	-0.649380	1.975692
49	1	0	1.415921	-2.617238	1.149186
50	1	0	1.730397	-4.045228	3.150272
51	1	0	5.468184	-2.081086	3.970886
52	1	0	3.756583	-3.778631	4.564900
53	53	0	-0.328914	-2.141749	-1.591380
54	8	0	-0.312065	2.052066	0.308988
55	16	0	0.335711	3.280049	-0.679324
56	8	0	-0.033448	3.077846	-2.087825
57	6	0	-0.929329	4.515138	-0.033069
58	9	0	-0.778421	5.628868	-0.731092
59	9	0	-2.168559	4.079542	-0.157897
60	9	0	-0.664113	4.746363	1.241571
61	6	0	-4.424563	0.065558	-0.416552
62	6	0	-5.589118	-0.282307	-0.508384
63	6	0	-6.944608	-0.696191	-0.584329
64	6	0	-9.617386	-1.499103	-0.714912
65	6	0	-7.671224	-0.552908	-1.777666
66	6	0	-7.576143	-1.249400	0.542007
67	6	0	-8.903508	-1.645903	0.472924
68	6	0	-8.998372	-0.953462	-1.837549
69	1	0	-7.179127	-0.125231	-2.649259
70	1	0	-7.008810	-1.361657	1.464687
71	1	0	-9.385452	-2.073944	1.350041
72	1	0	-9.554027	-0.840280	-2.766570
73	1	0	-10.658754	-1.811803	-0.765545

Zero-point correction=	0.537403 (Hartree/Particle)
Thermal correction to Energy=	0.580261
Thermal correction to Enthalpy=	0.581205
Thermal correction to Gibbs Free Energy=	0.452540
Sum of electronic and zero-point Energies=	-2751.846380
Sum of electronic and thermal Energies=	-2751.803522
Sum of electronic and thermal Enthalpies=	-2751.802577
Sum of electronic and thermal Free Energies=	-2751.931242

3ba



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.476801	-1.718467	-0.378236

2	6	0	-0.424311	-0.572297	-0.996924
3	1	0	-0.271921	-0.475038	-2.080196
4	1	0	-0.060565	-2.409165	0.278616
5	1	0	1.058470	-2.288048	-1.108513
6	6	0	1.185424	-0.580092	0.302240
7	6	0	0.433530	0.424356	-0.188241
8	6	0	0.381090	1.873985	-0.079878
9	6	0	0.274790	4.680203	0.086932
10	6	0	1.376928	2.590222	0.614304
11	6	0	-0.665720	2.590115	-0.688227
12	6	0	-0.716742	3.980594	-0.603567
13	6	0	1.321040	3.978645	0.694275
14	1	0	2.196493	2.050738	1.077944
15	1	0	-1.446659	2.049298	-1.214375
16	1	0	-1.534214	4.518101	-1.076716
17	1	0	2.097545	4.517501	1.230910
18	1	0	0.234176	5.764142	0.152103
19	6	0	-1.847313	-0.644179	-0.693460
20	6	0	-3.032399	-0.704784	-0.437715
21	8	0	2.207109	-0.544024	1.234401
22	16	0	3.531987	-1.594712	1.117960
23	8	0	3.131511	-2.943847	0.656447
24	6	0	4.268367	-0.771313	-0.428513
25	9	0	5.486686	-1.295809	-0.608612
26	9	0	3.528228	-0.996585	-1.514386
27	9	0	4.383444	0.543764	-0.224710
28	6	0	-4.426196	-0.781169	-0.131023
29	6	0	-5.344888	-1.263432	-1.083947
30	6	0	-4.904572	-0.376940	1.130982
31	6	0	-6.702017	-1.338400	-0.779455
32	1	0	-4.980873	-1.576936	-2.057633
33	6	0	-6.263273	-0.455195	1.427414
34	1	0	-4.200060	-0.004008	1.868059
35	6	0	-7.166269	-0.935467	0.475354
36	1	0	-7.399713	-1.713067	-1.523658
37	1	0	-6.618734	-0.140283	2.404879
38	1	0	-8.225538	-0.995505	0.709916

Zero-point correction=	0.273758	(Hartree/Particle)
Thermal correction to Energy=	0.296080	
Thermal correction to Enthalpy=	0.297024	
Thermal correction to Gibbs Free Energy=	0.216048	
Sum of electronic and zero-point Energies=	-1579.544676	
Sum of electronic and thermal Energies=	-1579.522354	
Sum of electronic and thermal Enthalpies=	-1579.521410	
Sum of electronic and thermal Free Energies=	-1579.602385	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.272476	(Hartree/Particle)
Thermal correction to Energy=	0.293658	
Thermal correction to Enthalpy=	0.294603	
Thermal correction to Gibbs Free Energy=	0.220169	
Sum of electronic and zero-point Energies=	-1578.812587	
Sum of electronic and thermal Energies=	-1578.791405	
Sum of electronic and thermal Enthalpies=	-1578.790461	
Sum of electronic and thermal Free Energies=	-1578.864895	

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

```
Zero-point correction=                           0.269793 (Hartree/Particle)
Thermal correction to Energy=                    0.291573
Thermal correction to Enthalpy=                  0.292517
Thermal correction to Gibbs Free Energy=         0.217003
Sum of electronic and zero-point Energies=          -1579.175258
Sum of electronic and thermal Energies=             -1579.153478
Sum of electronic and thermal Enthalpies=           -1579.152534
Sum of electronic and thermal Free Energies=        -1579.228049
```

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.496966	-1.919144	-0.107322
2	6	0	-0.346417	-0.805631	-0.823673
3	1	0	-0.140166	-0.776833	-1.905291
4	1	0	-0.085368	-2.542251	0.583018
5	1	0	1.081086	-2.563148	-0.775000
6	6	0	1.212348	-0.761527	0.510269
7	6	0	0.485551	0.218157	-0.050902
8	6	0	0.427887	1.663463	-0.027398
9	6	0	0.302298	4.457764	-0.028279
10	6	0	1.289534	2.413176	0.787445
11	6	0	-0.498432	2.333541	-0.836550
12	6	0	-0.558384	3.721462	-0.837429
13	6	0	1.224559	3.799017	0.784146
14	1	0	2.010858	1.894849	1.418293
15	1	0	-1.178514	1.753488	-1.460320
16	1	0	-1.282336	4.230763	-1.471167
17	1	0	1.896859	4.373118	1.419719
18	1	0	0.254461	5.545284	-0.027901
19	6	0	-1.776521	-0.807338	-0.574306
20	6	0	-2.970290	-0.777186	-0.361576
21	8	0	2.252667	-0.694796	1.410440
22	16	0	3.679935	-1.489875	1.060668
23	8	0	3.421556	-2.852795	0.566211
24	6	0	4.025519	-0.533781	-0.527715
25	9	0	5.293670	-0.775145	-0.834032
26	9	0	3.255367	-0.948810	-1.516344
27	9	0	3.857636	0.763545	-0.340081
28	6	0	-4.374572	-0.744498	-0.108368
29	6	0	-5.263974	-1.445787	-0.936121
30	6	0	-4.884020	-0.007763	0.971260
31	6	0	-6.629254	-1.410153	-0.686142
32	1	0	-4.868366	-2.017166	-1.774146
33	6	0	-6.250563	0.023081	1.215080
34	1	0	-4.193424	0.538806	1.611193
35	6	0	-7.126450	-0.677166	0.388820
36	1	0	-7.310244	-1.959422	-1.334031
37	1	0	-6.635012	0.598057	2.055773
38	1	0	-8.197347	-0.651234	0.582647

```
Zero-point correction=                           0.274927 (Hartree/Particle)
Thermal correction to Energy=                    0.296562
Thermal correction to Enthalpy=                  0.297506
Thermal correction to Gibbs Free Energy=         0.221008
Sum of electronic and zero-point Energies=          -1578.813039
Sum of electronic and thermal Energies=             -1578.791403
Sum of electronic and thermal Enthalpies=           -1578.790459
Sum of electronic and thermal Free Energies=        -1578.866957
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$[Pd^{II}]I^{+}$

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.663672	-0.311868	0.143258
2	46	0	-0.581147	1.409702	-0.500323
3	53	0	-2.958228	0.375340	-0.478556
4	6	0	0.383635	-1.029176	1.767210
5	6	0	0.014045	-2.128300	4.302404
6	6	0	-0.256451	-0.277033	2.770924
7	6	0	0.819969	-2.341077	2.031752
8	6	0	0.636904	-2.880718	3.303636
9	6	0	-0.432684	-0.829338	4.036130
10	1	0	-0.633236	0.718371	2.554654
11	1	0	1.296625	-2.932067	1.256702
12	1	0	0.975106	-3.891071	3.511317
13	1	0	-0.931573	-0.253892	4.809568
14	1	0	-0.134235	-2.557747	5.288660
15	6	0	1.882143	1.032611	0.147366
16	6	0	3.422913	3.369078	0.063287
17	6	0	2.422753	1.566061	1.338961
18	6	0	2.117160	1.692842	-1.090982
19	6	0	2.882898	2.863343	-1.118244
20	6	0	3.200588	2.715530	1.285685
21	1	0	2.240929	1.071279	2.287376
22	1	0	1.768253	1.255781	-2.023339
23	1	0	3.067291	3.361614	-2.064775
24	1	0	3.637077	3.111305	2.197542
25	1	0	4.026359	4.271385	0.038348
26	6	0	1.048108	-1.560741	-1.096248
27	6	0	1.641723	-3.559464	-2.947233
28	6	0	2.385473	-1.791354	-1.472880
29	6	0	0.009082	-2.328638	-1.653779
30	6	0	0.313748	-3.326604	-2.576439
31	6	0	2.673706	-2.795127	-2.396284
32	1	0	3.191912	-1.202726	-1.046674
33	1	0	-1.024678	-2.134804	-1.383205
34	1	0	-0.486747	-3.915937	-3.012470
35	1	0	3.704049	-2.978422	-2.685156
36	1	0	1.872355	-4.335698	-3.670673

Zero-point correction= 0.277100 (Hartree/Particle)
Thermal correction to Energy= 0.297289
Thermal correction to Enthalpy= 0.298233
Thermal correction to Gibbs Free Energy= 0.222753
Sum of electronic and zero-point Energies= -1173.976398
Sum of electronic and thermal Energies= -1173.956209
Sum of electronic and thermal Enthalpies= -1173.955264
Sum of electronic and thermal Free Energies= -1174.030745

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction= 0.275018 (Hartree/Particle)
Thermal correction to Energy= 0.295070

Thermal correction to Enthalpy=	0.296014
Thermal correction to Gibbs Free Energy=	0.222768
Sum of electronic and zero-point Energies=	-1173.406127
Sum of electronic and thermal Energies=	-1173.386075
Sum of electronic and thermal Enthalpies=	-1173.385130
Sum of electronic and thermal Free Energies=	-1173.458377

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.272190	(Hartree/Particle)
Thermal correction to Energy=	0.291363	
Thermal correction to Enthalpy=	0.292307	
Thermal correction to Gibbs Free Energy=	0.221511	
Sum of electronic and zero-point Energies=	-1174.816824	
Sum of electronic and thermal Energies=	-1174.797652	
Sum of electronic and thermal Enthalpies=	-1174.796708	
Sum of electronic and thermal Free Energies=	-1174.867503	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.500938	0.436373	0.241017
2	46	0	0.005920	-1.451504	-0.801996
3	53	0	2.573964	-0.979767	-0.857135
4	6	0	0.204148	0.773137	1.845914
5	6	0	1.216399	1.293610	4.371662
6	6	0	0.653733	-0.287247	2.645553
7	6	0	0.278557	2.095659	2.301761
8	6	0	0.783979	2.347218	3.571463
9	6	0	1.152478	-0.021520	3.911292
10	1	0	0.628007	-1.308734	2.264862
11	1	0	-0.054300	2.920551	1.673738
12	1	0	0.844143	3.370475	3.934265
13	1	0	1.505343	-0.838538	4.535898
14	1	0	1.618377	1.497458	5.361795
15	6	0	-2.045694	-0.488007	0.313462
16	6	0	-4.144138	-2.320017	0.249235
17	6	0	-2.534216	-1.037569	1.513519
18	6	0	-2.613606	-0.878194	-0.926600
19	6	0	-3.659686	-1.800253	-0.943974
20	6	0	-3.589867	-1.931056	1.473750
21	1	0	-2.093383	-0.746217	2.465578
22	1	0	-2.291995	-0.406251	-1.856466
23	1	0	-4.102662	-2.092757	-1.892813
24	1	0	-3.987806	-2.335482	2.401545
25	1	0	-4.968346	-3.029520	0.234053
26	6	0	-0.639982	1.911891	-0.759444
27	6	0	-0.838791	4.259147	-2.220096
28	6	0	-1.893872	2.512234	-0.939094
29	6	0	0.514382	2.485360	-1.309524
30	6	0	0.407172	3.661079	-2.038355
31	6	0	-1.984584	3.689544	-1.670781
32	1	0	-2.788724	2.071192	-0.502558
33	1	0	1.485796	2.007951	-1.175267
34	1	0	1.298257	4.108967	-2.471743
35	1	0	-2.953488	4.163414	-1.810328
36	1	0	-0.916022	5.178620	-2.796338

Zero-point correction=	0.276145 (Hartree/Particle)
Thermal correction to Energy=	0.296138
Thermal correction to Enthalpy=	0.297082
Thermal correction to Gibbs Free Energy=	0.223567
Sum of electronic and zero-point Energies=	-1173.407134
Sum of electronic and thermal Energies=	-1173.387141
Sum of electronic and thermal Enthalpies=	-1173.386197
Sum of electronic and thermal Free Energies=	-1173.459712

V = $Et_3N[Pd^{II}]I^+$

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.034291	0.142209	-0.100504
2	7	0	-3.267269	0.408418	-0.281792
3	6	0	-3.664478	0.028582	-1.681897
4	1	0	-3.583752	-1.059221	-1.744951
5	1	0	-4.723768	0.289727	-1.821790
6	6	0	-2.814533	0.653389	-2.784967
7	1	0	-3.173961	0.292988	-3.754683
8	1	0	-1.762941	0.355317	-2.692243
9	1	0	-2.866576	1.746727	-2.806350
10	6	0	-3.624600	1.848112	-0.024918
11	1	0	-3.651721	2.362651	-0.987306
12	1	0	-4.645417	1.880545	0.377265
13	6	0	-2.666402	2.601351	0.896566
14	1	0	-2.574337	2.143451	1.883593
15	1	0	-3.034684	3.624215	1.036335
16	1	0	-1.665621	2.687621	0.454194
17	6	0	-4.027322	-0.492471	0.650729
18	1	0	-3.773939	-1.516189	0.370428
19	1	0	-5.099937	-0.349814	0.450843
20	6	0	-3.750156	-0.296356	2.136738
21	1	0	-4.275296	-1.080052	2.692598
22	1	0	-4.107936	0.665622	2.514671
23	1	0	-2.681624	-0.391779	2.361015
24	15	0	1.248935	0.224956	0.059805
25	6	0	2.246676	-0.024016	-1.443946
26	6	0	3.851109	-0.435022	-3.701183
27	6	0	1.938855	-1.051099	-2.350719
28	6	0	3.365295	0.800128	-1.678425
29	6	0	4.162370	0.588771	-2.802322
30	6	0	2.741832	-1.251505	-3.474030
31	1	0	1.079925	-1.690564	-2.180172
32	1	0	3.613740	1.602026	-0.989955
33	1	0	5.024581	1.225691	-2.976050
34	1	0	2.496333	-2.046350	-4.171807
35	1	0	4.472167	-0.593565	-4.577857
36	6	0	1.190413	2.026734	0.356881
37	6	0	0.911426	4.786037	0.761983
38	6	0	1.312545	2.569574	1.651000
39	6	0	0.912194	2.884294	-0.731730
40	6	0	0.779654	4.256717	-0.524810
41	6	0	1.178142	3.942258	1.845896
42	1	0	1.531936	1.922936	2.494440
43	1	0	0.833132	2.482193	-1.737537

44	1	0	0.582202	4.912198	-1.367732
45	1	0	1.290908	4.356910	2.843114
46	1	0	0.813495	5.855956	0.920393
47	6	0	2.049844	-0.592541	1.472205
48	6	0	3.266780	-1.787303	3.687734
49	6	0	1.309125	-0.827531	2.643522
50	6	0	3.399607	-0.974799	1.411866
51	6	0	4.001707	-1.569513	2.521000
52	6	0	1.920618	-1.416108	3.748469
53	1	0	0.254876	-0.569060	2.683135
54	1	0	3.976874	-0.818284	0.506814
55	1	0	5.044583	-1.867278	2.469033
56	1	0	1.343631	-1.598609	4.650002
57	1	0	3.738841	-2.255102	4.546581
58	53	0	-0.994447	-2.508527	-0.212476

Zero-point correction=	0.487319 (Hartree/Particle)
Thermal correction to Energy=	0.518044
Thermal correction to Enthalpy=	0.518988
Thermal correction to Gibbs Free Energy=	0.421124
Sum of electronic and zero-point Energies=	-1466.224427
Sum of electronic and thermal Energies=	-1466.193702
Sum of electronic and thermal Enthalpies=	-1466.192758
Sum of electronic and thermal Free Energies=	-1466.290622

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.482247 (Hartree/Particle)
Thermal correction to Energy=	0.512264
Thermal correction to Enthalpy=	0.513208
Thermal correction to Gibbs Free Energy=	0.419644
Sum of electronic and zero-point Energies=	-1465.423889
Sum of electronic and thermal Energies=	-1465.393872
Sum of electronic and thermal Enthalpies=	-1465.392927
Sum of electronic and thermal Free Energies=	-1465.486492

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.477401 (Hartree/Particle)
Thermal correction to Energy=	0.507273
Thermal correction to Enthalpy=	0.508217
Thermal correction to Gibbs Free Energy=	0.415465
Sum of electronic and zero-point Energies=	-1466.929557
Sum of electronic and thermal Energies=	-1466.899685
Sum of electronic and thermal Enthalpies=	-1466.898741
Sum of electronic and thermal Free Energies=	-1466.991493

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.020260	0.087490	0.068766
2	7	0	3.253355	0.260855	0.286756
3	6	0	3.508215	0.312681	1.750558
4	1	0	3.348147	-0.699559	2.143761
5	1	0	4.571684	0.561021	1.913419
6	6	0	2.609410	1.288664	2.483717
7	1	0	2.898308	1.339487	3.539921
8	1	0	1.555525	0.966039	2.446920

9	1	0	2.668265	2.307311	2.075887
10	6	0	3.727094	1.520270	-0.368360
11	1	0	3.995492	2.239485	0.415313
12	1	0	4.659091	1.301287	-0.908674
13	6	0	2.708362	2.149499	-1.294985
14	1	0	2.339411	1.442002	-2.051065
15	1	0	3.151818	2.999923	-1.828183
16	1	0	1.849282	2.544624	-0.731242
17	6	0	3.969317	-0.908658	-0.285362
18	1	0	3.650400	-1.791461	0.282183
19	1	0	5.049994	-0.771181	-0.101487
20	6	0	3.707407	-1.132466	-1.757890
21	1	0	4.225077	-2.042500	-2.081958
22	1	0	4.069525	-0.309520	-2.386524
23	1	0	2.634012	-1.274052	-1.951186
24	15	0	-1.224050	0.260898	-0.121750
25	6	0	-2.234044	0.299333	1.374863
26	6	0	-3.830362	0.410417	3.650150
27	6	0	-1.875949	-0.425969	2.514105
28	6	0	-3.389754	1.095892	1.382525
29	6	0	-4.186293	1.141661	2.518303
30	6	0	-2.677590	-0.367637	3.649342
31	1	0	-0.975144	-1.038057	2.511303
32	1	0	-3.664534	1.680798	0.504030
33	1	0	-5.085042	1.754618	2.522489
34	1	0	-2.397732	-0.933699	4.535029
35	1	0	-4.455600	0.451876	4.539661
36	6	0	-0.988813	1.985729	-0.624812
37	6	0	-0.357850	4.610317	-1.308495
38	6	0	-1.008088	2.383453	-1.969905
39	6	0	-0.638377	2.912939	0.376206
40	6	0	-0.328963	4.221575	0.029343
41	6	0	-0.699762	3.694615	-2.304016
42	1	0	-1.285154	1.671770	-2.746652
43	1	0	-0.632419	2.607888	1.423662
44	1	0	-0.071710	4.940917	0.803509
45	1	0	-0.731915	4.008531	-3.344882
46	1	0	-0.119109	5.637067	-1.577917
47	6	0	-2.034750	-0.671139	-1.433182
48	6	0	-3.234028	-2.098989	-3.495041
49	6	0	-1.298346	-0.996093	-2.580914
50	6	0	-3.364780	-1.082564	-1.312678
51	6	0	-3.960097	-1.795050	-2.348079
52	6	0	-1.903504	-1.700463	-3.611847
53	1	0	-0.245885	-0.713855	-2.656198
54	1	0	-3.933986	-0.855397	-0.412569
55	1	0	-4.994382	-2.118136	-2.253856
56	1	0	-1.332350	-1.953918	-4.502188
57	1	0	-3.703760	-2.659040	-4.300895
58	53	0	0.722779	-2.493328	0.577978

Zero-point correction= 0.484810 (Hartree/Particle)
Thermal correction to Energy= 0.514889
Thermal correction to Enthalpy= 0.515834
Thermal correction to Gibbs Free Energy= 0.421252
Sum of electronic and zero-point Energies= -1465.425078
Sum of electronic and thermal Energies= -1465.394998
Sum of electronic and thermal Enthalpies= -1465.394054
Sum of electronic and thermal Free Energies= -1465.488635

[Pd^{II}]HI

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.918853	-0.006109	-0.050756
2	46	0	-1.395255	0.009284	-0.061752
3	53	0	-4.030919	-0.004712	-0.119992
4	6	0	1.743981	1.316237	-1.023222
5	6	0	2.973048	3.291864	-2.589161
6	6	0	1.154882	1.738095	-2.225527
7	6	0	2.949549	1.904490	-0.606434
8	6	0	3.559231	2.886996	-1.388043
9	6	0	1.770790	2.716790	-3.006086
10	1	0	0.208279	1.309273	-2.541506
11	1	0	3.406117	1.604442	0.332162
12	1	0	4.489703	3.338911	-1.055301
13	1	0	1.304177	3.037000	-3.933346
14	1	0	3.447245	4.060112	-3.193737
15	6	0	1.701428	-1.581725	-0.578593
16	6	0	2.823931	-4.041043	-1.320751
17	6	0	3.033741	-1.649243	-1.016350
18	6	0	0.934848	-2.756497	-0.526540
19	6	0	1.496921	-3.980771	-0.891322
20	6	0	3.589911	-2.874455	-1.385366
21	1	0	3.633462	-0.746430	-1.080424
22	1	0	-0.104535	-2.705634	-0.212665
23	1	0	0.893823	-4.883302	-0.849263
24	1	0	4.620187	-2.916449	-1.728054
25	1	0	3.258751	-4.993143	-1.612520
26	6	0	1.461239	0.272300	1.684738
27	6	0	2.116262	0.748026	4.371164
28	6	0	2.275152	-0.629458	2.385341
29	6	0	0.971352	1.412678	2.347835
30	6	0	1.301836	1.649899	3.680920
31	6	0	2.600062	-0.388853	3.722355
32	1	0	2.653934	-1.518203	1.891049
33	1	0	0.334489	2.118044	1.818724
34	1	0	0.918535	2.534550	4.181508
35	1	0	3.231552	-1.093856	4.256035
36	1	0	2.368311	0.929688	5.412237
37	1	0	-1.375365	-0.372711	-1.533112

Zero-point correction=	0.283167	(Hartree/Particle)
Thermal correction to Energy=	0.304177	
Thermal correction to Enthalpy=	0.305121	
Thermal correction to Gibbs Free Energy=	0.226935	
Sum of electronic and zero-point Energies=	-1174.800357	
Sum of electronic and thermal Energies=	-1174.779348	
Sum of electronic and thermal Enthalpies=	-1174.778403	
Sum of electronic and thermal Free Energies=	-1174.856590	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.281125	(Hartree/Particle)
Thermal correction to Energy=	0.301919	
Thermal correction to Enthalpy=	0.302863	
Thermal correction to Gibbs Free Energy=	0.227195	

```
 Sum of electronic and zero-point Energies=          -1174.188438
 Sum of electronic and thermal Energies=             -1174.167644
 Sum of electronic and thermal Enthalpies=           -1174.166700
 Sum of electronic and thermal Free Energies=        -1174.242368
```

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

```
 Zero-point correction=                           0.278748 (Hartree/Particle)
 Thermal correction to Energy=                    0.299377
 Thermal correction to Enthalpy=                  0.300321
 Thermal correction to Gibbs Free Energy=         0.226321
 Sum of electronic and zero-point Energies=          -1175.605043
 Sum of electronic and thermal Energies=             -1175.584414
 Sum of electronic and thermal Enthalpies=           -1175.583470
 Sum of electronic and thermal Free Energies=        -1175.657470
```

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.905836	0.008878	-0.038128
2	46	0	1.401117	-0.035209	0.123371
3	53	0	4.051531	0.001232	-0.041198
4	6	0	-1.642093	-1.305303	-1.065965
5	6	0	-2.749557	-3.253142	-2.727553
6	6	0	-0.963384	-1.719087	-2.215854
7	6	0	-2.876707	-1.882463	-0.747776
8	6	0	-3.426603	-2.852634	-1.578642
9	6	0	-1.519001	-2.686185	-3.046288
10	1	0	0.009615	-1.287818	-2.453160
11	1	0	-3.407205	-1.575676	0.154289
12	1	0	-4.386154	-3.300122	-1.325975
13	1	0	-0.983314	-3.004108	-3.938596
14	1	0	-3.180157	-4.015631	-3.374099
15	6	0	-1.617238	1.571768	-0.644220
16	6	0	-2.666110	4.023985	-1.456739
17	6	0	-2.898332	1.637206	-1.201496
18	6	0	-0.864949	2.741098	-0.501194
19	6	0	-1.390875	3.964566	-0.902496
20	6	0	-3.418185	2.861227	-1.607234
21	1	0	-3.488331	0.728613	-1.324669
22	1	0	0.141364	2.684562	-0.082941
23	1	0	-0.798795	4.870838	-0.791697
24	1	0	-4.413128	2.907791	-2.046198
25	1	0	-3.074275	4.979787	-1.780491
26	6	0	-1.621294	-0.247284	1.620729
27	6	0	-2.593146	-0.733591	4.190827
28	6	0	-2.521465	0.643189	2.209744
29	6	0	-1.205135	-1.380784	2.331737
30	6	0	-1.692727	-1.624036	3.609136
31	6	0	-3.004750	0.396562	3.492228
32	1	0	-2.846437	1.531521	1.669216
33	1	0	-0.501037	-2.080590	1.876508
34	1	0	-1.367782	-2.508249	4.154124
35	1	0	-3.707424	1.093474	3.945409
36	1	0	-2.972375	-0.920991	5.193708
37	1	0	1.409763	0.387182	-1.348708

```
Zero-point correction=                           0.281772 (Hartree/Particle)
```

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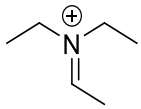
Thermal correction to Energy=                  0.301699
Thermal correction to Enthalpy=                0.302643
Thermal correction to Gibbs Free Energy=       0.227593
Sum of electronic and zero-point Energies=         -1174.189058
Sum of electronic and thermal Energies=            -1174.169130
Sum of electronic and thermal Enthalpies=          -1174.168186
Sum of electronic and thermal Free Energies=       -1174.243237
```

$[Et_2N{=}CHCH_3]^+$



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.093120	-0.150238	-0.099593
2	6	0	-0.403622	1.050224	0.637071
3	1	0	-1.042634	0.712397	1.453710
4	1	0	0.476761	1.516730	1.083183
5	6	0	-1.132124	2.023848	-0.291337
6	1	0	-2.032759	1.575367	-0.721365
7	1	0	-0.488838	2.365973	-1.107825
8	1	0	-1.432110	2.901805	0.288462
9	6	0	1.482917	-0.049516	-0.643615
10	1	0	1.583670	0.961620	-1.046935
11	1	0	1.560524	-0.751559	-1.477020
12	6	0	2.539273	-0.336817	0.423252
13	1	0	2.480613	0.359591	1.265022
14	1	0	3.529278	-0.227126	-0.029594
15	1	0	2.450462	-1.358504	0.805119
16	6	0	-0.604476	-1.219796	-0.284101
17	6	0	-1.982688	-1.496104	0.187314
18	1	0	-2.601916	-1.753878	-0.682404
19	1	0	-2.454810	-0.680381	0.733238
20	1	0	-1.963164	-2.395283	0.818253
21	1	0	-0.112596	-2.006114	-0.856198

```
Zero-point correction=                         0.196923  (Hartree/Particle)
Thermal correction to Energy=                  0.206238
Thermal correction to Enthalpy=                0.207182
Thermal correction to Gibbs Free Energy=       0.162942
Sum of electronic and zero-point Energies=          -291.390210
Sum of electronic and thermal Energies=             -291.380895
Sum of electronic and thermal Enthalpies=           -291.379951
Sum of electronic and thermal Free Energies=        -291.424190
```

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

```
Zero-point correction=                         0.195237 (Hartree/Particle)
Thermal correction to Energy=                  0.204547
Thermal correction to Enthalpy=                0.205492
Thermal correction to Gibbs Free Energy=       0.161582
Sum of electronic and zero-point Energies=          -291.190903
Sum of electronic and thermal Energies=             -291.181592
Sum of electronic and thermal Enthalpies=           -291.180648
```

Sum of electronic and thermal Free Energies= -291.224558

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

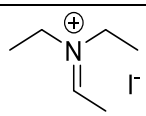
Zero-point correction= 0.192924 (Hartree/Particle)
Thermal correction to Energy= 0.202047
Thermal correction to Enthalpy= 0.202992
Thermal correction to Gibbs Free Energy= 0.159851
Sum of electronic and zero-point Energies= -291.284915
Sum of electronic and thermal Energies= -291.275792
Sum of electronic and thermal Enthalpies= -291.274848
Sum of electronic and thermal Free Energies= -291.317989

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.112385	-0.125329	-0.101344
2	6	0	-0.432154	1.041723	0.635650
3	1	0	-1.011916	0.678112	1.488832
4	1	0	0.432998	1.577655	1.040260
5	6	0	-1.251120	1.925392	-0.283883
6	1	0	-2.139278	1.402402	-0.657577
7	1	0	-0.662099	2.264602	-1.144049
8	1	0	-1.583316	2.811126	0.266991
9	6	0	1.486818	0.035749	-0.640458
10	1	0	1.563844	1.070012	-0.995920
11	1	0	1.582294	-0.622771	-1.509956
12	6	0	2.522232	-0.280583	0.418155
13	1	0	2.414693	0.356919	1.303434
14	1	0	3.522915	-0.114775	0.006105
15	1	0	2.451900	-1.328550	0.733076
16	6	0	-0.536479	-1.220956	-0.286225
17	6	0	-1.890682	-1.540683	0.186397
18	1	0	-2.517734	-1.770528	-0.686405
19	1	0	-2.370541	-0.755770	0.773325
20	1	0	-1.851089	-2.467122	0.774719
21	1	0	-0.011047	-1.987864	-0.861251

Zero-point correction= 0.195747 (Hartree/Particle)
Thermal correction to Energy= 0.204820
Thermal correction to Enthalpy= 0.205764
Thermal correction to Gibbs Free Energy= 0.162623
Sum of electronic and zero-point Energies= -291.191078
Sum of electronic and thermal Energies= -291.182005
Sum of electronic and thermal Enthalpies= -291.181061
Sum of electronic and thermal Free Energies= -291.224202

$[Et_2N{=}CHCH_3]^+I^-$



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	-1.633987	0.063848	-0.214736
2	6	0	-2.137939	1.412842	0.077472
3	1	0	-2.094609	2.001389	-0.841880
4	1	0	-3.199314	1.302845	0.328359
5	6	0	-1.394710	2.134235	1.208111
6	1	0	-0.335828	2.261833	0.969450
7	1	0	-1.457739	1.577278	2.148698
8	1	0	-1.845500	3.120383	1.367235
9	6	0	-1.998468	-1.010859	0.724508
10	1	0	-2.475331	-0.545867	1.592006
11	1	0	-1.070673	-1.475564	1.081255
12	6	0	-2.935441	-2.048197	0.101728
13	1	0	-3.874291	-1.589435	-0.227270
14	1	0	-3.172133	-2.825909	0.836060
15	1	0	-2.472862	-2.535831	-0.763303
16	6	0	-0.615820	-0.166424	-1.061611
17	6	0	-0.326875	0.773092	-2.202861
18	1	0	0.526127	0.401346	-2.771507
19	1	0	-0.088022	1.784332	-1.867222
20	1	0	-1.204106	0.820265	-2.866027
21	1	0	-0.459637	-1.218517	-1.266530
22	53	0	1.719195	-0.190446	0.201882

Zero-point correction=	0.197641	(Hartree/Particle)
Thermal correction to Energy=	0.208782	
Thermal correction to Enthalpy=	0.209727	
Thermal correction to Gibbs Free Energy=	0.158026	
Sum of electronic and zero-point Energies=	-303.015384	
Sum of electronic and thermal Energies=	-303.004243	
Sum of electronic and thermal Enthalpies=	-303.003299	
Sum of electronic and thermal Free Energies=	-303.054999	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.195080	(Hartree/Particle)
Thermal correction to Energy=	0.205806	
Thermal correction to Enthalpy=	0.206750	
Thermal correction to Gibbs Free Energy=	0.156695	
Sum of electronic and zero-point Energies=	-302.753726	
Sum of electronic and thermal Energies=	-302.743001	
Sum of electronic and thermal Enthalpies=	-302.742056	
Sum of electronic and thermal Free Energies=	-302.792111	

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.193377	(Hartree/Particle)
Thermal correction to Energy=	0.204605	
Thermal correction to Enthalpy=	0.205549	
Thermal correction to Gibbs Free Energy=	0.154391	
Sum of electronic and zero-point Energies=	-302.881090	
Sum of electronic and thermal Energies=	-302.869862	
Sum of electronic and thermal Enthalpies=	-302.868918	
Sum of electronic and thermal Free Energies=	-302.920076	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.641717	0.050616	0.205736
2	6	0	2.184648	1.330634	-0.255370
3	1	0	2.255663	2.006474	0.604462
4	1	0	3.213817	1.132624	-0.584644
5	6	0	1.361470	1.948039	-1.372238
6	1	0	0.332764	2.142470	-1.045834
7	1	0	1.306879	1.285095	-2.244874
8	1	0	1.816295	2.892863	-1.691317
9	6	0	1.981950	-1.138705	-0.581675
10	1	0	2.205333	-0.807318	-1.604125
11	1	0	1.080152	-1.763100	-0.645603
12	6	0	3.154279	-1.886956	0.021408
13	1	0	4.046100	-1.249092	0.075803
14	1	0	3.402597	-2.766102	-0.583941
15	1	0	2.917718	-2.228276	1.037335
16	6	0	0.686895	-0.038824	1.114925
17	6	0	0.388396	1.071954	2.058315
18	1	0	-0.477116	0.815395	2.673268
19	1	0	0.169762	2.012670	1.542546
20	1	0	1.257936	1.230905	2.716172
21	1	0	0.453440	-1.053571	1.428856
22	53	0	-1.773947	-0.221174	-0.170386

Zero-point correction= 0.196030 (Hartree/Particle)
Thermal correction to Energy= 0.207153
Thermal correction to Enthalpy= 0.208097
Thermal correction to Gibbs Free Energy= 0.157414
Sum of electronic and zero-point Energies= -302.754042
Sum of electronic and thermal Energies= -302.742919
Sum of electronic and thermal Enthalpies= -302.741975
Sum of electronic and thermal Free Energies= -302.792658

V-I $[Et_3N[Pd^{II}]I]^+I^-$

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.001573	-0.354015	-0.033729
2	7	0	2.134311	-0.664119	-0.062412
3	6	0	2.621576	-1.308326	1.208755
4	1	0	2.284529	-2.346081	1.168167
5	1	0	3.720899	-1.287976	1.170796
6	6	0	2.138048	-0.666705	2.505725
7	1	0	2.464015	-1.300313	3.337555
8	1	0	1.043869	-0.604733	2.545173
9	1	0	2.562359	0.327614	2.670758
10	6	0	2.485836	0.781862	-0.050101
11	1	0	1.892172	1.254374	0.746252
12	1	0	3.555866	0.852272	0.279332
13	6	0	2.364141	1.576573	-1.352066
14	1	0	3.130024	1.277737	-2.071476
15	1	0	2.548985	2.627554	-1.106623
16	1	0	1.378710	1.512424	-1.824201
17	6	0	2.738689	-1.425285	-1.208576
18	1	0	2.770190	-2.468493	-0.886536
19	1	0	3.778923	-1.078913	-1.303044

20	6	0	2.005620	-1.373114	-2.547861
21	1	0	2.543491	-2.024625	-3.246545
22	1	0	1.969753	-0.377420	-2.991747
23	1	0	0.985872	-1.757924	-2.452814
24	15	0	-2.146438	0.568041	0.035774
25	6	0	-2.941035	0.642594	1.688978
26	6	0	-4.168429	0.669266	4.210398
27	6	0	-2.817486	-0.460782	2.549605
28	6	0	-3.683547	1.760752	2.105721
29	6	0	-4.293393	1.770729	3.360843
30	6	0	-3.432227	-0.444725	3.802251
31	1	0	-2.245038	-1.329514	2.238227
32	1	0	-3.780567	2.625243	1.456144
33	1	0	-4.863520	2.640809	3.674646
34	1	0	-3.329288	-1.302931	4.460238
35	1	0	-4.640718	0.681257	5.188817
36	6	0	-1.860378	2.323471	-0.441833
37	6	0	-1.214531	4.954560	-1.183411
38	6	0	-2.312607	2.849124	-1.661863
39	6	0	-1.075419	3.133319	0.401710
40	6	0	-0.760037	4.440124	0.034454
41	6	0	-1.989985	4.157775	-2.027100
42	1	0	-2.919548	2.240275	-2.324035
43	1	0	-0.721872	2.745362	1.353899
44	1	0	-0.158611	5.055702	0.697423
45	1	0	-2.349024	4.553949	-2.972907
46	1	0	-0.964285	5.971523	-1.471760
47	6	0	-3.417525	-0.060474	-1.126149
48	6	0	-5.305352	-0.978415	-2.981906
49	6	0	-3.001262	-0.709934	-2.298642
50	6	0	-4.789146	0.115367	-0.885886
51	6	0	-5.726708	-0.343709	-1.811295
52	6	0	-3.942511	-1.160089	-3.224910
53	1	0	-1.943381	-0.879653	-2.474548
54	1	0	-5.126620	0.600244	0.024783
55	1	0	-6.786685	-0.209159	-1.614498
56	1	0	-3.610110	-1.666031	-4.126793
57	1	0	-6.038204	-1.338593	-3.698631
58	53	0	-0.717383	-2.962873	0.072067
59	53	0	6.081494	0.622405	0.128022

Zero-point correction=	0.486466	(Hartree/Particle)
Thermal correction to Energy=	0.519705	
Thermal correction to Enthalpy=	0.520650	
Thermal correction to Gibbs Free Energy=	0.412366	
Sum of electronic and zero-point Energies=	-1477.811189	
Sum of electronic and thermal Energies=	-1477.777950	
Sum of electronic and thermal Enthalpies=	-1477.777006	
Sum of electronic and thermal Free Energies=	-1477.885289	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.481505	(Hartree/Particle)
Thermal correction to Energy=	0.513402	
Thermal correction to Enthalpy=	0.514347	
Thermal correction to Gibbs Free Energy=	0.411832	
Sum of electronic and zero-point Energies=	-1476.961305	
Sum of electronic and thermal Energies=	-1476.929407	
Sum of electronic and thermal Enthalpies=	-1476.928463	
Sum of electronic and thermal Free Energies=	-1477.030978	

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.476972	(Hartree/Particle)
Thermal correction to Energy=	0.508513	
Thermal correction to Enthalpy=	0.509457	
Thermal correction to Gibbs Free Energy=	0.409772	
Sum of electronic and zero-point Energies=	-1478.503904	
Sum of electronic and thermal Energies=	-1478.472364	
Sum of electronic and thermal Enthalpies=	-1478.471419	
Sum of electronic and thermal Free Energies=	-1478.571105	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.093165	-0.324316	0.019024
2	7	0	2.040291	-0.627948	0.017300
3	6	0	2.484008	-1.368818	1.233333
4	1	0	2.140148	-2.402568	1.104640
5	1	0	3.588762	-1.369390	1.228967
6	6	0	1.958377	-0.818499	2.541648
7	1	0	2.210611	-1.520122	3.345085
8	1	0	0.860849	-0.718394	2.523866
9	1	0	2.399215	0.149811	2.804549
10	6	0	2.444696	0.797756	0.138241
11	1	0	1.865649	1.236423	0.967292
12	1	0	3.513512	0.805649	0.456669
13	6	0	2.316739	1.667990	-1.097110
14	1	0	3.030198	1.375952	-1.876043
15	1	0	2.568369	2.694718	-0.804661
16	1	0	1.303958	1.690492	-1.527196
17	6	0	2.631054	-1.301223	-1.175316
18	1	0	2.697800	-2.367285	-0.925064
19	1	0	3.668830	-0.934054	-1.274118
20	6	0	1.854693	-1.169888	-2.471058
21	1	0	2.393805	-1.714792	-3.256019
22	1	0	1.738037	-0.136278	-2.811724
23	1	0	0.857509	-1.621486	-2.379778
24	15	0	-2.213724	0.531780	0.027104
25	6	0	-3.114168	0.592877	1.598228
26	6	0	-4.490813	0.659806	4.016853
27	6	0	-2.956550	-0.444926	2.521499
28	6	0	-3.957387	1.671793	1.895864
29	6	0	-4.646122	1.699763	3.101858
30	6	0	-3.648211	-0.408667	3.728073
31	1	0	-2.293326	-1.279535	2.291325
32	1	0	-4.069646	2.489651	1.182847
33	1	0	-5.300916	2.537830	3.332123
34	1	0	-3.522546	-1.215968	4.446564
35	1	0	-5.028130	0.687033	4.962969
36	6	0	-1.626835	2.225099	-0.292058
37	6	0	-0.421509	4.697113	-0.763561
38	6	0	-1.714029	2.819477	-1.557085
39	6	0	-0.916855	2.875137	0.731958
40	6	0	-0.321441	4.107371	0.495098
41	6	0	-1.117502	4.054508	-1.784764
42	1	0	-2.257234	2.320686	-2.359305
43	1	0	-0.843114	2.417424	1.720405

44	1	0	0.220117	4.609446	1.294196
45	1	0	-1.198279	4.518783	-2.765596
46	1	0	0.045656	5.662387	-0.948363
47	6	0	-3.363476	0.084534	-1.298044
48	6	0	-5.047555	-0.550877	-3.420814
49	6	0	-2.825615	-0.343267	-2.517639
50	6	0	-4.748664	0.177256	-1.141151
51	6	0	-5.586313	-0.142142	-2.204539
52	6	0	-3.666927	-0.651139	-3.578726
53	1	0	-1.743517	-0.439921	-2.626169
54	1	0	-5.174414	0.491465	-0.188964
55	1	0	-6.665183	-0.073653	-2.080430
56	1	0	-3.246098	-0.983626	-4.525360
57	1	0	-5.706802	-0.801730	-4.249598
58	53	0	-0.885535	-2.867791	0.073183
59	53	0	6.131536	0.408212	0.102843

Zero-point correction= 0.484861 (Hartree/Particle)
Thermal correction to Energy= 0.517364
Thermal correction to Enthalpy= 0.518309
Thermal correction to Gibbs Free Energy= 0.414435
Sum of electronic and zero-point Energies= -1476.962609
Sum of electronic and thermal Energies= -1476.930105
Sum of electronic and thermal Enthalpies= -1476.929161
Sum of electronic and thermal Free Energies= -1477.033034

$Et_3N.HI$

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.513164	-0.001124	-0.001225
2	6	0	1.934987	-1.279676	0.677154
3	1	0	1.494092	-1.243391	1.673664
4	1	0	3.026278	-1.247856	0.778359
5	6	0	1.928325	0.046818	-1.449512
6	1	0	1.474929	-0.828876	-1.914661
7	1	0	3.018264	-0.068939	-1.478816
8	6	0	1.460984	-2.546063	-0.031286
9	1	0	1.991651	-2.736612	-0.968408
10	1	0	0.384452	-2.499330	-0.225229
11	1	0	1.649551	-3.397159	0.631215
12	6	0	1.463636	1.299342	-2.188184
13	1	0	1.644365	1.150520	-3.257752
14	1	0	2.005709	2.200009	-1.886377
15	1	0	0.389402	1.454748	-2.044213
16	6	0	1.942741	1.224760	0.763152
17	1	0	1.501697	2.070571	0.235143
18	1	0	3.033872	1.293402	0.679604
19	6	0	1.476346	1.246474	2.216602
20	1	0	0.399655	1.057497	2.279200
21	1	0	1.669329	2.245435	2.621086
22	1	0	2.008765	0.529149	2.847498
23	1	0	0.428671	0.001978	0.003217
24	53	0	-1.848207	0.001449	0.002028

Zero-point correction= 0.221882 (Hartree/Particle)

```
Thermal correction to Energy=                  0.233421
Thermal correction to Enthalpy=                0.234365
Thermal correction to Gibbs Free Energy=       0.182605
Sum of electronic and zero-point Energies=          -304.206491
Sum of electronic and thermal Energies=             -304.194951
Sum of electronic and thermal Enthalpies=           -304.194007
Sum of electronic and thermal Free Energies=        -304.245767
```

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

```
Zero-point correction=                         0.220024 (Hartree/Particle)
Thermal correction to Energy=                  0.231727
Thermal correction to Enthalpy=                0.232671
Thermal correction to Gibbs Free Energy=       0.180571
Sum of electronic and zero-point Energies=          -303.945145
Sum of electronic and thermal Energies=             -303.933442
Sum of electronic and thermal Enthalpies=           -303.932498
Sum of electronic and thermal Free Energies=        -303.984599
```

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

```
Zero-point correction=                         0.217954 (Hartree/Particle)
Thermal correction to Energy=                  0.229336
Thermal correction to Enthalpy=                0.230280
Thermal correction to Gibbs Free Energy=       0.179540
Sum of electronic and zero-point Energies=          -304.080667
Sum of electronic and thermal Energies=             -304.069285
Sum of electronic and thermal Enthalpies=           -304.068341
Sum of electronic and thermal Free Energies=        -304.119082
```

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.522326	-0.002417	-0.002242
2	6	0	-1.930470	-1.134581	-0.896799
3	1	0	-1.447496	-0.942485	-1.860284
4	1	0	-3.018629	-1.054274	-1.033422
5	6	0	-1.951313	-0.213812	1.418717
6	1	0	-1.465659	-1.140419	1.741008
7	1	0	-3.037899	-0.380345	1.402171
8	6	0	-1.510752	-2.493778	-0.382048
9	1	0	-2.094068	-2.822860	0.484300
10	1	0	-0.443724	-2.501456	-0.123193
11	1	0	-1.663957	-3.230035	-1.178364
12	6	0	-1.552612	0.914154	2.344257
13	1	0	-1.721004	0.592342	3.377573
14	1	0	-2.136934	1.827003	2.184997
15	1	0	-0.484549	1.146093	2.238606
16	6	0	-1.954527	1.329666	-0.537266
17	1	0	-1.491392	2.077809	0.114229
18	1	0	-3.044975	1.386128	-0.407301
19	6	0	-1.528881	1.572593	-1.968184
20	1	0	-0.456128	1.375036	-2.094849
21	1	0	-1.702667	2.627311	-2.207510
22	1	0	-2.093163	0.975104	-2.692158
23	1	0	-0.457788	0.006847	0.003867
24	53	0	1.886559	0.004333	0.003660

```
---------------------------------------------------------------------
Zero-point correction=                           0.220806 (Hartree/Particle)
Thermal correction to Energy=                    0.232318
Thermal correction to Enthalpy=                  0.233262
Thermal correction to Gibbs Free Energy=         0.181335
Sum of electronic and zero-point Energies=           -303.945379
Sum of electronic and thermal Energies=              -303.933868
Sum of electronic and thermal Enthalpies=            -303.932923
Sum of electronic and thermal Free Energies=         -303.984851
```

I^-

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

```
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1         53           0        0.000000    0.000000    0.000000
---------------------------------------------------------------------
Zero-point correction=                           0.000000 (Hartree/Particle)
Thermal correction to Energy=                    0.001416
Thermal correction to Enthalpy=                  0.002360
Thermal correction to Gibbs Free Energy=        -0.016848
Sum of electronic and zero-point Energies=           -11.472110
Sum of electronic and thermal Energies=              -11.470694
Sum of electronic and thermal Enthalpies=            -11.469750
Sum of electronic and thermal Free Energies=         -11.488958
```

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

```
Zero-point correction=                           0.000000 (Hartree/Particle)
Thermal correction to Energy=                    0.001416
Thermal correction to Enthalpy=                  0.002360
Thermal correction to Gibbs Free Energy=        -0.016848
Sum of electronic and zero-point Energies=           -11.494130
Sum of electronic and thermal Energies=              -11.492714
Sum of electronic and thermal Enthalpies=            -11.491769
Sum of electronic and thermal Free Energies=         -11.510978
```

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

```
Zero-point correction=                           0.000000 (Hartree/Particle)
Thermal correction to Energy=                    0.001416
Thermal correction to Enthalpy=                  0.002360
Thermal correction to Gibbs Free Energy=        -0.016848
Sum of electronic and zero-point Energies=           -11.535746
Sum of electronic and thermal Energies=              -11.534330
Sum of electronic and thermal Enthalpies=            -11.533385
Sum of electronic and thermal Free Energies=         -11.552594
```

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

```
---------------------------------------------------------------------
Center     Atomic      Atomic             Coordinates (Angstroms)
Number     Number       Type              X           Y           Z
---------------------------------------------------------------------
     1         53           0        0.000000    0.000000    0.000000
```

Zero-point correction=	0.000000 (Hartree/Particle)
Thermal correction to Energy=	0.001416
Thermal correction to Enthalpy=	0.002360
Thermal correction to Gibbs Free Energy=	-0.016848
Sum of electronic and zero-point Energies=	-11.494130
Sum of electronic and thermal Energies=	-11.492714
Sum of electronic and thermal Enthalpies=	-11.491769
Sum of electronic and thermal Free Energies=	-11.510978

$TS_{1Pd\text{-}VII}$

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Imaginary frequency: -19.7232 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.362773	-1.421422	-2.298744
2	6	0	1.729001	-0.729373	-1.738341
3	6	0	2.489307	-0.069900	-0.551075
4	1	0	1.220620	-0.041329	-2.417172
5	6	0	1.632210	-0.877612	0.422798
6	6	0	0.890193	-1.375602	-0.638010
7	6	0	1.774193	-1.128607	1.852612
8	6	0	2.080065	-1.662323	4.606533
9	6	0	2.955072	-0.765033	2.533555
10	6	0	0.752098	-1.768116	2.585434
11	6	0	0.907880	-2.036021	3.941227
12	6	0	3.097937	-1.025922	3.896089
13	1	0	3.774152	-0.303364	1.994613
14	1	0	-0.172976	-2.034823	2.083611
15	1	0	0.106322	-2.528653	4.485206
16	1	0	4.015682	-0.734451	4.399295
17	1	0	2.194781	-1.863659	5.668023
18	53	0	-0.109760	-3.389061	-0.902720
19	8	0	2.339232	1.353298	-0.609861
20	8	0	3.864430	-0.407430	-0.422280
21	16	0	4.950232	0.399881	-1.475014
22	8	0	4.926506	-0.232038	-2.816055
23	6	0	6.356212	-0.445459	-0.533744
24	9	0	6.295069	-1.769022	-0.633466
25	9	0	7.494795	-0.010883	-1.091343
26	9	0	6.335102	-0.080462	0.751027
27	16	0	2.400031	2.219784	0.853124
28	8	0	3.802386	2.466668	1.263223
29	6	0	1.915613	3.767363	-0.125196
30	9	0	2.878507	4.128793	-0.964229
31	9	0	1.718113	4.742302	0.775773
32	9	0	0.775470	3.574510	-0.799183
33	46	0	-1.039170	-0.712848	-0.351136
34	15	0	-3.177469	0.280600	-0.092213
35	6	0	-4.402091	-0.698741	0.884951
36	6	0	-6.167531	-2.208488	2.465975
37	6	0	-5.762321	-0.781906	0.551748
38	6	0	-3.936697	-1.390579	2.015014
39	6	0	-4.814136	-2.133526	2.804231
40	6	0	-6.638136	-1.534500	1.338099

41	1	0	-6.139060	-0.264863	-0.325425
42	1	0	-2.880978	-1.348921	2.271239
43	1	0	-4.439600	-2.662259	3.676658
44	1	0	-7.688555	-1.594430	1.065620
45	1	0	-6.849977	-2.795259	3.074945
46	6	0	-3.191606	1.934033	0.731662
47	6	0	-3.070196	4.474910	1.925403
48	6	0	-4.234317	2.382373	1.556466
49	6	0	-2.086716	2.773187	0.519794
50	6	0	-2.026692	4.037028	1.106508
51	6	0	-4.171245	3.645986	2.149036
52	1	0	-5.091926	1.743514	1.744385
53	1	0	-1.267680	2.429596	-0.104922
54	1	0	-1.159166	4.667811	0.934203
55	1	0	-4.982947	3.979853	2.790087
56	1	0	-3.022401	5.454869	2.392648
57	6	0	-4.028590	0.575189	-1.705122
58	6	0	-5.271045	0.899148	-4.204442
59	6	0	-4.835090	1.694822	-1.959113
60	6	0	-3.844849	-0.374871	-2.723740
61	6	0	-4.467491	-0.217489	-3.961908
62	6	0	-5.450792	1.854639	-3.202801
63	1	0	-4.977606	2.447602	-1.189767
64	1	0	-3.205844	-1.236178	-2.544281
65	1	0	-4.316419	-0.961354	-4.739525
66	1	0	-6.068808	2.729248	-3.388113
67	1	0	-5.748791	1.027281	-5.172045

Zero-point correction=	0.460701 (Hartree/Particle)
Thermal correction to Energy=	0.504668
Thermal correction to Enthalpy=	0.505612
Thermal correction to Gibbs Free Energy=	0.372122
Sum of electronic and zero-point Energies=	-3331.604930
Sum of electronic and thermal Energies=	-3331.560962
Sum of electronic and thermal Enthalpies=	-3331.560018
Sum of electronic and thermal Free Energies=	-3331.693508

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Imaginary frequency: -46.1575 cm^{-1}

Zero-point correction=	0.457904 (Hartree/Particle)
Thermal correction to Energy=	0.500459
Thermal correction to Enthalpy=	0.501404
Thermal correction to Gibbs Free Energy=	0.377249
Sum of electronic and zero-point Energies=	-3330.348221
Sum of electronic and thermal Energies=	-3330.305665
Sum of electronic and thermal Enthalpies=	-3330.304721
Sum of electronic and thermal Free Energies=	-3330.428875

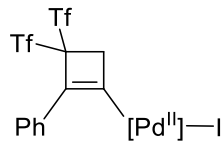
M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Imaginary frequency: -48.8120 cm^{-1}

Zero-point correction=	0.452784 (Hartree/Particle)
Thermal correction to Energy=	0.495184
Thermal correction to Enthalpy=	0.496128
Thermal correction to Gibbs Free Energy=	0.372471
Sum of electronic and zero-point Energies=	-3332.202035

Sum of electronic and thermal Energies= -3332.159635
Sum of electronic and thermal Enthalpies= -3332.158691
Sum of electronic and thermal Free Energies= -3332.282348

VII



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.839110	-1.515570	-1.997107
2	6	0	1.645016	-0.532540	-1.559076
3	6	0	2.765775	-0.068788	-0.581669
4	1	0	1.380819	0.188756	-2.337664
5	6	0	1.796618	-0.286119	0.576069
6	6	0	0.787181	-0.557289	-0.294665
7	6	0	1.963282	-0.232525	2.024853
8	6	0	2.252868	-0.180409	4.825811
9	6	0	3.233992	-0.358467	2.619006
10	6	0	0.842278	-0.083904	2.864035
11	6	0	0.985462	-0.061528	4.247918
12	6	0	3.372735	-0.331013	4.005971
13	1	0	4.107828	-0.512477	1.994736
14	1	0	-0.143988	0.010533	2.416464
15	1	0	0.107093	0.052017	4.877713
16	1	0	4.360435	-0.435903	4.446597
17	1	0	2.364965	-0.158433	5.906361
18	53	0	-0.900082	-3.086259	0.172408
19	8	0	3.123317	1.283386	-0.909009
20	8	0	3.930140	-0.870821	-0.460897
21	16	0	4.980587	-0.915262	-1.823845
22	8	0	4.591470	-2.023860	-2.726041
23	6	0	6.299137	-1.633815	-0.671467
24	9	0	5.939376	-2.825136	-0.205755
25	9	0	7.415371	-1.759764	-1.400690
26	9	0	6.534370	-0.798545	0.344249
27	16	0	4.117641	2.095916	0.204518
28	8	0	5.486525	2.213181	-0.352428
29	6	0	3.246467	3.706570	-0.251734
30	9	0	3.316001	3.962695	-1.554077
31	9	0	3.851005	4.689997	0.426751
32	9	0	1.966009	3.637964	0.131147
33	46	0	-1.165052	-0.466121	-0.175045
34	15	0	-3.550289	0.246912	-0.220259
35	6	0	-4.892694	-0.890631	-0.753231
36	6	0	-6.918186	-2.689827	-1.477154
37	6	0	-5.945459	-0.476351	-1.584469
38	6	0	-4.859202	-2.217917	-0.295822
39	6	0	-5.871454	-3.109092	-0.653425
40	6	0	-6.952138	-1.374134	-1.943877
41	1	0	-5.977709	0.543646	-1.955357
42	1	0	-4.034732	-2.558653	0.323166
43	1	0	-5.833432	-4.134654	-0.296987

44	1	0	-7.760892	-1.044707	-2.590673
45	1	0	-7.701073	-3.387981	-1.760903
46	6	0	-4.152607	0.980487	1.359114
47	6	0	-4.950635	2.146663	3.786258
48	6	0	-5.489717	0.907212	1.776673
49	6	0	-3.219458	1.638053	2.177813
50	6	0	-3.616326	2.223700	3.379436
51	6	0	-5.883638	1.486478	2.985043
52	1	0	-6.222541	0.393606	1.162273
53	1	0	-2.176047	1.691780	1.874259
54	1	0	-2.883232	2.730705	4.000740
55	1	0	-6.921538	1.418944	3.299731
56	1	0	-5.259853	2.594243	4.726810
57	6	0	-3.610090	1.641519	-1.426710
58	6	0	-3.573411	3.702646	-3.334771
59	6	0	-4.288042	2.845705	-1.184923
60	6	0	-2.907741	1.485825	-2.635474
61	6	0	-2.894635	2.507587	-3.584855
62	6	0	-4.267702	3.869192	-2.134996
63	1	0	-4.828001	2.987334	-0.253844
64	1	0	-2.373247	0.559076	-2.834278
65	1	0	-2.349446	2.372692	-4.514895
66	1	0	-4.794801	4.798231	-1.935075
67	1	0	-3.557153	4.502202	-4.070246

Zero-point correction=	0.460690 (Hartree/Particle)
Thermal correction to Energy=	0.504811
Thermal correction to Enthalpy=	0.505755
Thermal correction to Gibbs Free Energy=	0.369936
Sum of electronic and zero-point Energies=	-3331.612448
Sum of electronic and thermal Energies=	-3331.568327
Sum of electronic and thermal Enthalpies=	-3331.567383
Sum of electronic and thermal Free Energies=	-3331.703202

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.457049 (Hartree/Particle)
Thermal correction to Energy=	0.499821
Thermal correction to Enthalpy=	0.500765
Thermal correction to Gibbs Free Energy=	0.375215
Sum of electronic and zero-point Energies=	-3330.347632
Sum of electronic and thermal Energies=	-3330.304860
Sum of electronic and thermal Enthalpies=	-3330.303916
Sum of electronic and thermal Free Energies=	-3330.429466

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.453027 (Hartree/Particle)
Thermal correction to Energy=	0.496982
Thermal correction to Enthalpy=	0.497926
Thermal correction to Gibbs Free Energy=	0.370635
Sum of electronic and zero-point Energies=	-3332.203132
Sum of electronic and thermal Energies=	-3332.159178
Sum of electronic and thermal Enthalpies=	-3332.158234
Sum of electronic and thermal Free Energies=	-3332.285524

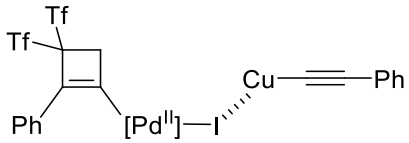
M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.108818	-2.429389	-1.366972
2	6	0	1.909268	-1.356560	-1.486644
3	6	0	2.852024	-0.467765	-0.648208
4	1	0	1.841320	-1.097685	-2.549625
5	6	0	1.689853	-0.128039	0.245618
6	6	0	0.837665	-0.807004	-0.563633
7	6	0	1.574516	0.649380	1.467902
8	6	0	1.284178	2.046799	3.881534
9	6	0	2.635891	0.720912	2.382403
10	6	0	0.377645	1.314385	1.774619
11	6	0	0.227810	1.995065	2.974693
12	6	0	2.487250	1.414382	3.577773
13	1	0	3.571048	0.206079	2.159710
14	1	0	-0.437108	1.321507	1.042888
15	1	0	-0.712508	2.500784	3.191823
16	1	0	3.316397	1.454312	4.281926
17	1	0	1.172404	2.585852	4.820605
18	53	0	-1.177903	-3.205090	-0.211526
19	8	0	3.360647	0.579770	-1.466535
20	8	0	3.909955	-1.077600	0.065212
21	16	0	5.182055	-1.693850	-0.851471
22	8	0	5.066392	-3.159803	-0.916383
23	6	0	6.280676	-1.386806	0.633419
24	9	0	5.868938	-2.090863	1.667787
25	9	0	7.505236	-1.763441	0.300458
26	9	0	6.286718	-0.097264	0.943205
27	16	0	4.132448	1.818349	-0.640933
28	8	0	5.432842	2.028464	-1.299363
29	6	0	3.004720	3.072296	-1.442835
30	9	0	3.070071	3.003813	-2.756504
31	9	0	3.396046	4.273763	-1.043443
32	9	0	1.759109	2.861425	-1.040484
33	46	0	-1.125160	-0.584426	-0.485477
34	15	0	-3.409637	0.155520	-0.149707
35	6	0	-4.222661	-0.366542	1.394280
36	6	0	-5.340108	-1.071809	3.849416
37	6	0	-5.609027	-0.344229	1.565901
38	6	0	-3.399520	-0.750271	2.458835
39	6	0	-3.957510	-1.094814	3.684603
40	6	0	-6.164155	-0.699840	2.790882
41	1	0	-6.256689	-0.052929	0.739123
42	1	0	-2.316182	-0.780987	2.322286
43	1	0	-3.312222	-1.392714	4.508709
44	1	0	-7.245115	-0.686875	2.918461
45	1	0	-5.777962	-1.351590	4.806051
46	6	0	-3.090568	1.945281	0.081201
47	6	0	-2.242902	4.589292	0.406784
48	6	0	-3.295446	2.605136	1.295669
49	6	0	-2.463419	2.627169	-0.973029
50	6	0	-2.044664	3.941876	-0.811209
51	6	0	-2.873578	3.923203	1.452977
52	1	0	-3.780993	2.087931	2.123185
53	1	0	-2.304274	2.120579	-1.927993
54	1	0	-1.555163	4.459816	-1.633859
55	1	0	-3.037623	4.430721	2.402424
56	1	0	-1.905639	5.615596	0.538829
57	6	0	-4.674124	0.059112	-1.455159
58	6	0	-6.604975	-0.217664	-3.445167

59	6	0	-5.617877	1.070676	-1.662392
60	6	0	-4.698271	-1.086896	-2.255677
61	6	0	-5.665372	-1.225102	-3.246091
62	6	0	-6.580760	0.929744	-2.655561
63	1	0	-5.596148	1.969846	-1.045232
64	1	0	-3.953045	-1.868738	-2.099865
65	1	0	-5.680268	-2.118501	-3.867453
66	1	0	-7.314610	1.717865	-2.814909
67	1	0	-7.358830	-0.324664	-4.223279

Zero-point correction=	0.462797 (Hartree/Particle)
Thermal correction to Energy=	0.506236
Thermal correction to Enthalpy=	0.507180
Thermal correction to Gibbs Free Energy=	0.379654
Sum of electronic and zero-point Energies=	-3330.352200
Sum of electronic and thermal Energies=	-3330.308761
Sum of electronic and thermal Enthalpies=	-3330.307817
Sum of electronic and thermal Free Energies=	-3330.435343

VII-Cu



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.320352	-1.513620	-2.255541
2	6	0	2.154913	-0.603854	-1.672025
3	6	0	3.148662	-0.433964	-0.476972
4	1	0	2.083039	0.264844	-2.332929
5	6	0	1.971502	-0.617865	0.462852
6	6	0	1.103309	-0.706009	-0.575772
7	6	0	1.786721	-0.693040	1.907096
8	6	0	1.250862	-0.971972	4.656465
9	6	0	2.764809	-1.209737	2.774229
10	6	0	0.548989	-0.291891	2.450258
11	6	0	0.273749	-0.444540	3.808253
12	6	0	2.493947	-1.344460	4.136000
13	1	0	3.720559	-1.530898	2.371868
14	1	0	-0.174883	0.225226	1.811132
15	1	0	-0.687505	-0.127042	4.202360
16	1	0	3.256510	-1.751516	4.794437
17	1	0	1.049391	-1.080927	5.718365
18	53	0	-1.151861	-2.033272	-2.698270
19	8	0	3.755911	0.859286	-0.548016
20	8	0	4.138079	-1.434122	-0.265691
21	16	0	5.394241	-1.537802	-1.434927
22	8	0	5.027414	-2.521179	-2.479808
23	6	0	6.385636	-2.507923	-0.147927
24	9	0	5.785397	-3.653718	0.162051
25	9	0	7.580208	-2.766065	-0.693106
26	9	0	6.557590	-1.772641	0.954600
27	16	0	4.616792	1.349646	0.835354
28	8	0	6.053166	1.465951	0.492254

29	6	0	3.892360	3.082019	0.640965
30	9	0	4.123369	3.597192	-0.559222
31	9	0	4.452301	3.859154	1.576387
32	9	0	2.572181	3.015398	0.864234
33	46	0	-0.841067	-0.873451	-0.212683
34	15	0	-3.187590	-0.893655	0.611285
35	6	0	-4.597796	-0.706062	-0.555428
36	6	0	-6.667896	-0.466216	-2.434985
37	6	0	-5.359223	0.469058	-0.625111
38	6	0	-4.880430	-1.759831	-1.442068
39	6	0	-5.912999	-1.640449	-2.370722
40	6	0	-6.388096	0.585856	-1.562616
41	1	0	-5.152953	1.294370	0.047845
42	1	0	-4.295636	-2.673988	-1.407818
43	1	0	-6.122854	-2.463143	-3.048564
44	1	0	-6.970637	1.501915	-1.606280
45	1	0	-7.468786	-0.372701	-3.163242
46	6	0	-3.579593	-2.417339	1.562512
47	6	0	-4.072888	-4.744735	3.050626
48	6	0	-4.897089	-2.812333	1.848056
49	6	0	-2.515198	-3.206805	2.024983
50	6	0	-2.760367	-4.362964	2.767532
51	6	0	-5.139713	-3.969037	2.589635
52	1	0	-5.731732	-2.221454	1.482650
53	1	0	-1.490773	-2.919770	1.799133
54	1	0	-1.927109	-4.967062	3.115250
55	1	0	-6.162605	-4.266896	2.803273
56	1	0	-4.265249	-5.647957	3.623162
57	6	0	-3.338451	0.499928	1.807209
58	6	0	-3.453699	2.684684	3.565380
59	6	0	-3.905294	0.353706	3.083096
60	6	0	-2.821874	1.751659	1.423084
61	6	0	-2.888221	2.838118	2.297683
62	6	0	-3.959309	1.442393	3.956091
63	1	0	-4.303234	-0.605905	3.397328
64	1	0	-2.371259	1.889769	0.442271
65	1	0	-2.488915	3.797915	1.982565
66	1	0	-4.399838	1.318172	4.941834
67	1	0	-3.497619	3.528821	4.248245
68	1	0	0.792101	4.656989	-0.034490
69	6	0	-0.020694	5.339629	-0.261592
70	6	0	-2.114598	7.088218	-0.860024
71	6	0	-1.107210	4.876123	-1.034629
72	6	0	0.010570	6.653156	0.201629
73	6	0	-1.033725	7.533568	-0.094213
74	6	0	-2.154622	5.775949	-1.325456
75	1	0	0.856239	6.993020	0.794314
76	1	0	-1.004259	8.558256	0.266638
77	1	0	-2.991980	5.429391	-1.923787
78	1	0	-2.929549	7.767442	-1.097442
79	6	0	-1.147690	3.527445	-1.503161
80	29	0	-1.206816	0.554211	-2.383085
81	6	0	-1.186695	2.364309	-1.901252

Zero-point correction=	0.562508 (Hartree/Particle)
Thermal correction to Energy=	0.617147
Thermal correction to Enthalpy=	0.618092
Thermal correction to Gibbs Free Energy=	0.456979
Sum of electronic and zero-point Energies=	-3835.499389
Sum of electronic and thermal Energies=	-3835.444749
Sum of electronic and thermal Enthalpies=	-3835.443805

Sum of electronic and thermal Free Energies= -3835.604917

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.558476	(Hartree/Particle)
Thermal correction to Energy=	0.610062	
Thermal correction to Enthalpy=	0.611006	
Thermal correction to Gibbs Free Energy=	0.465262	
Sum of electronic and zero-point Energies=	-3834.039410	
Sum of electronic and thermal Energies=	-3833.987825	
Sum of electronic and thermal Enthalpies=	-3833.986881	
Sum of electronic and thermal Free Energies=	-3834.132625	

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.553478	(Hartree/Particle)
Thermal correction to Energy=	0.605256	
Thermal correction to Enthalpy=	0.606200	
Thermal correction to Gibbs Free Energy=	0.462493	
Sum of electronic and zero-point Energies=	-3837.181072	
Sum of electronic and thermal Energies=	-3837.129294	
Sum of electronic and thermal Enthalpies=	-3837.128349	
Sum of electronic and thermal Free Energies=	-3837.272057	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.566284	-1.818858	-1.976460
2	6	0	2.318657	-0.813330	-1.613068
3	6	0	3.250167	-0.316059	-0.474651
4	1	0	2.208355	-0.120500	-2.456861
5	6	0	2.080338	-0.391971	0.460331
6	6	0	1.248920	-0.746322	-0.543646
7	6	0	1.781386	-0.155191	1.859640
8	6	0	0.919455	0.062540	4.516260
9	6	0	2.657419	-0.450511	2.908141
10	6	0	0.485686	0.301022	2.166883
11	6	0	0.043913	0.384347	3.481949
12	6	0	2.223522	-0.337061	4.225431
13	1	0	3.662946	-0.807018	2.683953
14	1	0	-0.140695	0.723664	1.361545
15	1	0	-0.968161	0.732006	3.692183
16	1	0	2.907800	-0.578405	5.036895
17	1	0	0.591969	0.138460	5.551166
18	53	0	-0.899697	-2.801617	-2.028812
19	8	0	3.740532	0.979949	-0.787634
20	8	0	4.316530	-1.147460	-0.061836
21	16	0	5.595893	-1.306107	-1.151725
22	8	0	5.372271	-2.494837	-1.991578
23	6	0	6.618423	-1.934756	0.284071
24	9	0	6.100840	-3.041330	0.776660
25	9	0	7.829708	-2.186889	-0.189186
26	9	0	6.698918	-1.010276	1.228576
27	16	0	4.429733	1.778219	0.514985
28	8	0	5.767858	2.229661	0.099506
29	6	0	3.299703	3.236135	0.214141
30	9	0	3.394233	3.684246	-1.021008

31	9	0	3.647290	4.195366	1.059934
32	9	0	2.053929	2.857932	0.463800
33	46	0	-0.689113	-0.858252	-0.090598
34	15	0	-3.008003	-0.752966	0.639138
35	6	0	-4.292396	-0.617083	-0.651015
36	6	0	-6.103524	-0.445891	-2.771285
37	6	0	-4.900913	0.601161	-0.961560
38	6	0	-4.597631	-1.751630	-1.414205
39	6	0	-5.502329	-1.664913	-2.464921
40	6	0	-5.802061	0.683936	-2.018306
41	1	0	-4.672996	1.491478	-0.377131
42	1	0	-4.130101	-2.709843	-1.184853
43	1	0	-5.738702	-2.553423	-3.047584
44	1	0	-6.271930	1.638145	-2.250471
45	1	0	-6.809403	-0.378793	-3.597125
46	6	0	-3.509482	-2.158204	1.681033
47	6	0	-4.168887	-4.237387	3.417229
48	6	0	-4.851081	-2.471057	1.923558
49	6	0	-2.502835	-2.898143	2.308207
50	6	0	-2.832364	-3.933794	3.176969
51	6	0	-5.177265	-3.508598	2.789277
52	1	0	-5.638664	-1.898848	1.431972
53	1	0	-1.455151	-2.661741	2.107750
54	1	0	-2.043868	-4.507194	3.660537
55	1	0	-6.222151	-3.749910	2.976111
56	1	0	-4.428261	-5.050546	4.092820
57	6	0	-3.201874	0.720141	1.706252
58	6	0	-3.324355	3.008888	3.304302
59	6	0	-3.761370	0.655001	2.985443
60	6	0	-2.699212	1.941537	1.235729
61	6	0	-2.767107	3.081537	2.029365
62	6	0	-3.820557	1.798018	3.779100
63	1	0	-4.146795	-0.290029	3.366987
64	1	0	-2.257412	2.001583	0.236958
65	1	0	-2.377678	4.025012	1.647174
66	1	0	-4.256903	1.739024	4.774821
67	1	0	-3.368933	3.898365	3.930313
68	1	0	0.541481	4.510784	-1.356961
69	6	0	-0.468693	4.895955	-1.230651
70	6	0	-3.062187	5.864110	-0.912491
71	6	0	-1.557456	4.066414	-1.545375
72	6	0	-0.679199	6.186350	-0.761342
73	6	0	-1.973811	6.675737	-0.599545
74	6	0	-2.858558	4.572290	-1.379427
75	1	0	0.175184	6.817094	-0.520288
76	1	0	-2.133545	7.688188	-0.232441
77	1	0	-3.704671	3.932282	-1.629013
78	1	0	-4.076521	6.241997	-0.792602
79	6	0	-1.369992	2.724196	-1.990702
80	29	0	-1.174252	-0.305045	-2.565682
81	6	0	-1.270253	1.550808	-2.348779

Zero-point correction=	0.564561 (Hartree/Particle)
Thermal correction to Energy=	0.617339
Thermal correction to Enthalpy=	0.618283
Thermal correction to Gibbs Free Energy=	0.469982
Sum of electronic and zero-point Energies=	-3834.044612
Sum of electronic and thermal Energies=	-3833.991834
Sum of electronic and thermal Enthalpies=	-3833.990890
Sum of electronic and thermal Free Energies=	-3834.139191

$TS_{VIICu\text{-}VIIICu}$

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Imaginary frequency: -48.6491 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.830415	1.550395	-1.647896
2	6	0	-1.970325	0.477845	-1.498586
3	6	0	-3.004679	0.086512	-0.401422
4	1	0	-2.137945	-0.018159	-2.459068
5	6	0	-1.871764	-0.555363	0.383861
6	6	0	-0.973814	-0.192704	-0.567047
7	6	0	-1.807585	-1.256138	1.666218
8	6	0	-1.601175	-2.585797	4.140378
9	6	0	-2.699754	-0.963435	2.713474
10	6	0	-0.816307	-2.234713	1.878350
11	6	0	-0.710593	-2.887261	3.105763
12	6	0	-2.594914	-1.625452	3.937240
13	1	0	-3.458610	-0.199914	2.573649
14	1	0	-0.149479	-2.502928	1.060823
15	1	0	0.057893	-3.642400	3.248056
16	1	0	-3.290428	-1.384992	4.736922
17	1	0	-1.524566	-3.100031	5.094451
18	53	0	1.028185	-2.798683	-2.261684
19	8	0	-4.013522	-0.753205	-0.967565
20	8	0	-3.609988	1.137531	0.355463
21	16	0	-4.546755	2.278792	-0.508083
22	8	0	-3.691679	3.428722	-0.894747
23	6	0	-5.323614	2.776477	1.144323
24	9	0	-4.412125	3.309958	1.954260
25	9	0	-6.261841	3.691078	0.870382
26	9	0	-5.894410	1.724889	1.733584
27	16	0	-5.179266	-1.366581	0.110095
28	8	0	-6.474816	-0.695692	-0.154346
29	6	0	-5.218556	-2.967466	-0.887466
30	9	0	-5.520593	-2.753381	-2.163317
31	9	0	-6.153729	-3.752588	-0.335346
32	9	0	-4.030947	-3.569423	-0.790907
33	15	0	3.279454	-0.298843	0.633917
34	6	0	4.786637	0.264423	-0.257679
35	6	0	7.036678	1.254967	-1.608454
36	6	0	6.079098	-0.084816	0.165732
37	6	0	4.631872	1.106000	-1.371174
38	6	0	5.754524	1.603879	-2.036210
39	6	0	7.196348	0.406403	-0.510422
40	1	0	6.214945	-0.744586	1.016966
41	1	0	3.636607	1.362309	-1.722338
42	1	0	5.623094	2.256251	-2.895313
43	1	0	8.192077	0.124038	-0.179296
44	1	0	7.909046	1.636377	-2.132321
45	6	0	3.029371	0.920570	1.993592
46	6	0	2.409826	2.804741	3.982346
47	6	0	3.738671	2.126858	2.073853
48	6	0	1.998364	0.671049	2.920082
49	6	0	1.695556	1.606147	3.909384
50	6	0	3.429392	3.061254	3.064544

51	1	0	4.532317	2.338341	1.364653
52	1	0	1.437590	-0.260084	2.878479
53	1	0	0.899136	1.398425	4.618533
54	1	0	3.987282	3.992234	3.115906
55	1	0	2.170011	3.535859	4.749396
56	6	0	3.790191	-1.849601	1.486932
57	6	0	4.606730	-4.264036	2.663559
58	6	0	4.297964	-1.866420	2.796322
59	6	0	3.693063	-3.056960	0.775315
60	6	0	4.103237	-4.255241	1.360892
61	6	0	4.701314	-3.069027	3.379801
62	1	0	4.376244	-0.943044	3.361351
63	1	0	3.282955	-3.064302	-0.230553
64	1	0	4.021861	-5.181461	0.798846
65	1	0	5.090272	-3.069963	4.394568
66	1	0	4.920988	-5.198648	3.120346
67	46	0	0.980784	-0.298756	-0.327929
68	6	0	1.154712	1.474088	-2.173800
69	6	0	1.133559	2.635822	-1.744979
70	29	0	1.179704	-0.315459	-2.829374
71	6	0	1.144843	3.999660	-1.329293
72	6	0	2.330125	4.761793	-1.412248
73	6	0	-0.032058	4.620245	-0.856188
74	6	0	2.336569	6.100806	-1.032268
75	1	0	3.235383	4.290094	-1.781974
76	6	0	-0.013042	5.958385	-0.472683
77	1	0	-0.956517	4.054131	-0.799767
78	6	0	1.166849	6.702894	-0.559690
79	1	0	3.254717	6.677521	-1.106733
80	1	0	-0.926396	6.422530	-0.111379
81	1	0	1.174151	7.748560	-0.263882

Zero-point correction=	0.562140 (Hartree/Particle)
Thermal correction to Energy=	0.613395
Thermal correction to Enthalpy=	0.614340
Thermal correction to Gibbs Free Energy=	0.461932
Sum of electronic and zero-point Energies=	-3835.480588
Sum of electronic and thermal Energies=	-3835.429332
Sum of electronic and thermal Enthalpies=	-3835.428388
Sum of electronic and thermal Free Energies=	-3835.580795

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Imaginary frequency: -55.0764 cm^{-1}

Zero-point correction=	0.559850 (Hartree/Particle)
Thermal correction to Energy=	0.610905
Thermal correction to Enthalpy=	0.611849
Thermal correction to Gibbs Free Energy=	0.468199
Sum of electronic and zero-point Energies=	-3834.019025
Sum of electronic and thermal Energies=	-3833.967970
Sum of electronic and thermal Enthalpies=	-3833.967026
Sum of electronic and thermal Free Energies=	-3834.110676

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.554492 (Hartree/Particle)
Thermal correction to Energy=	0.604844
Thermal correction to Enthalpy=	0.605788

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Thermal correction to Gibbs Free Energy=         0.469549
Sum of electronic and zero-point Energies=          -3837.163503
Sum of electronic and thermal Energies=             -3837.113152
Sum of electronic and thermal Enthalpies=           -3837.112207
Sum of electronic and thermal Free Energies=        -3837.248447
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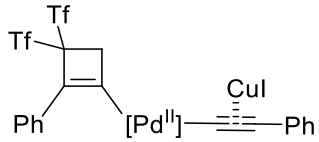
VIII-Cu



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.742429	1.304074	-2.068223
2	6	0	-1.821828	0.482443	-1.350049
3	6	0	-3.015295	0.606784	-0.357926
4	1	0	-1.776350	-0.476529	-1.874087
5	6	0	-2.007376	0.690874	0.785812
6	6	0	-0.968309	0.602767	-0.082986
7	6	0	-2.188037	0.830620	2.231132
8	6	0	-2.512125	1.128603	5.009456
9	6	0	-3.280421	1.550406	2.752774
10	6	0	-1.265156	0.257944	3.126080
11	6	0	-1.427157	0.408707	4.501671
12	6	0	-3.436388	1.697480	4.130324
13	1	0	-3.992790	2.010582	2.075319
14	1	0	-0.434075	-0.317706	2.732476
15	1	0	-0.709731	-0.045780	5.179800
16	1	0	-4.281503	2.260495	4.517094
17	1	0	-2.638307	1.241976	6.082799
18	53	0	0.727551	-2.816311	-3.551419
19	8	0	-3.811366	-0.576634	-0.456935
20	8	0	-3.833314	1.768640	-0.420474
21	16	0	-4.781403	1.972831	-1.838430
22	8	0	-4.036301	2.800021	-2.816640
23	6	0	-5.837540	3.196355	-0.853277
24	9	0	-5.123874	4.259530	-0.489333
25	9	0	-6.830860	3.585877	-1.661535
26	9	0	-6.356259	2.608420	0.226739
27	16	0	-5.036929	-0.784998	0.708020
28	8	0	-6.354277	-0.546743	0.071195
29	6	0	-4.750398	-2.648828	0.611796
30	9	0	-4.887182	-3.112484	-0.624385
31	9	0	-5.658578	-3.228188	1.408084
32	9	0	-3.526618	-2.925339	1.073540
33	46	0	0.990487	0.916273	0.004380
34	15	0	3.400627	1.530743	0.072197
35	6	0	3.652122	3.312939	-0.320906
36	6	0	3.922422	6.019059	-1.022574
37	6	0	4.884687	3.968976	-0.166800
38	6	0	2.562201	4.033877	-0.831048
39	6	0	2.693325	5.379160	-1.181586
40	6	0	5.016656	5.312418	-0.514344
41	1	0	5.741421	3.432515	0.229424

42	1	0	1.599366	3.542248	-0.967753
43	1	0	1.838902	5.920625	-1.577201
44	1	0	5.975123	5.809021	-0.390898
45	1	0	4.029995	7.065466	-1.294093
46	6	0	4.125912	1.283775	1.743724
47	6	0	5.022723	0.803049	4.363361
48	6	0	4.563586	0.003564	2.124188
49	6	0	4.129032	2.314415	2.696494
50	6	0	4.576908	2.073652	3.996894
51	6	0	5.014067	-0.230750	3.423773
52	1	0	4.558698	-0.810044	1.405136
53	1	0	3.788501	3.309237	2.425958
54	1	0	4.578869	2.883381	4.721421
55	1	0	5.361612	-1.222843	3.699139
56	1	0	5.374810	0.618792	5.374555
57	6	0	4.497823	0.607809	-1.076426
58	6	0	6.091653	-0.768510	-2.928523
59	6	0	3.914006	-0.044264	-2.172714
60	6	0	5.893030	0.559400	-0.914291
61	6	0	6.682905	-0.124186	-1.837295
62	6	0	4.707252	-0.730386	-3.095040
63	1	0	2.836144	-0.032515	-2.305946
64	1	0	6.362377	1.037448	-0.059437
65	1	0	7.760577	-0.158871	-1.701984
66	1	0	4.232601	-1.243931	-3.925728
67	1	0	6.710408	-1.306319	-3.641562
68	1	0	0.364071	-4.583669	0.344896
69	6	0	0.884867	-4.543576	1.297175
70	6	0	2.225506	-4.426787	3.747786
71	6	0	1.382178	-3.311637	1.762536
72	6	0	1.062847	-5.700218	2.052506
73	6	0	1.729975	-5.646435	3.278796
74	6	0	2.060157	-3.265334	2.997531
75	1	0	0.676941	-6.645610	1.682065
76	1	0	1.864501	-6.550657	3.865801
77	1	0	2.450158	-2.316580	3.353700
78	1	0	2.745684	-4.380563	4.700775
79	6	0	1.200468	-2.101312	1.011441
80	29	0	0.960956	-2.040797	-1.199925
81	6	0	1.105461	-0.960238	0.531629

Zero-point correction=	0.562205 (Hartree/Particle)
Thermal correction to Energy=	0.616104
Thermal correction to Enthalpy=	0.617048
Thermal correction to Gibbs Free Energy=	0.455456
Sum of electronic and zero-point Energies=	-3835.517861
Sum of electronic and thermal Energies=	-3835.463961
Sum of electronic and thermal Enthalpies=	-3835.463017
Sum of electronic and thermal Free Energies=	-3835.624609

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I).

Zero-point correction=	0.558061 (Hartree/Particle)
Thermal correction to Energy=	0.608952
Thermal correction to Enthalpy=	0.609897
Thermal correction to Gibbs Free Energy=	0.465709
Sum of electronic and zero-point Energies=	-3834.051705
Sum of electronic and thermal Energies=	-3834.000814
Sum of electronic and thermal Enthalpies=	-3833.999869
Sum of electronic and thermal Free Energies=	-3834.144057

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.553330	(Hartree/Particle)
Thermal correction to Energy=	0.604446	
Thermal correction to Enthalpy=	0.605390	
Thermal correction to Gibbs Free Energy=	0.461502	
Sum of electronic and zero-point Energies=	-3837.190409	
Sum of electronic and thermal Energies=	-3837.139293	
Sum of electronic and thermal Enthalpies=	-3837.138349	
Sum of electronic and thermal Free Energies=	-3837.282238	

M06/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I), PCM(Triethylamine)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.947219	0.363593	-2.761993
2	6	0	-1.880660	-0.057247	-1.750132
3	6	0	-2.998763	0.402194	-0.792895
4	1	0	-1.753730	-1.146734	-1.808823
5	6	0	-1.960145	1.121031	0.029993
6	6	0	-0.970428	0.687542	-0.784662
7	6	0	-2.069041	1.906715	1.252064
8	6	0	-2.270595	3.431162	3.595044
9	6	0	-3.230519	2.643565	1.525878
10	6	0	-1.012279	1.944182	2.173564
11	6	0	-1.111908	2.702566	3.331984
12	6	0	-3.327100	3.398157	2.689383
13	1	0	-4.053241	2.637238	0.810869
14	1	0	-0.114597	1.357137	1.978374
15	1	0	-0.280926	2.719721	4.035763
16	1	0	-4.233135	3.968224	2.887408
17	1	0	-2.349400	4.022934	4.505358
18	53	0	0.925212	-3.395712	-2.908338
19	8	0	-3.585006	-0.748108	-0.199006
20	8	0	-4.004777	1.271925	-1.271480
21	16	0	-5.093338	0.634601	-2.387682
22	8	0	-4.739241	1.118384	-3.732502
23	6	0	-6.324764	1.892874	-1.754812
24	9	0	-5.861178	3.117490	-1.907400
25	9	0	-7.434785	1.750497	-2.461546
26	9	0	-6.585490	1.667659	-0.474724
27	16	0	-4.579851	-0.462361	1.120118
28	8	0	-5.854554	-1.149443	0.852248
29	6	0	-3.585291	-1.681551	2.130961
30	9	0	-3.546934	-2.865060	1.553986
31	9	0	-4.172214	-1.786105	3.315675
32	9	0	-2.356633	-1.211832	2.288903
33	46	0	1.008971	1.000188	-0.752789
34	15	0	3.392262	1.312020	-0.260422
35	6	0	4.347035	2.549024	-1.205771
36	6	0	5.732652	4.465146	-2.685381
37	6	0	5.689830	2.823105	-0.921200
38	6	0	3.709573	3.239396	-2.238715
39	6	0	4.400405	4.196501	-2.977306
40	6	0	6.377877	3.777918	-1.657806
41	1	0	6.197463	2.289788	-0.116882
42	1	0	2.665330	3.023972	-2.472694
43	1	0	3.896552	4.728608	-3.781868

44	1	0	7.421741	3.988186	-1.432321
45	1	0	6.274703	5.212899	-3.261399
46	6	0	3.451906	1.888391	1.473058
47	6	0	3.246573	2.794318	4.111387
48	6	0	3.236419	0.980896	2.518652
49	6	0	3.547312	3.252906	1.762512
50	6	0	3.443965	3.701943	3.075798
51	6	0	3.143544	1.433550	3.829745
52	1	0	3.138408	-0.084732	2.307318
53	1	0	3.707875	3.972946	0.959945
54	1	0	3.523557	4.766476	3.288501
55	1	0	2.992086	0.716022	4.634875
56	1	0	3.174273	3.146141	5.139016
57	6	0	4.381614	-0.218257	-0.310152
58	6	0	5.836308	-2.591607	-0.519490
59	6	0	4.051760	-1.168003	-1.282180
60	6	0	5.451067	-0.465751	0.555922
61	6	0	6.175088	-1.648471	0.448226
62	6	0	4.773557	-2.352366	-1.385606
63	1	0	3.217324	-0.986513	-1.963333
64	1	0	5.706853	0.256380	1.331682
65	1	0	7.003034	-1.838060	1.129018
66	1	0	4.488449	-3.088897	-2.135146
67	1	0	6.399654	-3.520052	-0.593306
68	1	0	0.986007	-4.149459	1.147584
69	6	0	0.872886	-3.764103	2.161462
70	6	0	0.575391	-2.757288	4.746685
71	6	0	0.765061	-2.382732	2.366754
72	6	0	0.832144	-4.629666	3.246686
73	6	0	0.684665	-4.130560	4.538350
74	6	0	0.614922	-1.882978	3.669487
75	1	0	0.914783	-5.702134	3.081657
76	1	0	0.652081	-4.813550	5.385101
77	1	0	0.523556	-0.806342	3.818057
78	1	0	0.455236	-2.364743	5.754824
79	6	0	0.808015	-1.459052	1.275577
80	29	0	0.936645	-2.009120	-0.868789
81	6	0	0.884005	-0.522200	0.466392

Zero-point correction=	0.563697 (Hartree/Particle)
Thermal correction to Energy=	0.616748
Thermal correction to Enthalpy=	0.617692
Thermal correction to Gibbs Free Energy=	0.466719
Sum of electronic and zero-point Energies=	-3834.059368
Sum of electronic and thermal Energies=	-3834.006318
Sum of electronic and thermal Enthalpies=	-3834.005373
Sum of electronic and thermal Free Energies=	-3834.156347

H_2O

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

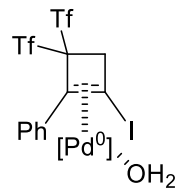
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.000000	0.762208	-0.478067
2	8	0	-0.000000	0.000000	0.119517
3	1	0	-0.000000	-0.762208	-0.478067

Zero-point correction=	0.021144 (Hartree/Particle)
Thermal correction to Energy=	0.023979
Thermal correction to Enthalpy=	0.024923
Thermal correction to Gibbs Free Energy=	0.003478
Sum of electronic and zero-point Energies=	-76.385879
Sum of electronic and thermal Energies=	-76.383045
Sum of electronic and thermal Enthalpies=	-76.382101
Sum of electronic and thermal Free Energies=	-76.403546

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.021994 (Hartree/Particle)
Thermal correction to Energy=	0.024831
Thermal correction to Enthalpy=	0.025775
Thermal correction to Gibbs Free Energy=	0.004401
Sum of electronic and zero-point Energies=	-76.401146
Sum of electronic and thermal Energies=	-76.398309
Sum of electronic and thermal Enthalpies=	-76.397365
Sum of electronic and thermal Free Energies=	-76.418739

IX



B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.945035	-1.209936	-2.277761
2	6	0	1.333622	-0.560474	-1.645862
3	6	0	2.186415	0.067846	-0.511353
4	1	0	0.756666	0.132345	-2.261760
5	6	0	1.416120	-0.752178	0.530805
6	6	0	0.586298	-1.289437	-0.521760
7	6	0	1.873479	-1.233872	1.847788
8	6	0	2.693362	-2.126612	4.404655
9	6	0	3.076777	-0.780710	2.424561
10	6	0	1.091100	-2.145228	2.587979
11	6	0	1.498948	-2.587327	3.843275
12	6	0	3.475218	-1.221643	3.687639
13	1	0	3.722559	-0.101140	1.881648
14	1	0	0.151973	-2.498015	2.175406
15	1	0	0.876551	-3.292515	4.388256
16	1	0	4.409452	-0.855691	4.105582
17	1	0	3.007852	-2.469422	5.386615
18	53	0	-0.050766	-3.347330	-0.823483
19	8	0	2.079879	1.511268	-0.530580
20	8	0	3.562971	-0.288471	-0.526040
21	16	0	4.555474	0.525753	-1.655258

22	8	0	4.364387	-0.032862	-3.015820
23	6	0	6.021200	-0.412633	-0.916212
24	9	0	5.890555	-1.727780	-1.047310
25	9	0	7.106091	-0.005533	-1.591121
26	9	0	6.167107	-0.091243	0.372011
27	16	0	2.193865	2.324285	0.935507
28	8	0	3.604380	2.620037	1.282581
29	6	0	1.570413	3.882876	0.066053
30	9	0	2.414575	4.296530	-0.869159
31	9	0	1.455302	4.825890	1.014043
32	9	0	0.361643	3.672823	-0.473055
33	46	0	-0.659767	-0.036793	0.544116
34	15	0	-2.934207	0.202760	-0.144208
35	6	0	-4.082516	-1.130534	0.407765
36	6	0	-5.760196	-3.167039	1.366710
37	6	0	-5.257087	-1.467520	-0.282370
38	6	0	-3.753812	-1.833572	1.578009
39	6	0	-4.591856	-2.840524	2.058342
40	6	0	-6.089374	-2.481306	0.195445
41	1	0	-5.519222	-0.944377	-1.197011
42	1	0	-2.833888	-1.593648	2.105332
43	1	0	-4.325130	-3.377061	2.964810
44	1	0	-6.993547	-2.737425	-0.350436
45	1	0	-6.407957	-3.958271	1.734551
46	6	0	-3.673943	1.747240	0.565394
47	6	0	-4.619354	4.145358	1.704468
48	6	0	-4.867319	1.767812	1.300584
49	6	0	-2.956907	2.950706	0.411723
50	6	0	-3.428349	4.139265	0.971966
51	6	0	-5.334442	2.958718	1.865366
52	1	0	-5.435137	0.853123	1.436511
53	1	0	-2.031104	2.958599	-0.158159
54	1	0	-2.865789	5.059132	0.834782
55	1	0	-6.260777	2.954189	2.433658
56	1	0	-4.984194	5.068601	2.145891
57	6	0	-3.262915	0.370679	-1.951869
58	6	0	-3.694169	0.525761	-4.723093
59	6	0	-4.250824	1.221540	-2.472340
60	6	0	-2.490724	-0.397954	-2.837936
61	6	0	-2.709966	-0.324458	-4.213756
62	6	0	-4.462432	1.298638	-3.850625
63	1	0	-4.852382	1.830075	-1.803827
64	1	0	-1.719413	-1.055490	-2.447896
65	1	0	-2.106088	-0.926667	-4.887022
66	1	0	-5.227499	1.964605	-4.240993
67	1	0	-3.858517	0.588760	-5.795415
68	1	0	-0.052958	1.702166	2.665955
69	8	0	-0.942646	1.381155	2.448661
70	1	0	-1.462785	2.161326	2.188465

Zero-point correction= 0.485502 (Hartree/Particle)
Thermal correction to Energy= 0.532957
Thermal correction to Enthalpy= 0.533901
Thermal correction to Gibbs Free Energy= 0.393193
Sum of electronic and zero-point Energies= -3408.007045
Sum of electronic and thermal Energies= -3407.959590
Sum of electronic and thermal Enthalpies= -3407.958646
Sum of electronic and thermal Free Energies= -3408.099354

M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Zero-point correction=	0.478950	(Hartree/Particle)
Thermal correction to Energy=	0.524109	
Thermal correction to Enthalpy=	0.525054	
Thermal correction to Gibbs Free Energy=	0.397410	
Sum of electronic and zero-point Energies=	-3408.620054	
Sum of electronic and thermal Energies=	-3408.574895	
Sum of electronic and thermal Enthalpies=	-3408.573951	
Sum of electronic and thermal Free Energies=	-3408.701594	

TS_{IX-I}

B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Imaginary frequency: -237.7616 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.747834	-1.398478	-2.054287
2	6	0	1.224250	-0.637950	-1.470329
3	6	0	2.088607	-0.081079	-0.326584
4	1	0	0.769026	0.097330	-2.132021
5	6	0	1.200547	-0.605525	0.716271
6	6	0	0.349030	-1.182982	-0.315988
7	6	0	1.479108	-0.809528	2.142310
8	6	0	1.989471	-1.100397	4.902222
9	6	0	2.457408	-0.021164	2.783493
10	6	0	0.759706	-1.741893	2.915034
11	6	0	1.017429	-1.885120	4.276608
12	6	0	2.705994	-0.169000	4.147784
13	1	0	3.029307	0.700599	2.210353
14	1	0	0.000586	-2.355679	2.443324
15	1	0	0.454223	-2.615308	4.851810
16	1	0	3.467156	0.446099	4.620630
17	1	0	2.186735	-1.214429	5.964473
18	53	0	-0.374851	-3.227148	-0.455708
19	8	0	3.402916	-0.215155	-0.204799
20	16	0	4.542621	-0.108143	-1.600901
21	8	0	3.929719	-0.629274	-2.837895
22	6	0	5.374330	-1.645026	-0.860681
23	9	0	4.561888	-2.697723	-0.844389
24	9	0	6.425606	-1.909280	-1.650408
25	9	0	5.812128	-1.382554	0.372544
26	46	0	-0.788939	0.337975	0.464342
27	15	0	-3.053989	0.456029	-0.162215
28	6	0	-3.666313	2.151278	-0.566606
29	6	0	-4.549440	4.763976	-1.094537
30	6	0	-4.694735	2.381415	-1.494490
31	6	0	-3.079030	3.246652	0.088722
32	6	0	-3.524120	4.543788	-0.172553
33	6	0	-5.132413	3.681087	-1.755837
34	1	0	-5.150356	1.546272	-2.017725
35	1	0	-2.268422	3.087619	0.794679
36	1	0	-3.061050	5.383006	0.339537
37	1	0	-5.926729	3.846284	-2.479060

38	1	0	-4.888852	5.775378	-1.301917
39	6	0	-3.549293	-0.539261	-1.634563
40	6	0	-4.207376	-2.000197	-3.941847
41	6	0	-2.721273	-0.496802	-2.768033
42	6	0	-4.706697	-1.329709	-1.669231
43	6	0	-5.030880	-2.057438	-2.817180
44	6	0	-3.051708	-1.215111	-3.915950
45	1	0	-1.812099	0.098542	-2.747617
46	1	0	-5.355332	-1.382365	-0.800507
47	1	0	-5.928481	-2.670141	-2.828727
48	1	0	-2.401608	-1.171031	-4.785513
49	1	0	-4.460075	-2.568707	-4.832779
50	6	0	-4.182156	-0.126413	1.179411
51	6	0	-5.814582	-1.104613	3.246399
52	6	0	-5.389859	0.513256	1.495359
53	6	0	-3.799534	-1.259718	1.916890
54	6	0	-4.613817	-1.748937	2.937865
55	6	0	-6.198665	0.026784	2.525315
56	1	0	-5.699206	1.394158	0.941905
57	1	0	-2.860310	-1.756039	1.688001
58	1	0	-4.306323	-2.628347	3.497396
59	1	0	-7.129254	0.535331	2.763153
60	1	0	-6.444776	-1.480451	4.048015
61	8	0	1.753014	1.806780	-0.292479
62	16	0	2.635795	2.904681	-1.030330
63	8	0	3.479513	2.271181	-2.100990
64	6	0	3.872940	3.245078	0.368511
65	9	0	4.634091	4.292623	0.026217
66	9	0	3.191732	3.555937	1.486774
67	9	0	4.676851	2.203604	0.640993
68	1	0	0.191706	1.950325	2.521240
69	8	0	-0.186981	2.336823	1.713567
70	1	0	0.572095	2.387987	1.089808

Zero-point correction=	0.484530	(Hartree/Particle)
Thermal correction to Energy=	0.531493	
Thermal correction to Enthalpy=	0.532437	
Thermal correction to Gibbs Free Energy=	0.392921	
Sum of electronic and zero-point Energies=	-3407.994488	
Sum of electronic and thermal Energies=	-3407.947525	
Sum of electronic and thermal Enthalpies=	-3407.946581	
Sum of electronic and thermal Free Energies=	-3408.086097	

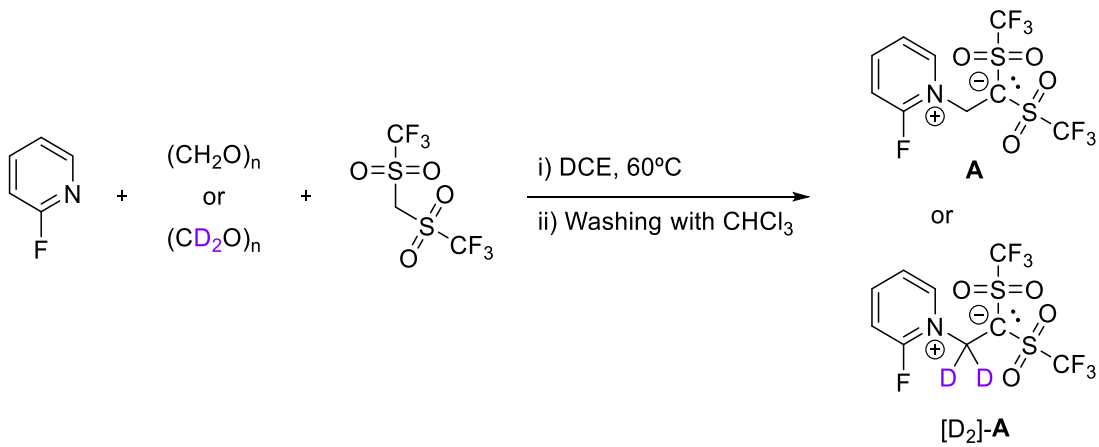
M06/ 6-311+G** (C,H,O,S,F,P,N), SDD (Pd,Cu,I), SMD(Triethylamine) // B3LYP/6-31G(d) (C,H,O,S,F,P,N), LANL2DZ (Pd,Cu,I)

Imaginary frequency: -306.6755 cm^{-1}

Zero-point correction=	0.477421	(Hartree/Particle)
Thermal correction to Energy=	0.523197	
Thermal correction to Enthalpy=	0.524141	
Thermal correction to Gibbs Free Energy=	0.395871	
Sum of electronic and zero-point Energies=	-3408.602495	
Sum of electronic and thermal Energies=	-3408.556719	
Sum of electronic and thermal Enthalpies=	-3408.555775	
Sum of electronic and thermal Free Energies=	-3408.684044	

General Methods: ^{1}H NMR, ^{13}C NMR, ^{19}F NMR, and D(^{2}H) NMR spectra were recorded on a Bruker Avance AMX-700, Bruker AMX-500, or Bruker Avance-DPX 300. NMR spectra were recorded in $CDCl_3$ or C_6D_6 solutions, except otherwise stated. Chemical shifts are given in ppm relative to TMS (^{1}H, 0.0 ppm), or $CDCl_3$ (^{1}H, 7.27 ppm; ^{13}C, 76.9 ppm), or C_6D_6 (^{1}H, 7.16 ppm; ^{13}C, 128.0 ppm). Chemical shifts in ^{19}F are given in ppm relative to (trifluoromethyl)benzene ($C_6H_5CF_3$) in $CDCl_3$ (^{19}F, –63.7 ppm). Low and high resolution mass spectra were taken on an AGILENT 6520 Accurate-Mass QTOF LC/MS spectrometer using the electronic impact (EI) or electrospray modes (ES) unless otherwise stated. IR spectra were recorded on a Bruker Tensor 27 spectrometer. All commercially available compounds were used without further purification.

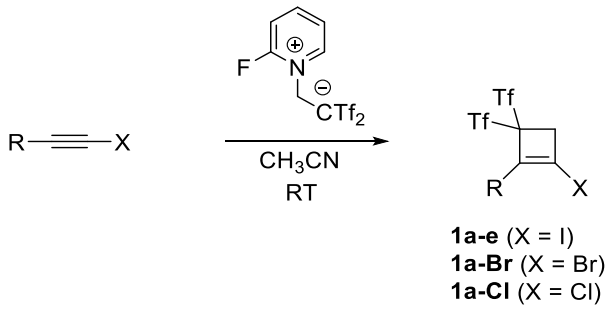
Yanai's reagent **A** was synthesized according to a literature procedure: H. Yanai, Y. Takahashi, H. Fukaya, Y. Dobashi, T. Matsumoto, *Chem. Commun.* **2013**, *49*, 10091. Deuterated azolium salt [D_2]-**A** was prepared adapting the same procedure: B. Alcaide, P. Almendros, C. Lázaro-Milla, *Chem. Eur. J.* **2019**, *25*, 7547.



To a solution of Tf_2CH_2 (281 mg, 1.00 mmol) in 1,2-dichloroethane (6.0 mL), paraformaldehyde (90% purity, 73.0 mg, 2.19 mmol) or paraformaldehyde-d_2 (98% purity, 98 atom % D, 64 mg, 2.00 mmol) and 2-fluoropyridine (172 µL, 2.00 mmol) were added at room temperature. After being

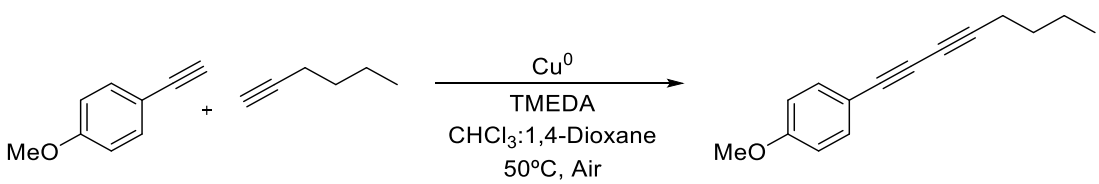
stirred for 8 h at 60 °C, the reaction mixture was concentrated under reduced pressure. The resulting residue was washed with $CHCl_3$ (1.0 mL x 3) to give zwitterion **A** in 91% yield (356 mg, 0.915 mmol) or [D_2]-**A** in 86% yield (336 mg, 0.858 mmol).

Bis(triflyl)iodocyclobutenes 1a–e, bis(triflyl)bromocyclobutene 1a–Br, and bis(triflyl)chlorocyclobutene 1a–Cl were prepared as described in the literature: 1a–Br, **1a–Cl**, **1a**, and **1e** (B. Alcaide, P. Almendros, C. Lázaro-Milla, *Adv. Synth. Catal.* **2017**, *359*, 2630); **[D_2]-1a** and **1b–d** (B. Alcaide, P. Almendros, C. Lázaro-Milla, *Chem. Eur. J.* **2019**, *25*, 7547).

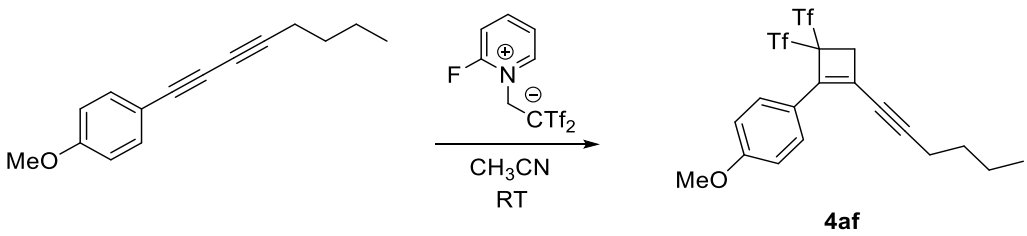


Yanai's reagent (0.2 mmol) was added at room temperature to a solution of the corresponding haloalkyne (0.2 mmol) in acetonitrile (5 mL). The reaction was stirred at room temperature until disappearance of the starting material (TLC), and then the mixture was concentrated under reduced pressure. Chromatography of the residue eluting with hexanes/ethyl acetate gave analytically pure bis(triflyl)halocyclobutenes **1a-e**, **1a-Br** or **1a-Cl**.

Novel bis(triflyl) cyclobutene 4af was prepared as follow:

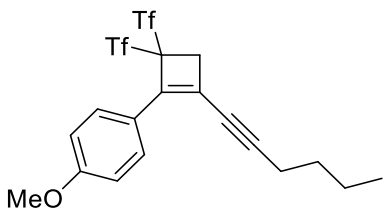


A Schlenk tube of 25 mL equipped with a magnetic stir bar was charged with copper powder (5 mol %), TMEDA (20 mol %) in $CHCl_3$/1,4-dioxane (0.3 mL/0.1 mL); then 1-ethynyl-4-methoxybenzene (0.20 mmol) and 1-hexyne (0.26 mmol) were added. The reaction mixture was stirred at 50ºC overnight. After completion of the reaction, the resulting solution was cooled to room temperature. Then $CHCl_3$ was added, and the solution was washed with saturated solution of NH_4Cl, and dried over anhydrous $MgSO_4$ and concentrated in vacuo. The crude product was purified by flash column chromatography on silica gel to give the desired 1-methoxy-4-(octa-1,3-diyn-1-yl)benzene (Procedure described in: Su, L.; Dong, J.; Liu, L.; Sun, M.; Qiu, R.; Zhou, Y.; Yin, S.-F. *J. Am. Chem. Soc.* **2016**, *138*, 12348).



4af

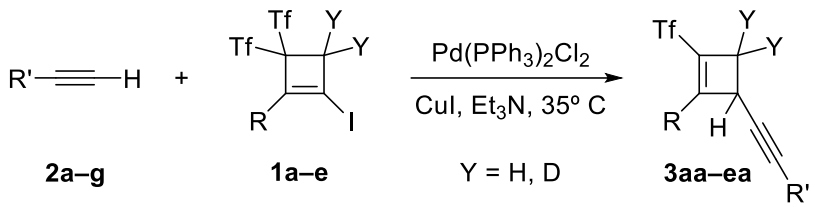
Yanai's reagent (0.24 mmol) was added at room temperature to a solution of the 1,3-diyne (50 mg, 0.24 mmol) in acetonitrile (5 mL). The reaction was stirred at room temperature until disappearance of the starting material (TLC), and then the mixture was concentrated under reduced pressure. Chromatography of the residue eluting with hexanes/diethyl ether (98:2) gave 76 mg (63%) of analytically pure compound **4af**. Spectroscopic and analytical data for bis(triflyl)cyclobutene **4af** follow.



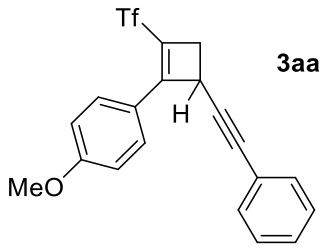
4af

1-(2-(Hex-1-yn-1-yl)-4,4-bis((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-4-methoxybenzene 4af. Colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.94 (m, 2H, $2CH^{Ar}$), 6.93 (m, 2H, $2CH^{Ar}$), 3.85 (s, 3H, OCH_3), 3.48 (s, 2H, CH_2), 2.55 (t, 2H, *J* = 7.0 Hz, CH_2), 1.65 (m, 2H, CH_2), 1.50 (m, 2H, CH_2), 0.98 (t, 3H, *J* = 7.3 Hz, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 161.0 ($C^{Ar\text{-}q}$-OMe), 136.9 (=C), 128.6 ($2CH^{Ar}$), 125.9 ($C^{Ar\text{-}q}$), 122.7 (=C-Tf), 119.8 (q, J_{CF} = 331.6 Hz, CF_3), 113.9 ($2CH^{Ar}$), 106.8 (*C*≡C), 86.6 (CTf_2), 74.8 (C≡*C*), 55.3 (OCH_3), 38.6 (CH_2), 30.0 (CH_2), 22.0 (CH_2), 19.8 (CH_2), 13.5 (CH_3); ^{19}F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –76.7 (s, 3F, CF_3); IR ($CHCl_3$): ν = 2211 (C≡C), 1383, 1104 (O=S=O), 1201 (C–F) cm^{-1}; HRMS (ES): calcd for $C_{19}H_{22}F_6N\,O_5S_2$ [*M* + NH_4]$^{+}$: 522.08381; found: 522.08373.

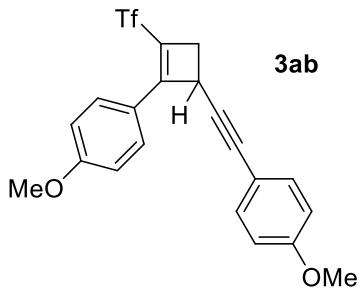
General procedure for the palladium-catalyzed reaction of bis(triflyl)iodocyclobutenes 1a–e with alkynes 2a–g. Synthesis of 1-triflyl-2-aryl-3-alkynyl-cyclobutenes 3.



A solution of the appropriate bis(triflyl)iodocyclobutene **1** (0.1 mmol), $Pd(PPh_3)_2Cl_2$ (0.005 mmol, 5.0 mol %), and CuI (0.005 mmol, 5.0 mol %) in triethylamine (2.5 mL) was stirred at rt for 10 minutes. Then, the corresponding alkyne (0.3 mmol) was slowly added. The resulting reaction mixture was gently heated at 35 ºC until disappearance of the starting material (TLC). After removal of the triethylamine in vacuum, the residue was purified by column chromatography on silica gel to give analytically pure compounds. Spectroscopic and analytical data for products **3** follow.

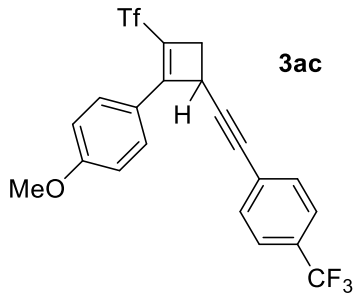


1-Methoxy-4-(4-(phenylethynyl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)benzene 3aa. From 50 mg (0.09 mmol) of iodocyclobutene **1a**, and after flash chromatography of the residue using hexanes/ethyl acetate (95:5) as eluent gave compound **3aa** (25 mg, 70%) as a pale yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$, 25 ºC): δ = 7.85 (m, 2H, $2CH^{Ar}$), 7.54 (m, 2H, $2CH^{Ar}$), 7.40 (m, 3H, $3CH^{Ar}$), 6.95 (m, 2H, $2CH^{Ar}$), 4.86 (dd, 1H, *J* = 4.4, 1.9 Hz, CH), 3.85 (s, 3H, OCH_3), 3.20 (d, 1H, *J* = 13.7 Hz, C*H*H), 3.15 (dd, 1H, *J* = 13.8, 4.5 Hz, CH*H*); ^{13}C NMR (125 MHz, $CDCl_3$, 25 ºC): δ = 160.6 ($C^{Ar\text{-}q}$-OMe), 139.1 (=C), 131.8 ($2CH^{Ar}$), 129.3 (CH^{Ar}), 128.5 ($2CH^{Ar}$), 128.2 ($2CH^{Ar}$), 124.8 ($C^{Ar\text{-}q}$), 122.0 ($C^{Ar\text{-}q}$), 120.7 (=C-Tf), 119.9 (q, J_{CF} = 329.2 Hz, CF_3), 114.0 ($2CH^{Ar}$), 98.4 (*C*≡C), 83.9 (C≡*C*), 57.3 (CH), 55.3 (OCH_3), 32.8 (CH_2); ^{19}F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –75.9 (s, 3F, CF_3); IR ($CHCl_3$): ν = 2197 (C≡C), 1372, 1089 (O=S=O), 1208 (C–F) cm^{-1}; HRMS (ES): calcd for $C_{20}H_{19}F_3NO_3S$ $[M + NH_4]^+$: 410.10323; found: 410.10476.

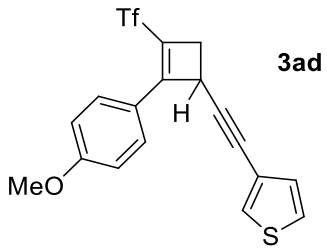


1-Methoxy-4-((2-(4-methoxyphenyl)-3-((trifluoromethyl)sulfonyl)cyclobut-2-en-1-yl)ethynyl)benzene 3ab. From 50 mg (0.09 mmol) of iodocyclobutene **1a**, and after flash chromatography of the residue using hexanes/toluene (1:1) as eluent gave compound **3ab** (25 mg, 65%) as a yellow solid; mp 122–124 ºC; ^{1}H NMR (500 MHz, $CDCl_3$, 25 ºC): δ = 7.84 (m, 2H,

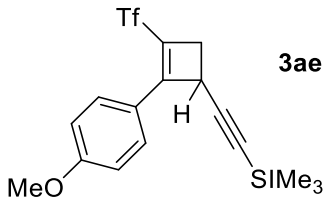
2CH^{Ar}), 7.48 (m, 2H, 2CH^{Ar}), 6.93 (m, 4H, 4CH^{Ar}), 4.85 (dd, 1H, *J* = 4.4, 1.9 Hz, CH), 3.85 (s, 3H, OCH_3), 3.85 (s, 3H, OCH_3), 3.13 (d, 1H, *J* = 13.8 Hz, C*H*H), 3.13 (dd, 1H, *J* = 13.8, 4.5 Hz, CH*H*); ^{13}C NMR (125 MHz, $CDCl_3$, 25 ºC): δ = 160.5 (2*C*$^{Ar\text{-}q}$-OMe), 138.1 (=C), 133.4 (2CH^{Ar}), 128.0 (2CH^{Ar}), 125.0 (*C*$^{Ar\text{-}q}$), 121.2 (=C-Tf), 119.9 (q, J_{CF} = 329.2 Hz, CF_3), 114.2 (2CH^{Ar}), 114.0 (*C*$^{Ar\text{-}q}$), 113.9 (2CH^{Ar}), 98.8 (*C*≡C), 82.0 (C≡*C*), 57.4 (CH), 55.4 (OCH_3), 55.3 (OCH_3), 32.8 (CH_2); ^{19}F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –75.9 (s, 3F, CF_3); IR ($CHCl_3$): ν = 2192 (C≡C), 1381, 1093 (O=S=O), 1210 (C–F) cm^{-1}; HRMS (ES): calcd for $C_{21}H_{21}F_3NO_4S$ [*M* + NH_4]$^+$: 440.11379; found: 440.11465.



1-Methoxy-4-(4-((4-(trifluoromethyl)phenyl)ethynyl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)benzene 3ac. From 50 mg (0.09 mmol) of iodocyclobutene **1a**, and after flash chromatography of the residue using hexanes/toluene (1:1) as eluent gave compound **3ac** (31 mg, 76%) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.83 (m, 2H, 2CH^{Ar}), 7.65 (m, 4H, 4CH^{Ar}), 6.96 (m, 2H, 2CH^{Ar}), 4.88 (m, 1H, CH), 3.86 (s, 3H, OCH_3), 3.17 (m, 2H, CH_2); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 160.9 (*C*$^{Ar\text{-}q}$-OMe), 140.5 (=C), 132.0 (2CH^{Ar}), 130.8 (q, J_{CF} = 32.9 Hz, *C*$^{Ar\text{-}q}$-CF_3), 128.3 (2CH^{Ar}), 125.8 (m, *C*$^{Ar\text{-}q}$), 125.5 (q, J_{CF} = 3.7 Hz, 2CH^{Ar}), 124.6 (*C*$^{Ar\text{-}q}$), 119.9 (=C-Tf), 119.9 (q, J_{CF} = 329.1 Hz, $2CF_3$), 114.1 (2CH^{Ar}), 96.4 (*C*≡C), 85.8 (C≡*C*), 57.3 (CH), 55.4 (OCH_3), 32.7 (CH_2); ^{19}F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –62.9 (s, 3F, CF_3), –75.9 (s, 3F, CF_3); IR ($CHCl_3$): ν = 1382, 1056 (O=S=O), 1204 (C–F) cm^{-1}; HRMS (ES): calcd for $C_{21}H_{14}F_6NaO_3S$ [*M* + Na]$^+$: 483.04601; found: 483.04672.

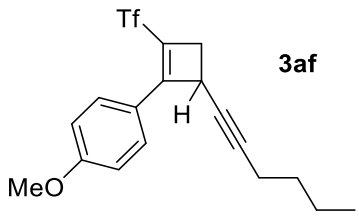


3-((2-(4-Methoxyphenyl)-3-((trifluoromethyl)sulfonyl)cyclobut-2-en-1-yl)ethynyl)thiophene 3ad. From 50 mg (0.09 mmol) of iodocyclobutene **1a**, and after flash chromatography of the residue using hexanes/toluene (7:3→6:4) as eluent gave compound **3ad** (22 mg, 63%) as a pale orange oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.83 (m, 2H, 2CH^{Ar}), 7.60 (dd, 1H, *J* = 2.9, 1.0 Hz, CH^{Ar}), 7.35 (dd, 1H, *J* = 5.0, 3.0 Hz, CH^{Ar}), 7.21 (dd, 1H, *J* = 5.0, 1.1 Hz, CH^{Ar}), 6.94 (m, 2H, 2CH^{Ar}), 4.85 (m, 1H, CH), 3.85 (s, 3H, OCH_3), 3.15 (m, 2H, CH_2); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 160.6 ($C^{Ar\text{-}q}$-OMe), 138.9 (=C), 130.2 (CH^{Ar}), 129.7 (CH^{Ar}), 128.1 (2CH^{Ar}), 125.9 (CH^{Ar}), 124.8 ($C^{Ar\text{-}q}$), 121.1 ($C^{Ar\text{-}q}$), 120.7 (=C-Tf), 119.9 (q, J_{CF} = 329.2 Hz, CF_3), 114.0 (2CH^{Ar}), 93.6 (*C*≡C), 83.5 (C≡*C*), 57.3 (CH), 55.3 (OCH_3), 32.8 (CH_2); ^{19}F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –75.9 (s, 3F, CF_3); IR ($CHCl_3$): ν = 1392, 1095 (O=S=O), 1210 (C–F) cm^{-1}; HRMS (ES): calcd for $C_{18}H_{17}F_3NO_3S_2$ [*M* + NH_4]$^{+}$: 416.05965; found: 416.05925.

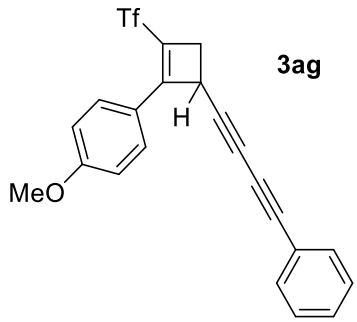


((2-(4-Methoxyphenyl)-3-((trifluoromethyl)sulfonyl)cyclobut-2-en-1-yl)ethynyl)trimethylsilane 3ae. From 50 mg (0.09 mmol) of iodocyclobutene **1a**, and after flash chromatography of the residue using hexanes/ethyl acetate (98:2) as eluent gave compound **3ae** (19 mg, 55%) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.79 (m, 2H, 2CH^{Ar}), 6.92 (m, 2H, 2CH^{Ar}), 4.79 (dd, 1H, *J* = 4.1, 2.3 Hz, CH), 3.85 (s, 3H, OCH_3), 3.06 (m, 2H, CH_2), 0.28 (s, 9H,

$3CH_3$); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 160.7 ($C^{Ar\text{-}q}$-OMe), 140.3 (=C), 128.2 ($2CH^{Ar}$), 124.7 ($C^{Ar\text{-}q}$), 120.6 (=C-Tf), 119.8 (q, J_{CF} = 329.1 Hz, CF_3), 113.9 ($2CH^{Ar}$), 105.6 (*C*≡C), 98.8 (C≡*C*), 57.1 (CH), 55.3 (OCH_3), 32.7 (CH_2), 0.36 ($3CH_3$); ^{19}F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –75.9 (s, 3F, CF_3); IR ($CHCl_3$): ν = 1373, 1090 (O=S=O), 1212 (C–F) cm^{-1}; HRMS (ES): calcd for $C_{17}H_{20}F_3O_3SSi$ $[M + H]^+$: 389.08490; found: 389.08376.

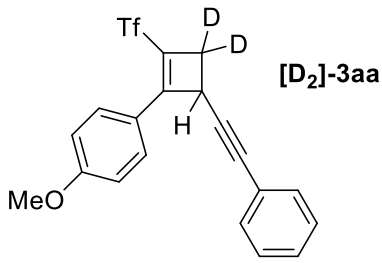


1-(4-(Hex-1-yn-1-yl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-4-methoxybenzene 3af. From 50 mg (0.09 mmol) of iodocyclobutene **1a**, and after flash chromatography of the residue using hexanes/toluene (1:1) as eluent gave compound **3af** (19 mg, 59%) as a colorless oil; ^1H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.77 (m, 2H, $2CH^{Ar}$), 6.91 (m, 2H, $2CH^{Ar}$), 4.78 (s, 1H, CH), 3.84 (s, 3H, OCH_3), 3.02 (m, 2H, CH_2), 2.49 (t, 2H, *J* = 6.9 Hz, CH_2), 1.63 (m, 2H, CH_2), 1.49 (m, 2H, CH_2), 0.97 (t, 3H, *J* = 7.2 Hz, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 160.3 ($C^{Ar\text{-}q}$-OMe), 137.8 (=C), 127.8 ($2CH^{Ar}$), 124.9 ($C^{Ar\text{-}q}$), 122.0 (=C-Tf), 119.9 (q, J_{CF} = 329.1 Hz, CF_3), 113.8 ($2CH^{Ar}$), 101.0 (*C*≡C), 75.7 (C≡*C*), 57.1 (CH), 55.3 (OCH_3), 32.9 (CH_2), 30.4 (CH_2), 22.0 (CH_2), 19.5 (CH_2), 13.5 (CH_3); ^{19}F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –76.0 (s, 3F, CF_3); IR ($CHCl_3$): ν = 1369, 1085 (O=S=O), 1207 (C–F) cm^{-1}; HRMS (ES): calcd for $C_{18}H_{23}F_3NO_3S$ $[M + NH_4]^+$: 390.13453; found: 390.13273.



3ag

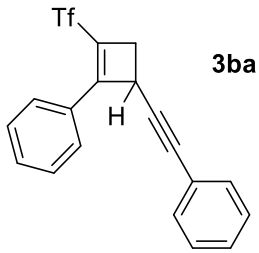
1-Methoxy-4-(4-(phenylbuta-1,3-diyn-1-yl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)benzene 3ag. From 50 mg (0.09 mmol) of iodocyclobutene **1a**, and after flash chromatography of the residue using hexanes/toluene (6:4) as eluent gave compound **3ag** (30 mg, 79%) as a pale orange oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.81 (m, 2H, 2CH^{Ar}), 7.56 (m, 2H, 2CH^{Ar}), 7.40 (m, 3H, 3CH^{Ar}), 6.95 (m, 2H, 2CH^{Ar}), 4.84 (m, 1H, CH), 3.86 (s, 3H, OCH_3), 3.12 (m, 2H, CH_2); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 161.1 ($C^{Ar\text{-}q}$-OMe), 143.0 (=C), 132.6 (2CH^{Ar}), 129.8 (CH^{Ar}), 128.5 (2CH^{Ar}), 128.3 (2CH^{Ar}), 124.6 ($C^{Ar\text{-}q}$), 121.1 ($C^{Ar\text{-}q}$), 118.9 (=C-Tf), 119.8 (q, J_{CF} = 329.1 Hz, CF_3), 114.0 (CH^{Ar}), 86.1 (*C*≡C), 82.7 (C≡*C*), 75.3 (*C*≡C), 73.4 (C≡*C*), 57.3 (CH), 55.4 (OCH_3), 32.7 (CH_2); ^{19}F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –75.8 (s, 3F, CF_3); IR ($CHCl_3$): ν = 1391, 1095 (O=S=O), 1211 (C–F) cm^{-1}; HRMS (ES): calcd for $C_{22}H_{19}F_3NO_3S$ [*M* + NH_4]$^{+}$: 434.10323; found: 434.10525.



[D$_2$]-3aa

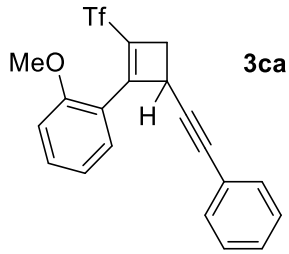
1-Methoxy-4-(4-(phenylethynyl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl-3,3-*d*$_2$)benzene [D$_2$]-3aa. From 50 mg (0.09 mmol) of iodocyclobutene **[D$_2$]-1a**, and after flash chromatography of the residue using hexanes/ethyl acetate (95:5) as eluent gave compound **[D$_2$]-3aa** (24 mg, 68%) as a pale yellow oil; ^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC): δ = 7.85 (m, 2H, 2CH^{Ar}), 7.54 (m, 2H, 2CH^{Ar}), 7.40 (m, 3H, 3CH^{Ar}), 6.95 (m, 2H, 2CH^{Ar}), 4.85 (s, 1H, CH), 3.85 (s, 3H,

OCH_3); ^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC): δ = 160.6 ($C^{Ar\text{-}q}$-OMe), 139.2 (=C), 131.8 ($2CH^{Ar}$), 129.3 (CH^{Ar}), 128.5 ($2CH^{Ar}$), 128.2 ($2CH^{Ar}$), 124.8 ($C^{Ar\text{-}q}$), 122.0 ($C^{Ar\text{-}q}$), 120.5 (=C-Tf), 119.9 (q, J_{CF} = 328.9 Hz, CF_3), 114.0 ($2CH^{Ar}$), 98.3 (*C*≡C), 83.9 (C≡*C*), 57.1 (CH), 55.3 (OCH_3), 32.2 (m, CD_2); ^{19}F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –75.9 (s, 3F, CF_3); D(^2H) NMR (107 MHz, $CDCl_3$, 25 ºC): δ = 3.17 (s, 2D, CD_2); IR ($CHCl_3$): ν = 2196 (C≡C), 1372, 1088 (O=S=O), 1207 (C–F) cm^{-1}; HRMS (ES): calcd for $C_{20}H_{17}D_2F_3NO_3S$ [M + NH_4]$^+$: 412.11578; found: 412.11648.



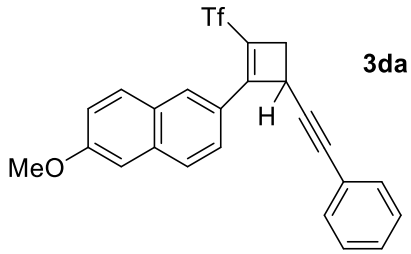
3ba

((2-Phenyl-3-((trifluoromethyl)sulfonyl)cyclobut-2-en-1-yl)ethynyl)benzene 3ba. From 50 mg (0.09 mmol) of iodocyclobutene **1b**, and after flash chromatography of the residue using hexanes/ethyl acetate (98:2) as eluent gave compound **3ba** (24 mg, 71%) as a pale yellow oil; ^1H NMR (700 MHz, $CDCl_3$, 25 ºC): δ = 7.90 (m, 2H, $2CH^{Ar}$), 7.56 (m, 2H, $2CH^{Ar}$), 7.42 (m, 4H, $4CH^{Ar}$), 4.91 (dd, 1H, *J* = 4.5, 1.8 Hz, CH), 3.23 (d, 1H, *J* = 13.8 Hz, C*H*H), 3.18 (dd, 1H, *J* = 13.9, 4.6 Hz, CH*H*); ^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC): δ = 139.4 (=C), 131.9 ($2CH^{Ar}$), 131.6 ($C^{Ar\text{-}q}$), 129.7 (CH^{Ar}), 129.5 (CH^{Ar}), 128.6 ($4CH^{Ar}$), 126.4 ($2CH^{Ar}$), 123.9 ($C^{Ar\text{-}q}$), 121.8 (=C-Tf), 119.9 (q, J_{CF} = 329.3 Hz, CF_3), 99.3 (*C*≡C), 83.6 (C≡*C*), 57.3 (CH), 33.0 (CH_2); ^{19}F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –75.9 (s, 3F, CF_3); IR ($CHCl_3$): ν = 2192 (C≡C), 1365, 1079 (O=S=O), 1211 (C–F) cm^{-1}; HRMS (ES): calcd for $C_{19}H_{17}F_3NO_2S$ [M + NH_4]$^+$: 380.09266; found: 380.09168.



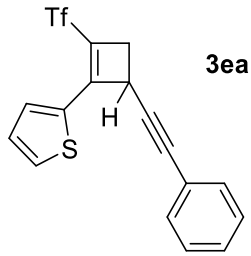
3ca

1-Methoxy-2-(4-(phenylethynyl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)benzene 3ca. From 50 mg (0.09 mmol) of iodocyclobutene **1c**, and after flash chromatography of the residue using hexanes/ethyl acetate (98:2) as eluent gave compound **3ca** (24 mg, 69%) as a colorless solid; mp 100–102 ºC; ^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC): δ = 7.83 (dd, 1H, *J* = 7.6, 1.6 Hz, CH^{Ar}), 7.49 (m, 2H, $2CH^{Ar}$), 7.37 (m, 4H, $4CH^{Ar}$), 7.01 (m, 1H, CH^{Ar}), 6.92 (d, 1H, *J* = 8.32 Hz, CH^{Ar}), 4.86 (dd, 1H, *J* = 4.6, 1.9 Hz, CH), 3.88 (s, 3H, OCH_3), 3.26 (dd, 1H, *J* = 13.8, 1.3 Hz, C*H*H), 3.21 (dd, 1H, *J* = 13.9, 4.6 Hz, CH*H*); ^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC): δ = 157.1 ($C^{Ar\text{-}q}$-OMe), 138.4 (=C), 131.8 ($2CH^{Ar}$), 131.0 (CH^{Ar}), 129.2 (CH^{Ar}), 128.9 (CH^{Ar}), 128.5 ($2CH^{Ar}$), 125.3 ($C^{Ar\text{-}q}$), 122.0 ($C^{Ar\text{-}q}$), 120.7 (=C-Tf), 119.8 (q, J_{CF} = 328.9 Hz, CF_3), 120.6 (CH^{Ar}), 110.9 (CH^{Ar}), 97.8 (*C*≡C), 83.4 (C≡*C*), 59.4 (CH), 55.1 (OCH_3), 33.6 (CH_2); ^{19}F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –77.0 (s, 3F, CF_3); IR ($CHCl_3$): ν = 2195 (C≡C), 1371, 1091 (O=S=O), 1209 (C–F) cm^{-1}; HRMS (ES): calcd for $C_{20}H_{19}F_3NO_3S$ $[M + NH_4]^+$: 410.10323; found: 410.10200.



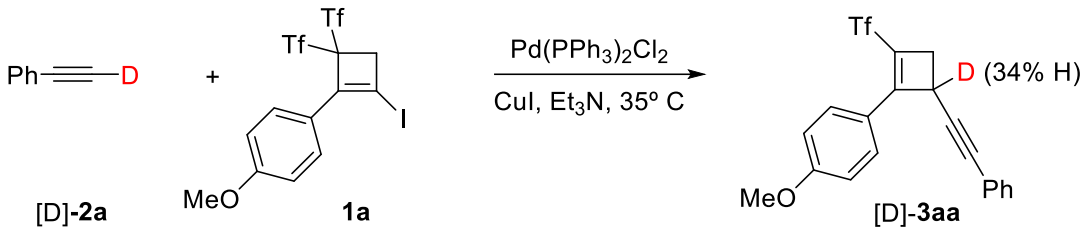
2-Methoxy-6-(4-(phenylethynyl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)naphthalene 3da. From 50 mg (0.09 mmol) of iodocyclobutene **1d**, and after flash chromatography of the residue using hexanes/diethyl ether (97:3) as eluent gave compound **3da** (25 mg, 68%) as a pale yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.21 (s, 1H, CH^{Ar}), 8.05 (dd, 1H, *J* = 8.6, 1.7 Hz, CH^{Ar}), 7.78 (m, 2H, $2CH^{Ar}$), 7.58 (m, 2H, $2CH^{Ar}$), 7.42 (m, 3H, $3CH^{Ar}$), 7.16 (m, 2H, $2CH^{Ar}$), 4.98 (m, 1H, CH), 3.94 (s, 3H, OCH_3), 3.22 (m, 2H, CH_2); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 158.8 ($C^{Ar\text{-}q}$-OMe), 139.6 (=C), 135.0 ($C^{Ar\text{-}q}$), 131.8 ($2CH^{Ar}$), 130.3 (CH^{Ar}), 129.4 (CH^{Ar}), 128.6 ($2CH^{Ar}$), 128.3 ($C^{Ar\text{-}q}$), 127.3 ($C^{Ar\text{-}q}$), 127.1 (CH^{Ar}), 126.5 (CH^{Ar}), 123.9 (CH^{Ar}), 122.7 (=C-Tf), 122.0 ($C^{Ar\text{-}q}$), 119.9

(q, J_{CF} = 329.3 Hz, CF_3), 119.5 (CH^{Ar}), 105.9 (CH^{Ar}), 99.1 (*C*≡C), 84.0 (C≡*C*), 57.4 (CH), 55.4 (OCH_3), 33.0 (CH_2); ^{19}F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –75.8 (s, 3F, CF_3); IR ($CHCl_3$): ν = 1391, 1095 (O=S=O), 1211 (C–F) cm^{-1}; HRMS (ES): calcd for $C_{24}H_{21}F_3NO_3S$ [*M* + NH_4]$^+$: 460.11888; found: 460.11940.



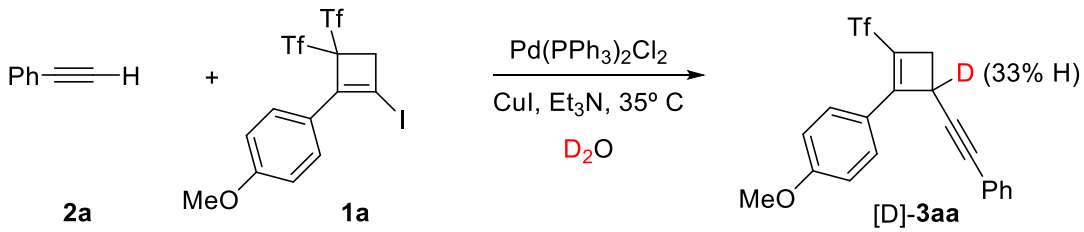
2-(4-(Phenylethynyl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)thiophene 3ea. From 45 mg (0.08 mmol) of iodocyclobutene **1e**, and after flash chromatography of the residue using hexanes/diethyl ether (95:5) as eluent gave compound **3ea** (25 mg, 81%) as a pale yellow oil; ^1H NMR (300 MHz, C_6D_6, 25 ºC): δ = 7.52 (m, 3H, 3CH^{Ar}), 6.98 (m, 3H, 3CH^{Ar}), 6.80 (m, 1H, *J* = 4.9 Hz, CH^{Ar}), 6.61 (m, 1H, CH^{Ar}), 3.87 (dd, 1H, *J* = 4.6, 1.7 Hz, CH), 2.89 (d, 1H, *J* = 14.0 Hz, C*H*H), 2.35 (dd, 1H, *J* = 14.0, 4.7 Hz, CH*H*); ^{13}C NMR (75 MHz, C_6D_6, 25 ºC): δ = 135.2 (=C), 134.8 ($C^{Ar\text{-}q}$), 132.0 (2CH^{Ar}), 129.5 (CH^{Ar}), 128.9 (CH^{Ar}), 128.8 (2CH^{Ar}), 127.5 (CH^{Ar}), 122.5 ($C^{Ar\text{-}q}$), 120.7 (=C-Tf), 120.4 (q, J_{CF} = 329.4 Hz, CF_3), 100.5 (*C*≡C), 84.2 (C≡*C*), 57.8 (CH), 33.4 (CH_2); ^{19}F NMR (282 MHz, C_6D_6, 25 ºC): δ = –76.6 (s, 3F, CF_3); IR (CH_2Cl_2): ν = 2195 (C≡C), 1362, 1088 (O=S=O), 1212 (C–F) cm^{-1}; HRMS (ES): calcd for $C_{17}H_{12}F_3O_2S_2$ [*M* + H]$^+$: 369.02253; found: 369.02182.

General procedure for the palladium-catalyzed reaction of bis(triflyl)iodocyclobutenes 1 with alkynes 2 using deuterated phenylacetylene as deuterium donor. Synthesis of deuterated 1-triflyl-2-aryl-3-alkynyl-cyclobutene [D]-3aa.



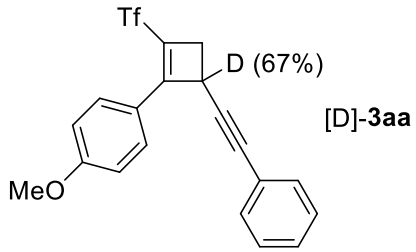
A solution of the appropriate bis(triflyl)iodocyclobutene **1** (0.1 mmol), $Pd(PPh_3)_2Cl_2$ (0.005 mmol, 5.0 mol %), and CuI (0.005 mmol, 5.0 mol %) in triethylamine (2.5 mL) was stirred at rt for 10 minutes. Then, the corresponding deuterated alkyne **[D]-2** (0.3 mmol) was slowly added. The resulting reaction mixture was gently heated at 36 °C until disappearance of the starting material (TLC). After removal of the triethylamine in vacuum, the residue was purified by column chromatography on silica gel to give analytically pure compounds. Spectroscopic and analytical data for deuterated 1-triflyl-2-aryl-3-alkynyl-cyclobutene **[D]-3aa** (34% H content) follow.

General procedure for the palladium-catalyzed reaction of bis(triflyl)iodocyclobutenes 1 with alkynes 2 using heavy water as deuterium donor. Synthesis of deuterated 1-triflyl-2-aryl-3-alkynyl-cyclobutene [D]-3aa.



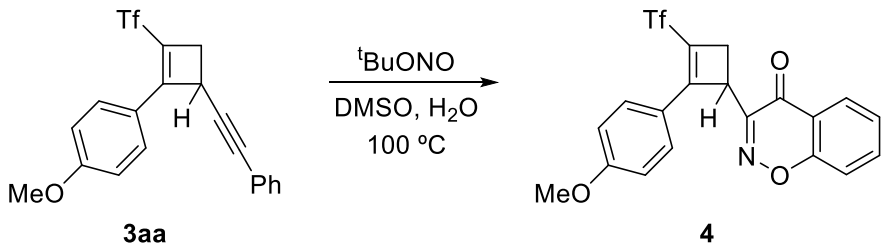
A solution of the appropriate bis(triflyl)iodocyclobutene **1** (0.1 mmol), $Pd(PPh_3)_2Cl_2$ (0.005 mmol, 5.0 mol %), CuI (0.005 mmol, 5.0 mol %), and D_2O (0.2 mmol) in triethylamine (2.5 mL) was stirred at rt for 10 minutes. Then, the corresponding alkyne **2** (0.3 mmol) was slowly added. The resulting reaction mixture was gently heated at 36 °C until disappearance of the starting material (TLC). After removal of the triethylamine in vacuum, the residue was purified by column chromatography on silica

gel to give analytically pure compounds. Spectroscopic and analytical data for deuterated 1-triflyl-2-aryl-3-alkynyl-cyclobutene **[D]-3aa** (33% H content) follow.

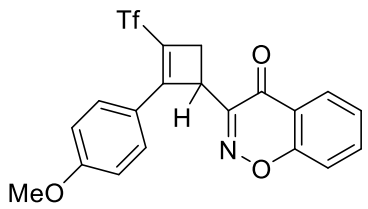


1-Methoxy-4-(4-(phenylethynyl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl-4-*d*)benzene [D]-3aa. From 60 mg (0.11 mmol) of iodocyclobutene **1a**, and after flash chromatography of the residue using hexanes/ethyl acetate (95:5) as eluent gave compound **[D]-3aa** (27 mg, 65%) as a pale yellow oil; ^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC): δ = 7.85 (m, 2H, 2CH^{Ar}), 7.54 (m, 2H, 2CH^{Ar}), 7.40 (m, 3H, 3CH^{Ar}), 6.95 (m, 2H, 2CH^{Ar}), 3.85 (s, 3H, OCH_3), 3.19 (d, 1H, *J* = 13.7 Hz, C*H*H), 3.14 (d, 1H, *J* = 13.7 Hz, CH*H*); ^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC): δ = 160.6 (*C*$^{Ar\text{-}q}$-OMe), 138.9 (=C), 131.7 (2CH^{Ar}), 129.3 (CH^{Ar}), 128.5 (2CH^{Ar}), 128.1 (2CH^{Ar}), 124.8 (*C*$^{Ar\text{-}q}$), 122.0 (*C*$^{Ar\text{-}q}$), 120.7 (=C-Tf), 119.9 (q, J_{CF} = 329. Hz, CF_3), 114.0 (2CH^{Ar}), 98.3 (*C*≡C), 83.8 (C≡*C*), 57.0 (m, CD), 55.3 (OCH_3), 32.6 (CH_2); ^{19}F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –75.9 (s, 3F, CF_3); D(^{2}H) NMR (107 MHz, $CDCl_3$, 25 ºC): δ = 4.88 (s, 1D, CD); IR ($CHCl_3$): ν = 2196 (C≡C), 1372, 1089 (O=S=O), 1207 (C–F) cm^{-1}; HRMS (ES): calcd for $C_{20}H_{18}DF_3NO_3S$ [*M* + NH_4]$^{+}$: 411.10950; found: 411.11096.

Procedure for the heterocyclization reaction of alkynyl-cyclobutene 3aa. Synthesis of cyclobutenyl-benzoxazinone 4.



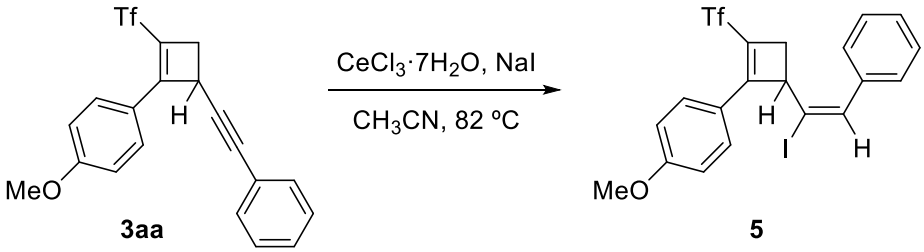
Alkynyl-cyclobutene **3aa** (0.05 mmol), H_2O (0.2 mmol), *tert*-butyl nitrite (0.25mmol) and DMSO (1 mL) were added into a Schlenk tube. Then, the tube was charged with argon, and the mixture was stirred at 100 ºC overnight until complete consumption of starting material as monitored by TLC. After the reaction was finished, brine (1 mL) was added to the reaction mixture. The aqueous phase was extracted with ethyl acetate (3 x 10 mL). The combined organic extracts were dried over $MgSO_4$, concentrated under vacuum, and the resulting residue was purified by silica gel flash column chromatography eluting with ethyl acetate/hexanes to afford the desired adduct **4**. Spectroscopic and analytical data for pure form of cyclobutenyl-benzo[*e*][1,2]oxazin-4-one **4** follow.



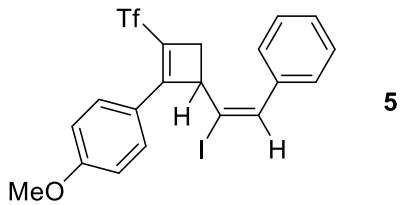
4

3-(2-(4-Methoxyphenyl)-3-((trifluoromethyl)sulfonyl)cyclobut-2-en-1-yl)-4*H*-benzo[*e*][1,2]oxazin-4-one 4. From 20 mg (0.05 mmol) of alkynyl-cyclobutene **3aa**, and after flash chromatography of the residue using hexanes/ethyl acetate (95:5→90:10→80:20) as eluent gave compound **4** (12 mg, 54%) as a yellow oil; ^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC): δ = 8.13 (m, 1H, 1CH^{Ar}), 7.95 (m, 2H, 2CH^{Ar}), 7.82 (m, 1H, CH^{Ar}), 7.56 (m, 1H, CH^{Ar}), 7.45 (m, 1H, CH^{Ar}), 6.95 (m, 2H, 2CH^{Ar}), 5.07 (m, 1H, CH), 3.86 (s, 3H, OCH_3), 3.65 (dd, 1H, *J* = 14.6, 4.6 Hz, C*H*H), 3.55 (d, 1H, *J* = 14.6 Hz, CH*H*); ^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC): δ = 168.0 (C=O), 161.6 (C=N), 161.3 ($C^{Ar\text{-}q}$-OMe), 152.2 ($C^{Ar\text{-}q}$), 139.6 (*C*=CTf), 136.1 (CH^{Ar}), 130.7 (2CH^{Ar}), 130.4 (C=*C*-Tf), 126.0 (CH^{Ar}), 125.2 (CH^{Ar}), 124.0 ($C^{Ar\text{-}q}$), 120.1 ($C^{Ar\text{-}q}$), 119.8 (q, J_{CF} = 328.8 Hz, CF_3), 116.5 (CH^{Ar}), 113.7 (2CH^{Ar}), 58.3 (CH), 55.3 (OCH_3), 31.9 (CH_2); ^{19}F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –75.9 (s, 3F, CF_3); IR ($CHCl_3$): ν = 1678 (C=O), 1345, 1079 (O=S=O), 1206 (C–F) cm^{-1}; HRMS (ES): calcd for $C_{20}H_{18}F_3N_2O_5S$ [*M* + NH_4]$^+$: 455.08830; found: 455.08910.

Procedure for the iodination reaction of alkynyl-cyclobutene 3aa. **Synthesis of iodoalkenyl-cyclobutene 5.**



Cerium(III) chloride heptahydrate (0.1 mmol) was added to a stirred suspension of alkynyl-cyclobutene **3aa** (0.06 mmol) and sodium iodide (0.18 mmol) in acetonitrile (2 mL). The resulting mixture was stirred at reflux until disappearance of the starting alkyne (TLC). The reaction mixture was allowed to cool to room temperature, was diluted with ether and treated with HCl (0.5 N). The organic layer was separated and extracted with diethyl ether (3 x 5 mL). The combined organic layers were washed with $NaHCO_3$ (10% aq. solution), $Na_2S_2O_3$ (10% aq. solution), and brine. The combined organic extracts were dried over $MgSO_4$, concentrated under vacuum, and the resulting residue was purified by silica gel flash column chromatography eluting with hexanes/diethyl ether to afford the desired adduct **5**. Spectroscopic and analytical data for pure form of iodoalkenyl-cyclobutene **5** follow.

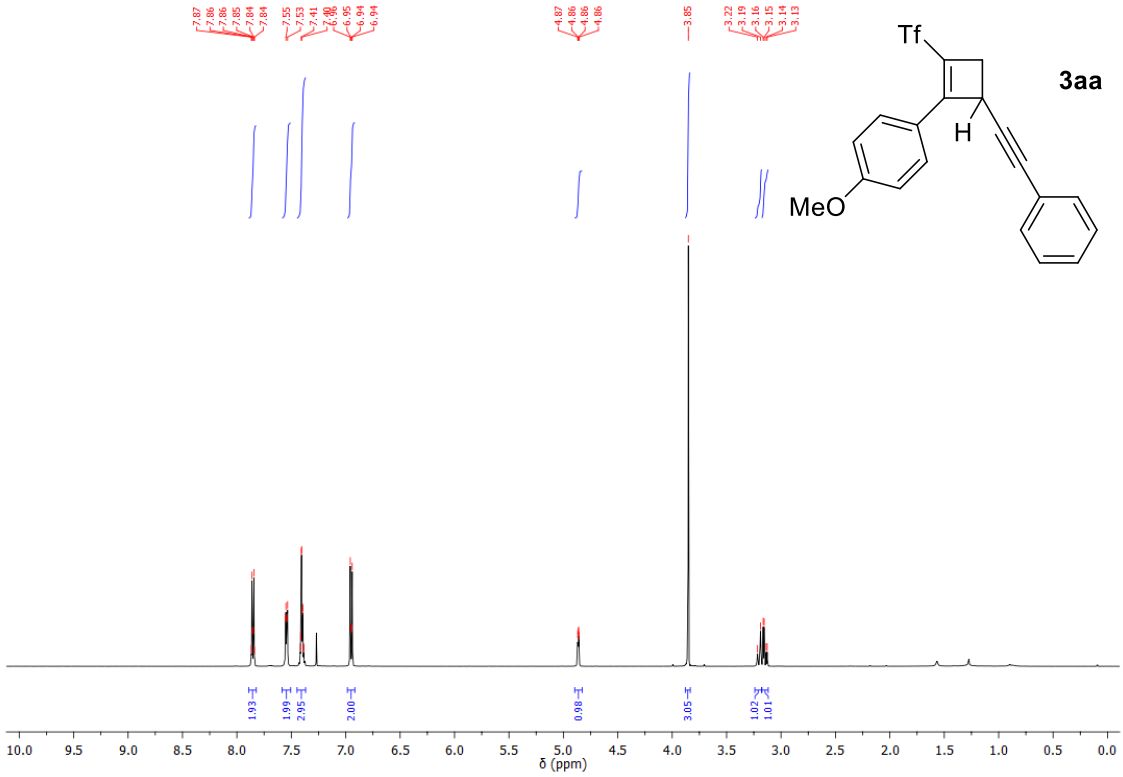


5

(*E*)-1-(4-(1-Iodo-2-phenylvinyl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-4-methoxybenzene 5. From 24 mg (0.06 mmol) of alkynyl-cyclobutene **3aa**, and after flash chromatography of the residue using hexanes/diethyl ether (98:2→96:4) as eluent gave compound **5** (19 mg, 61%) as a yellow oil; ^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC): δ = 7.46 (m, 4H, 4CH^{Ar}), 7.41 (s,

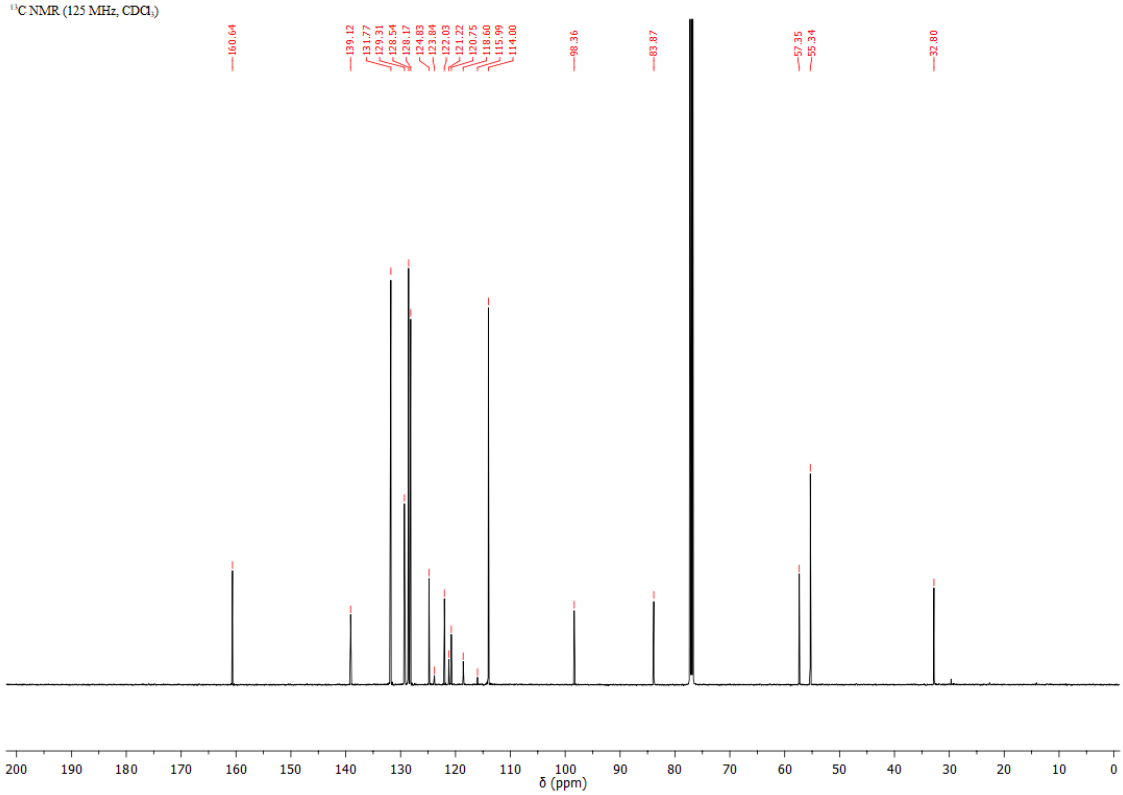
1H, =CH), 7.29 (m, 2H, 2CH^{Ar}), 7.25 (m, 1H, CH^{Ar}), 6.83 (m, 2H, 2CH^{Ar}), 4.84 (t, 1H, J = 3.1 Hz, CH), 3.80 (s, 3H, OCH_3), 3.16 (d, 1H, J = 3.3 Hz, CH_2); ^{13}C NMR (175 MHz, $CDCl_3$, 25 °C): δ = 160.5 ($C^{Ar\text{-}q}$-OMe), 144.9 (=CH), 141.1 (*C*=CTf), 136.4 ($C^{Ar\text{-}q}$), 132.7 (C=*C*-Tf), 129.3 (2CH^{Ar}), 128.9 (CH^{Ar}), 128.7 (2CH^{Ar}), 128.2 (2CH^{Ar}), 124.0 ($C^{Ar\text{-}q}$), 119.9 (q, J_{CF} = 329.1 Hz, CF_3), 113.9 (2CH^{Ar}), 88.5 (=CI), 55.6 (CH), 55.3 (OCH_3), 31.9 (CH_2); ^{19}F NMR (282 MHz, $CDCl_3$, 25 °C): δ = –76.1 (s, 3F, CF_3); IR ($CHCl_3$): ν = 1369, 1087 (O=S=O), 1205 (C–F) cm^{-1}; HRMS (ES): calcd for $C_{20}H_{20}F_3INO_3S$ $[M + NH_4]^+$: 538.01552; found: 538.01307.

^{1}H NMR (500 MHz, $CDCl_3$)

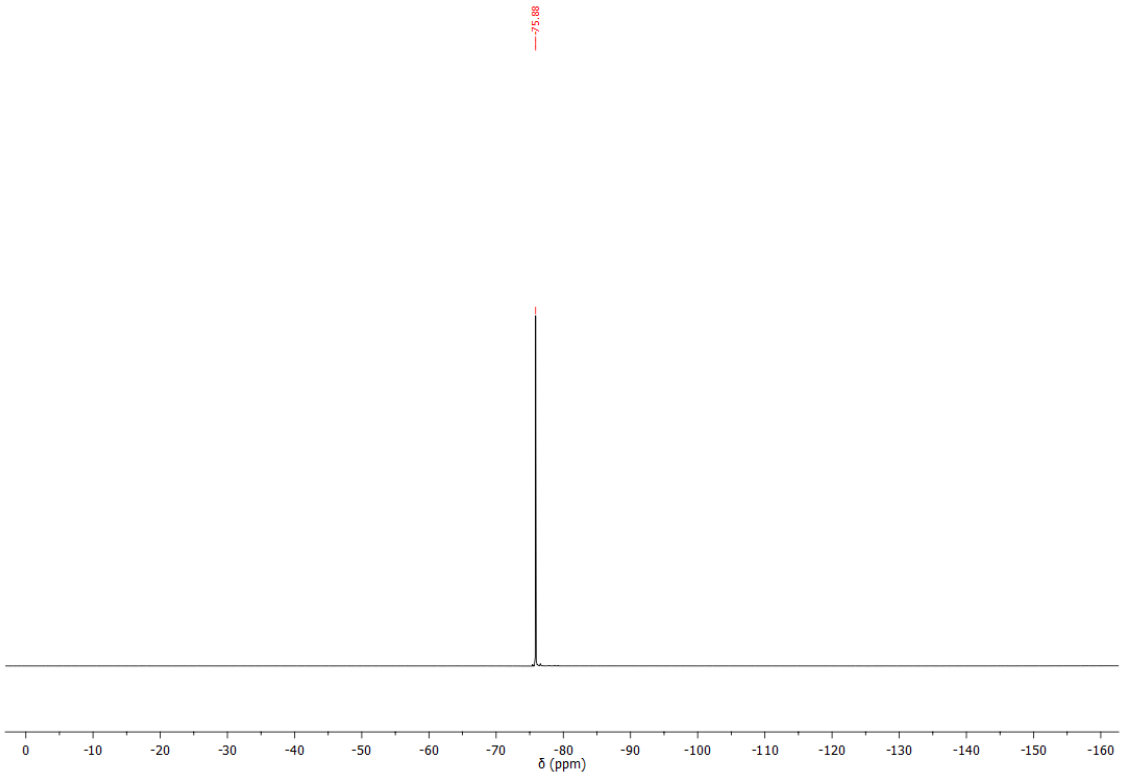


3aa

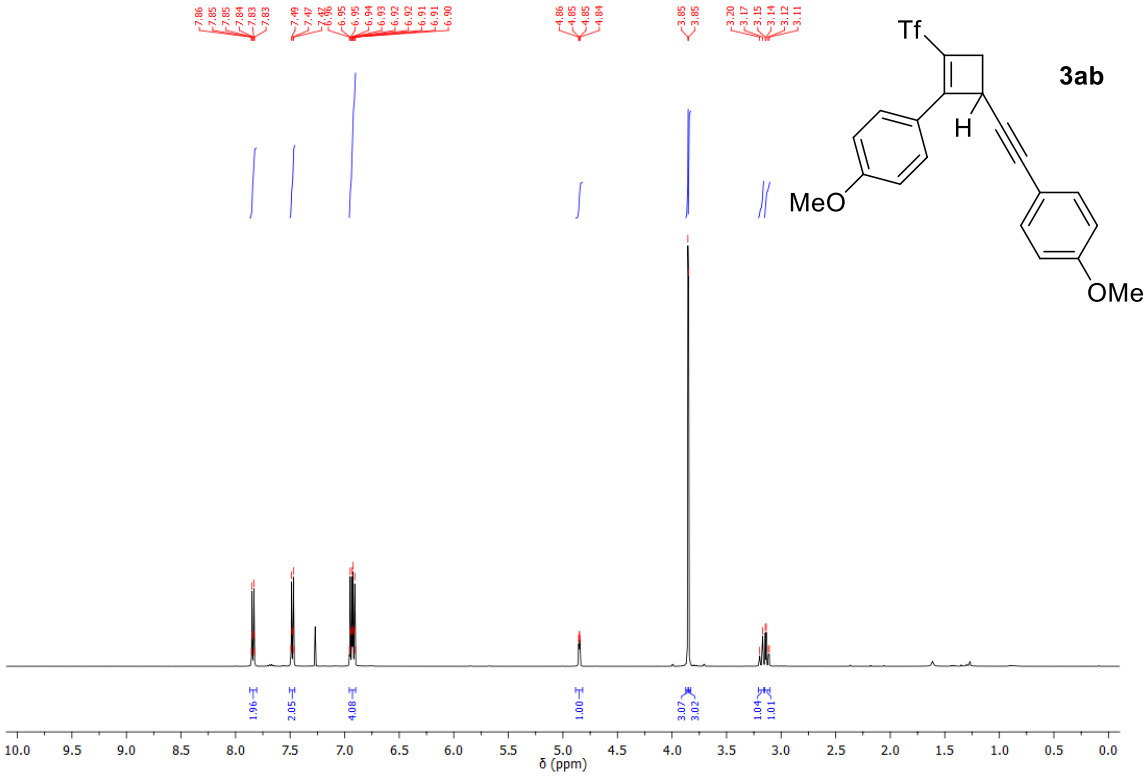
^{13}C NMR (125 MHz, $CDCl_3$)



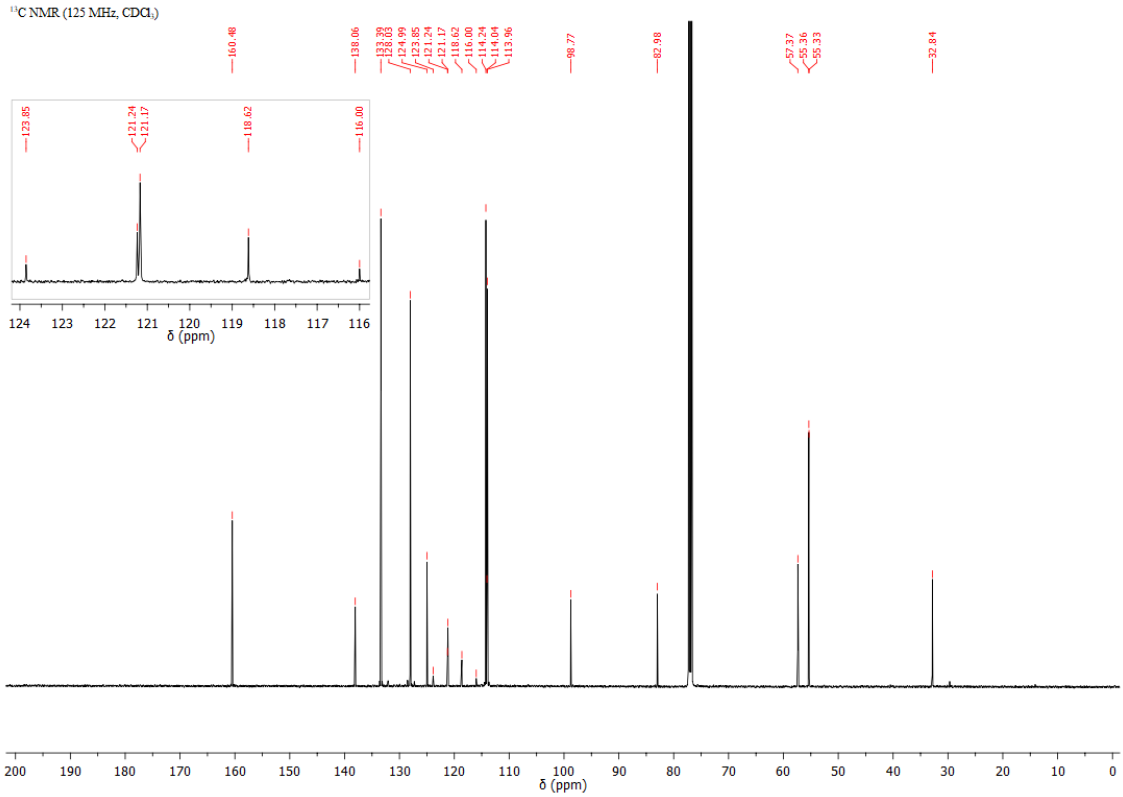
^{19}F NMR (282 MHz, $CDCl_3$)



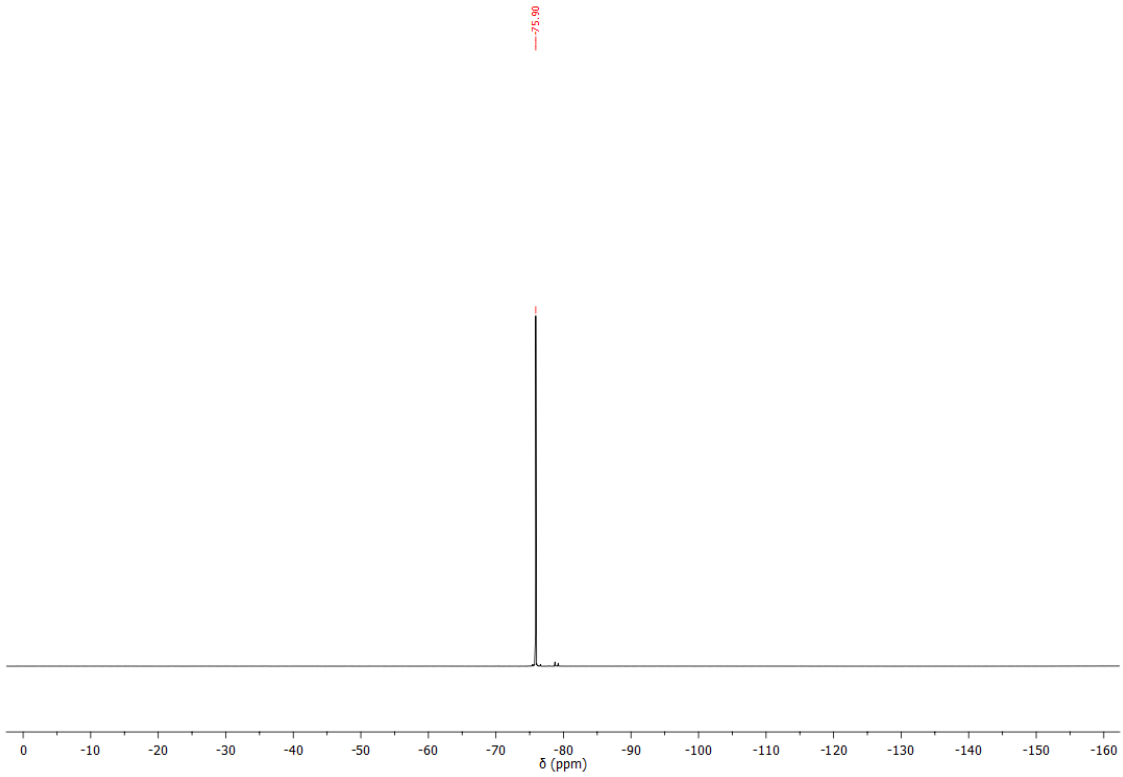
^{1}H NMR (500 MHz, $CDCl_3$)



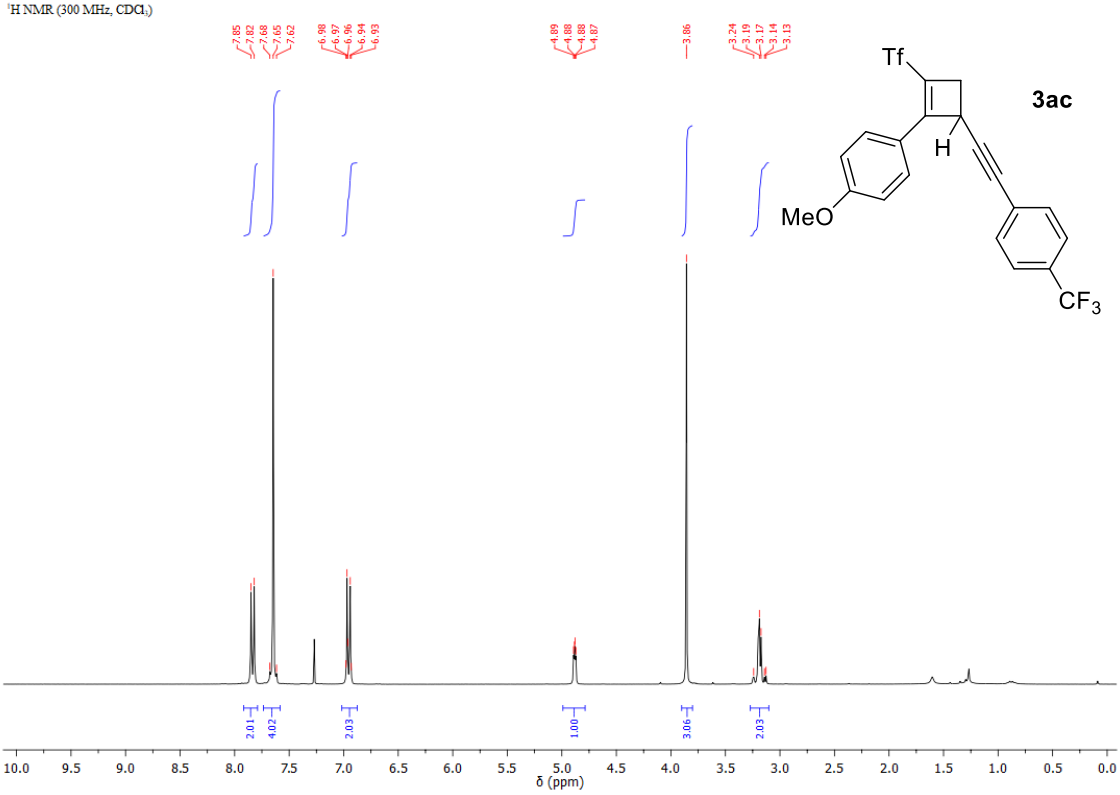
^{13}C NMR (125 MHz, $CDCl_3$)



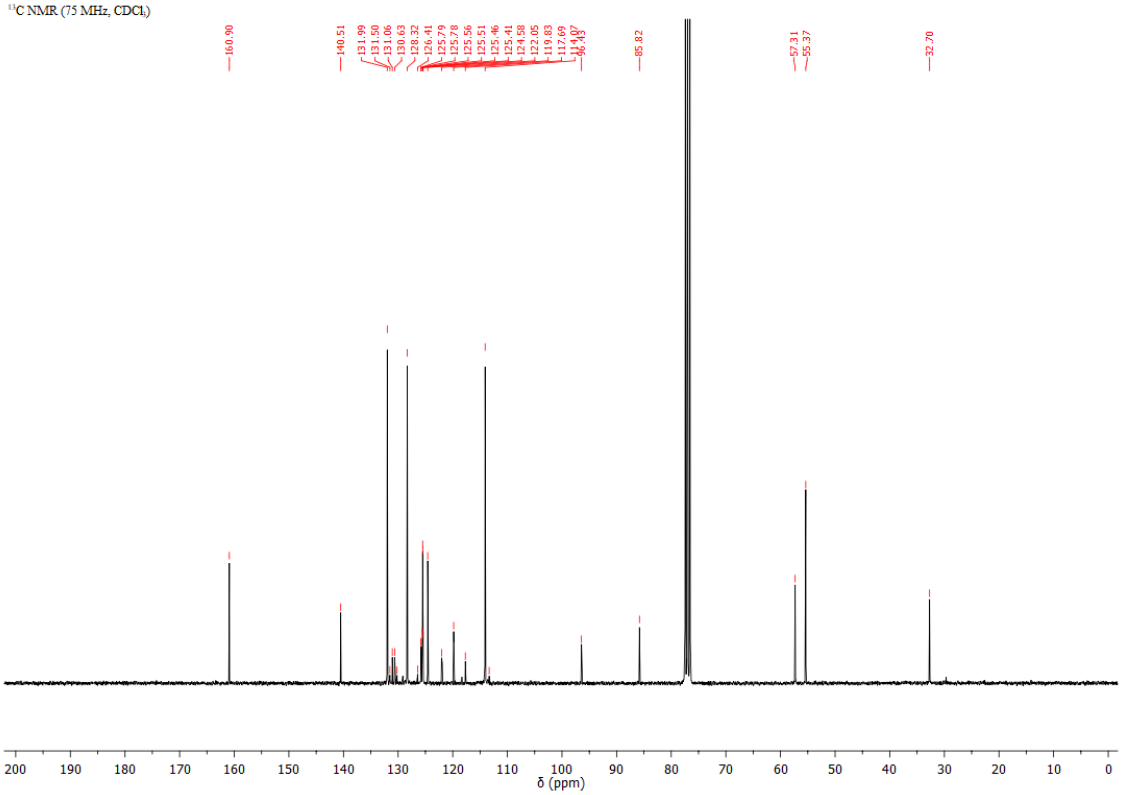
^{19}F NMR (282 MHz, $CDCl_3$)



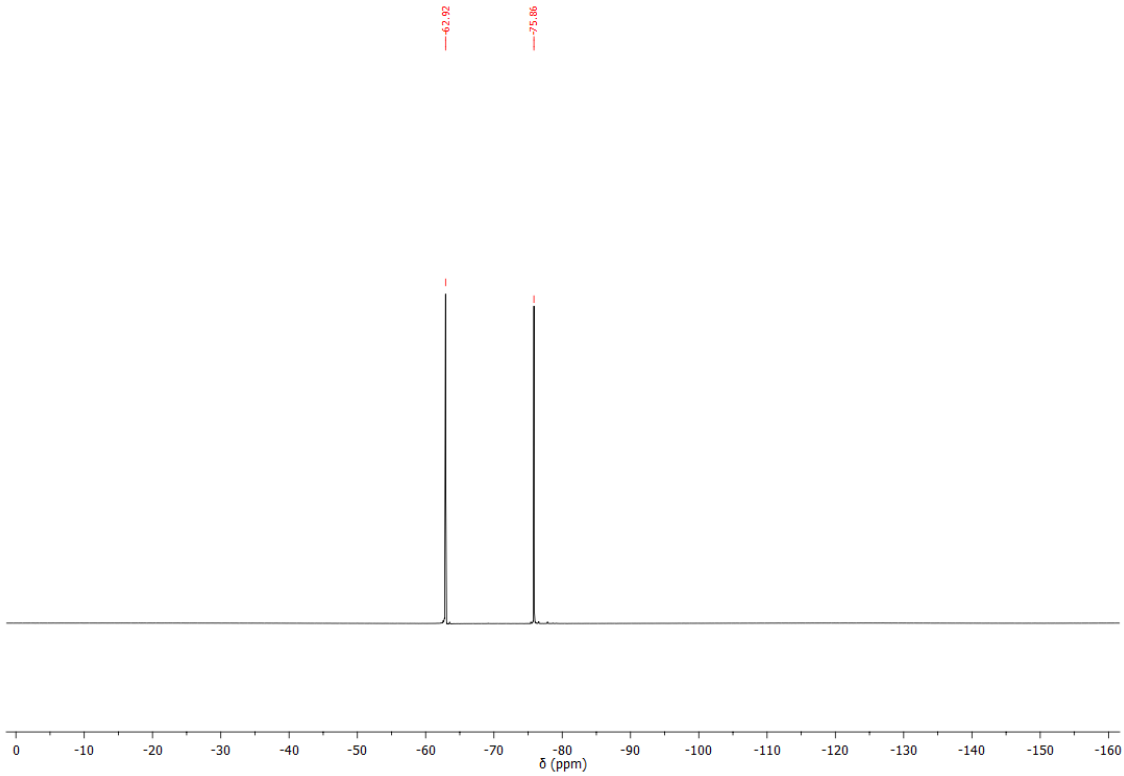
^{1}H NMR (300 MHz, $CDCl_3$)



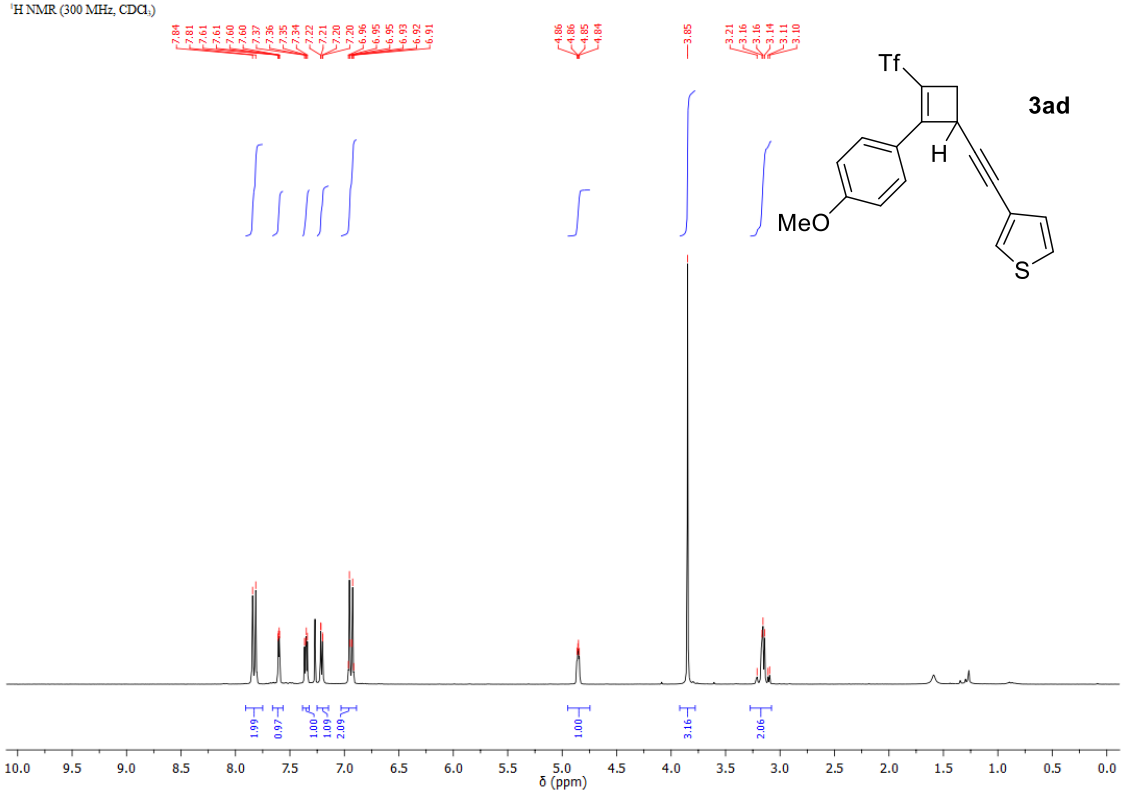
^{13}C NMR (75 MHz, $CDCl_3$)



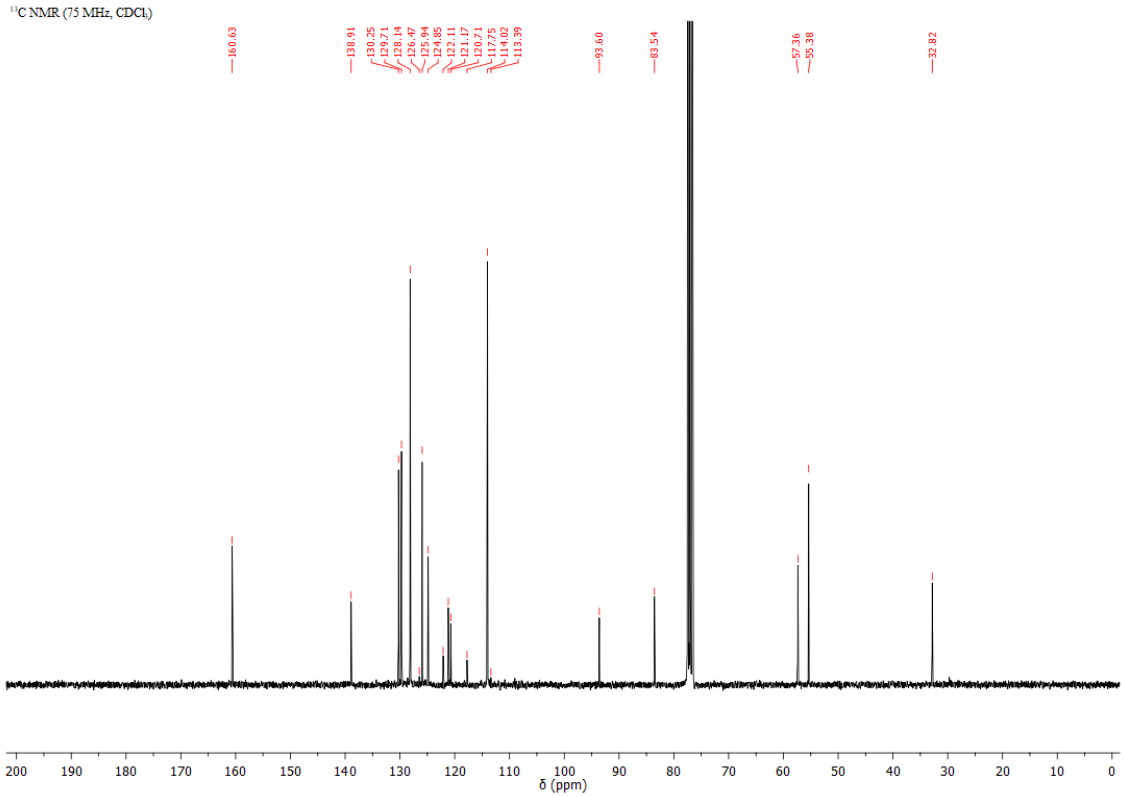
^{19}F NMR (282 MHz, $CDCl_3$)

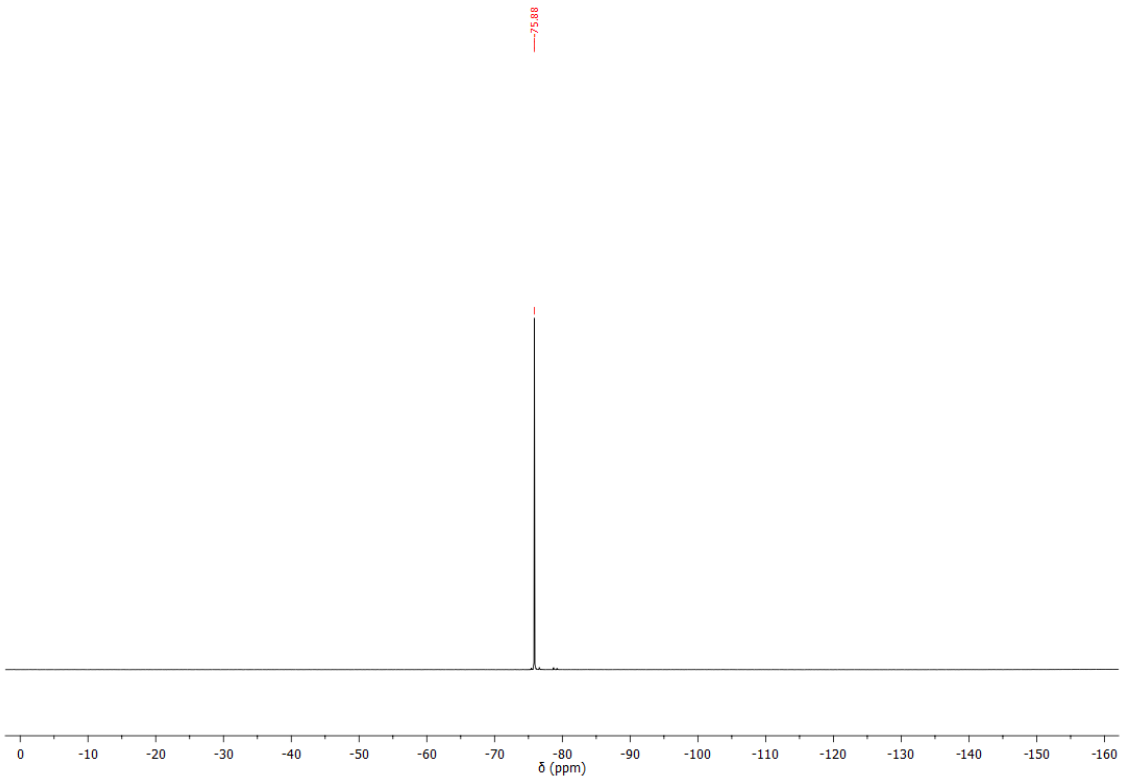


^{1}H NMR (300 MHz, $CDCl_3$)

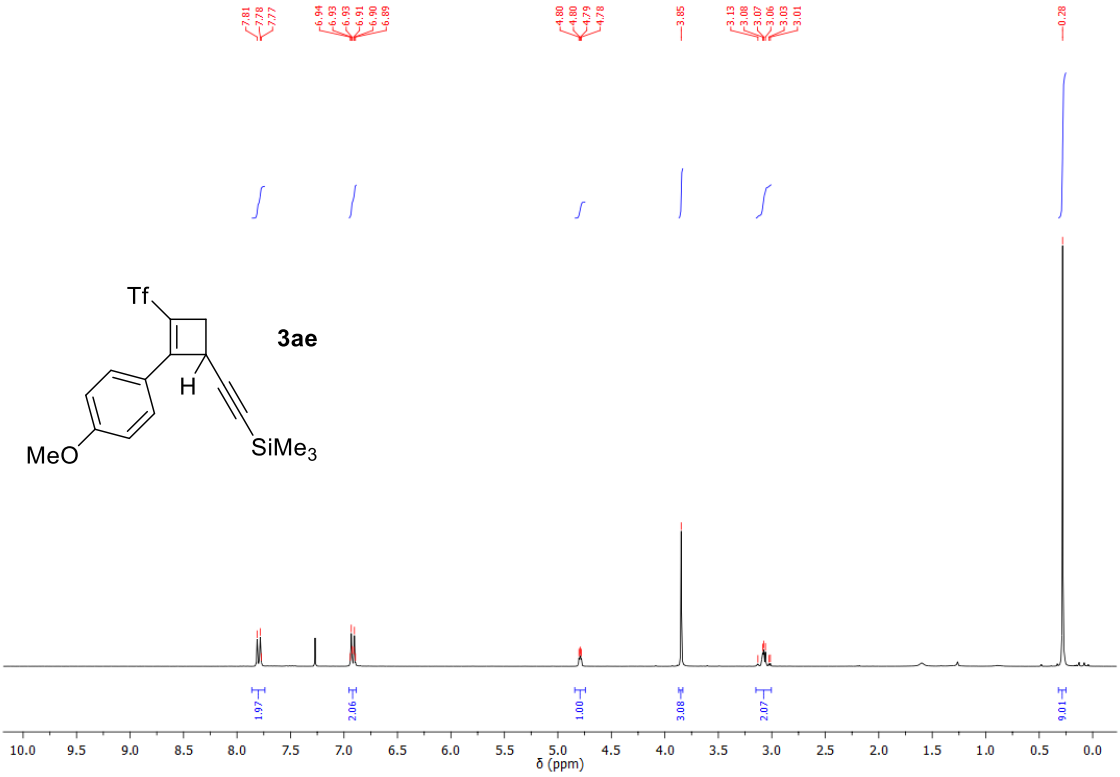


^{13}C NMR (75 MHz, $CDCl_3$)

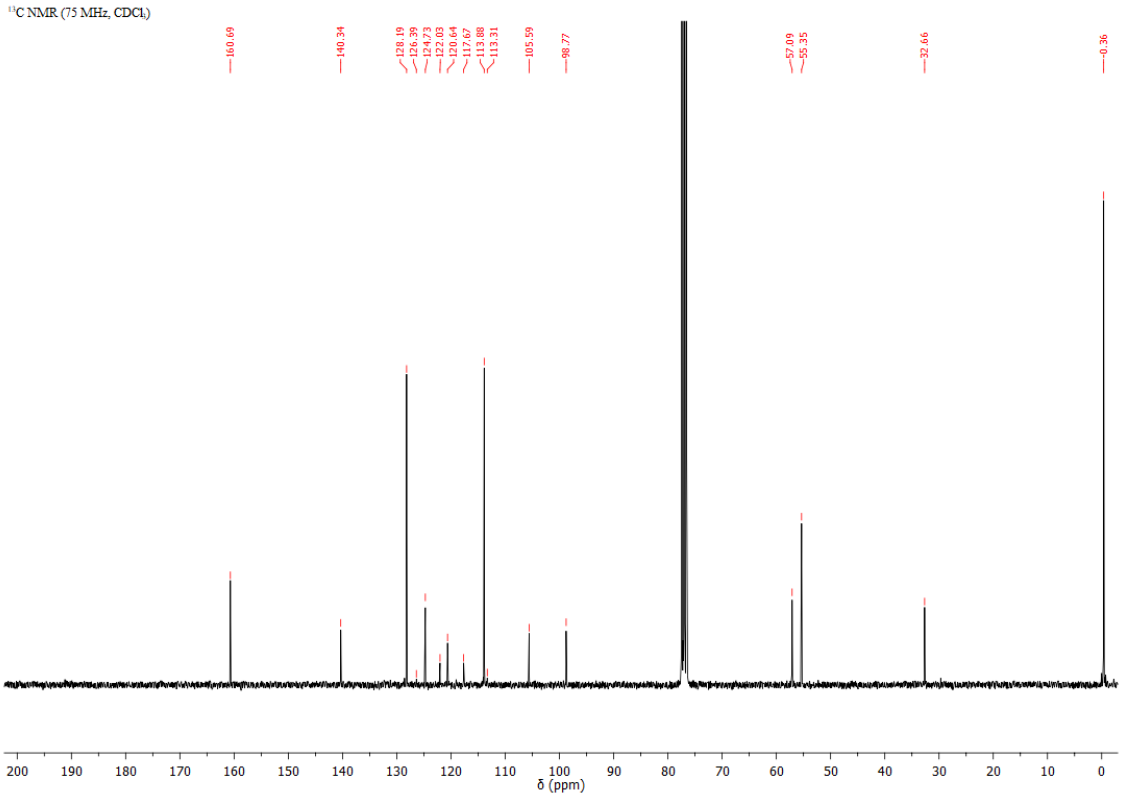



-75.88
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
δ (ppm)

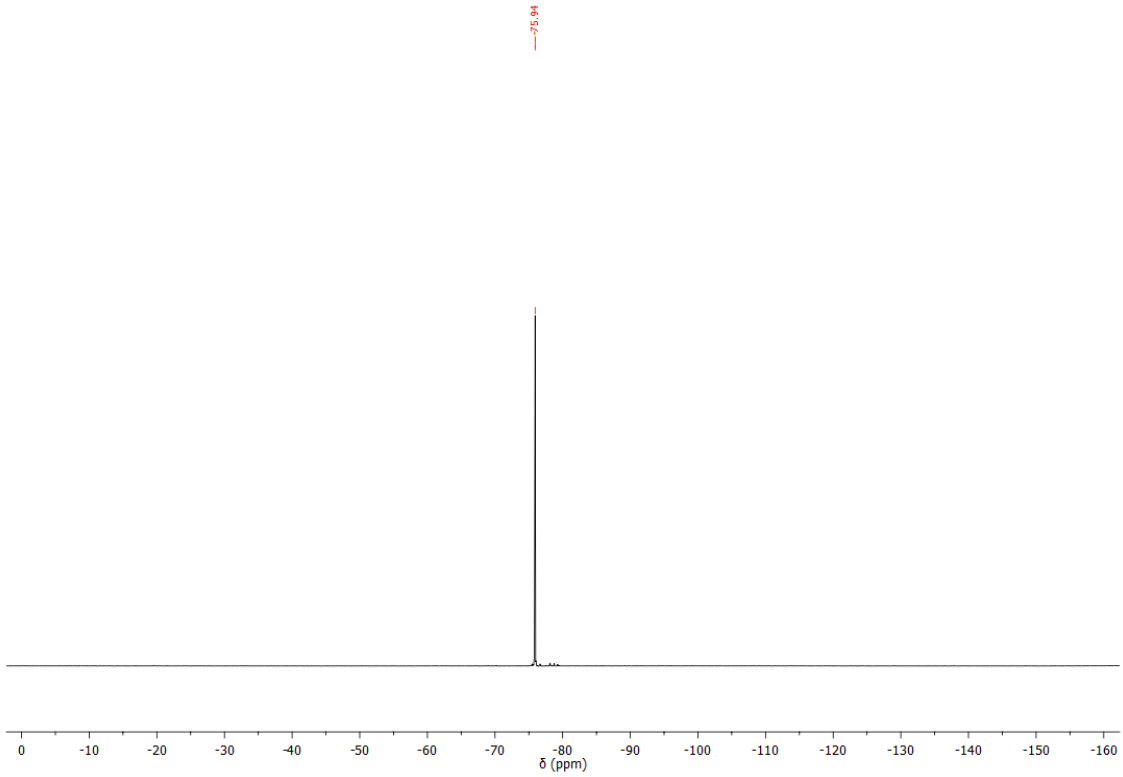
^{1}H NMR (300 MHz, $CDCl_3$)



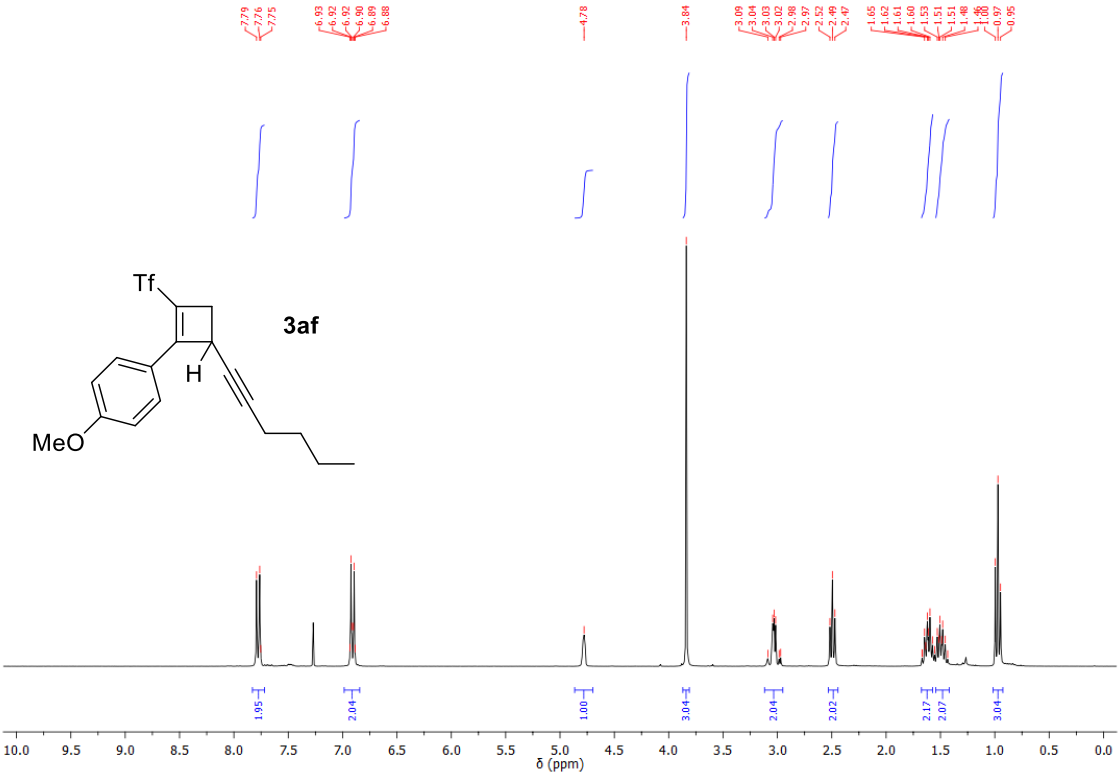
^{13}C NMR (75 MHz, $CDCl_3$)



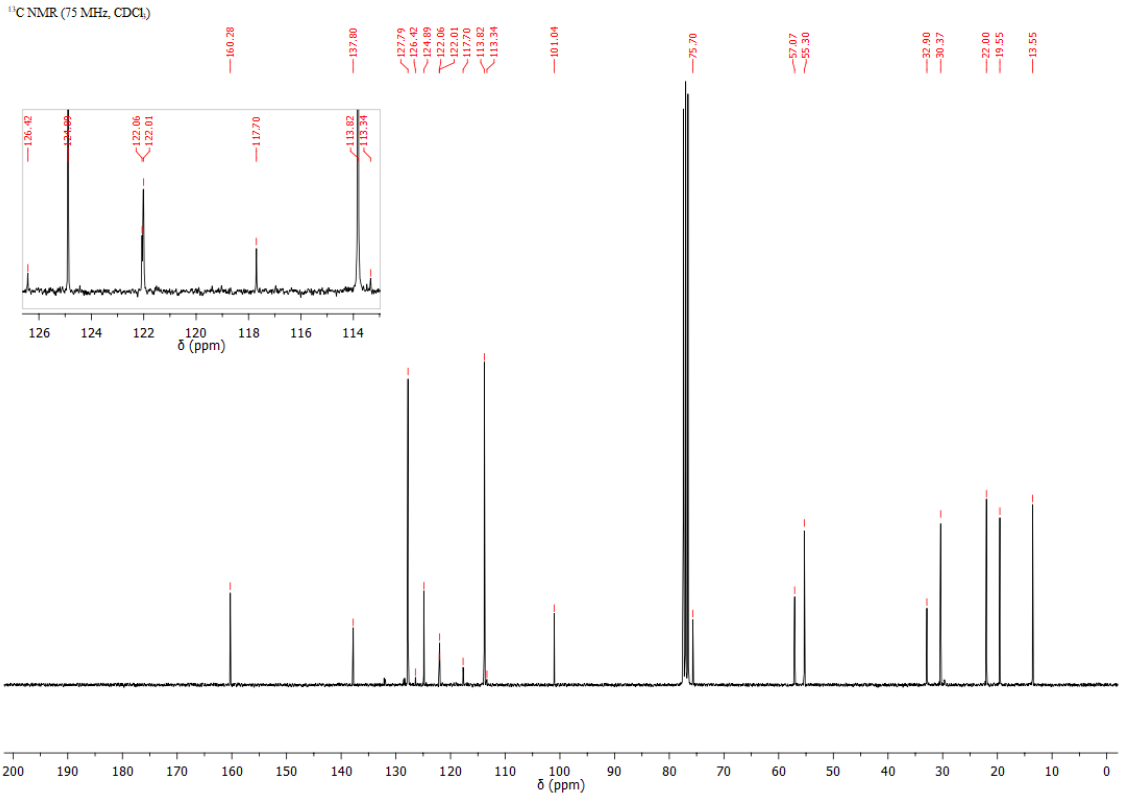
^{19}F NMR (282 MHz, $CDCl_3$)



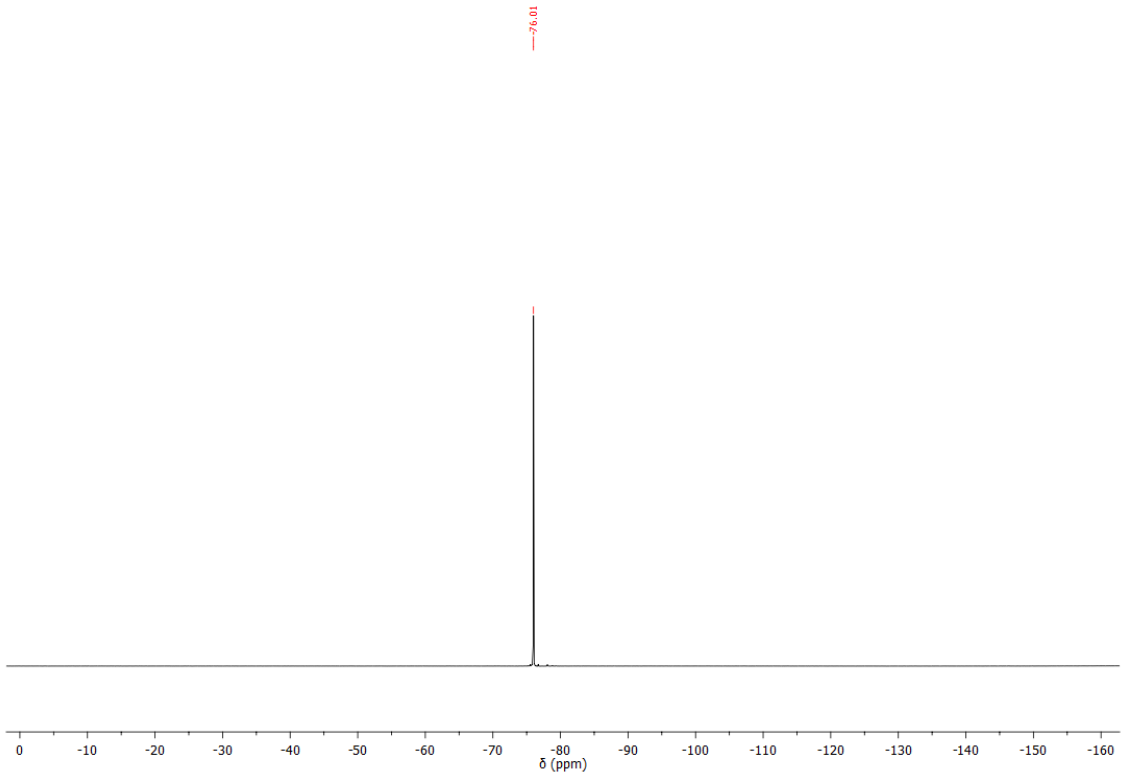
^{1}H NMR (300 MHz, $CDCl_3$)



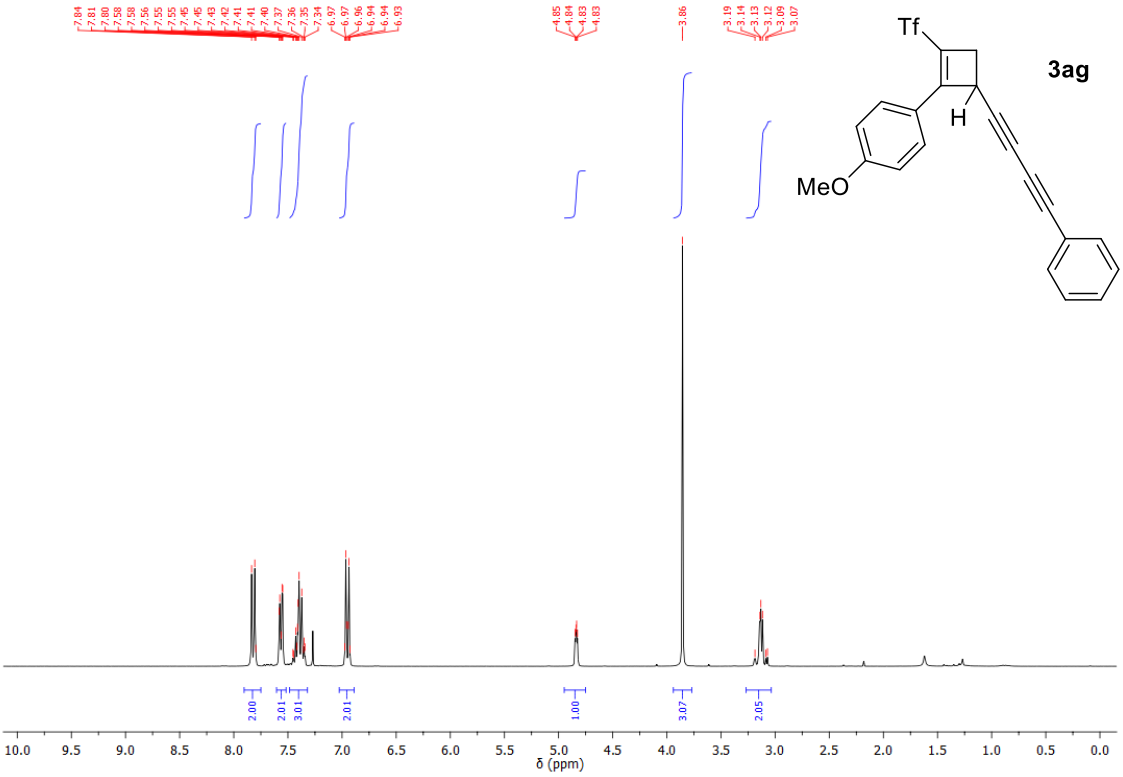
^{13}C NMR (75 MHz, $CDCl_3$)



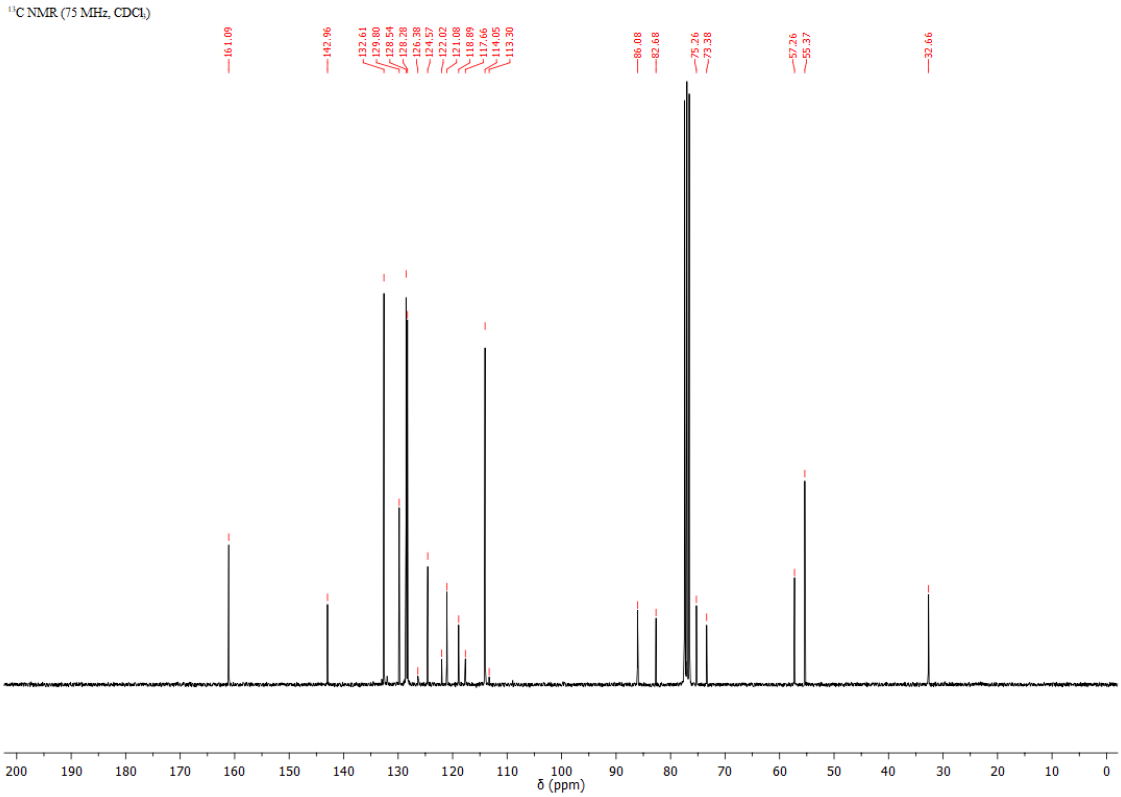
^{19}F NMR (282 MHz, $CDCl_3$)



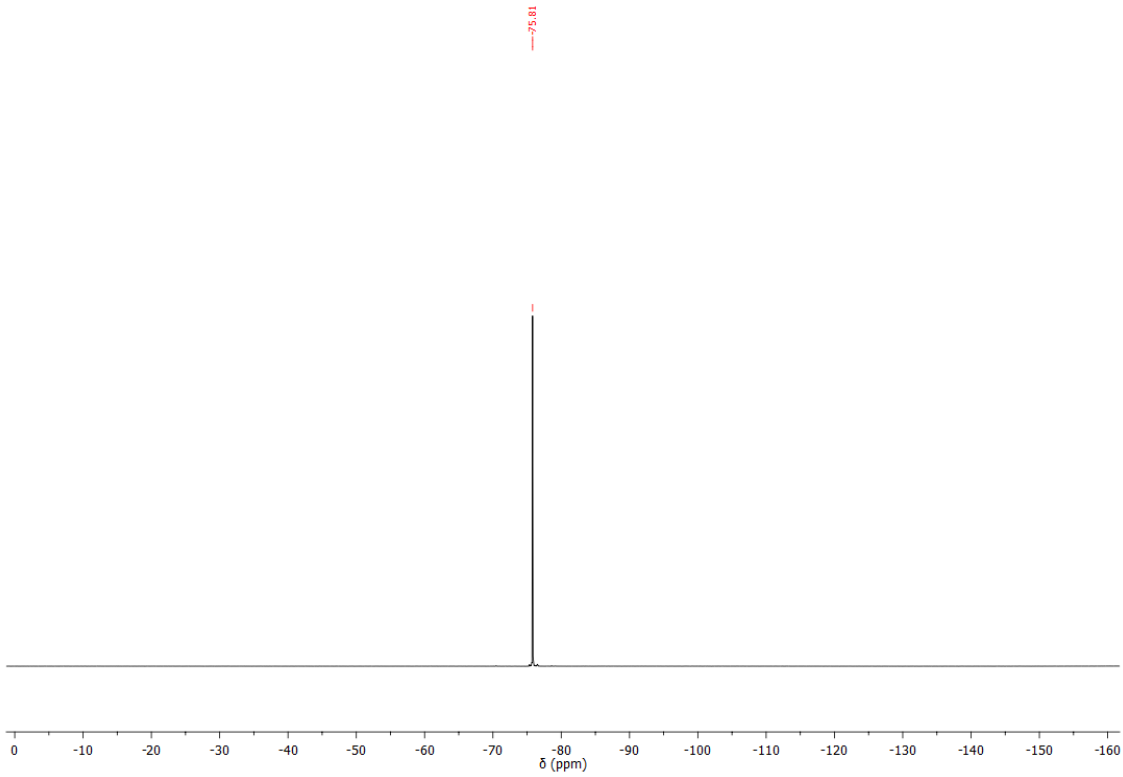
^{1}H NMR (300 MHz, $CDCl_3$)

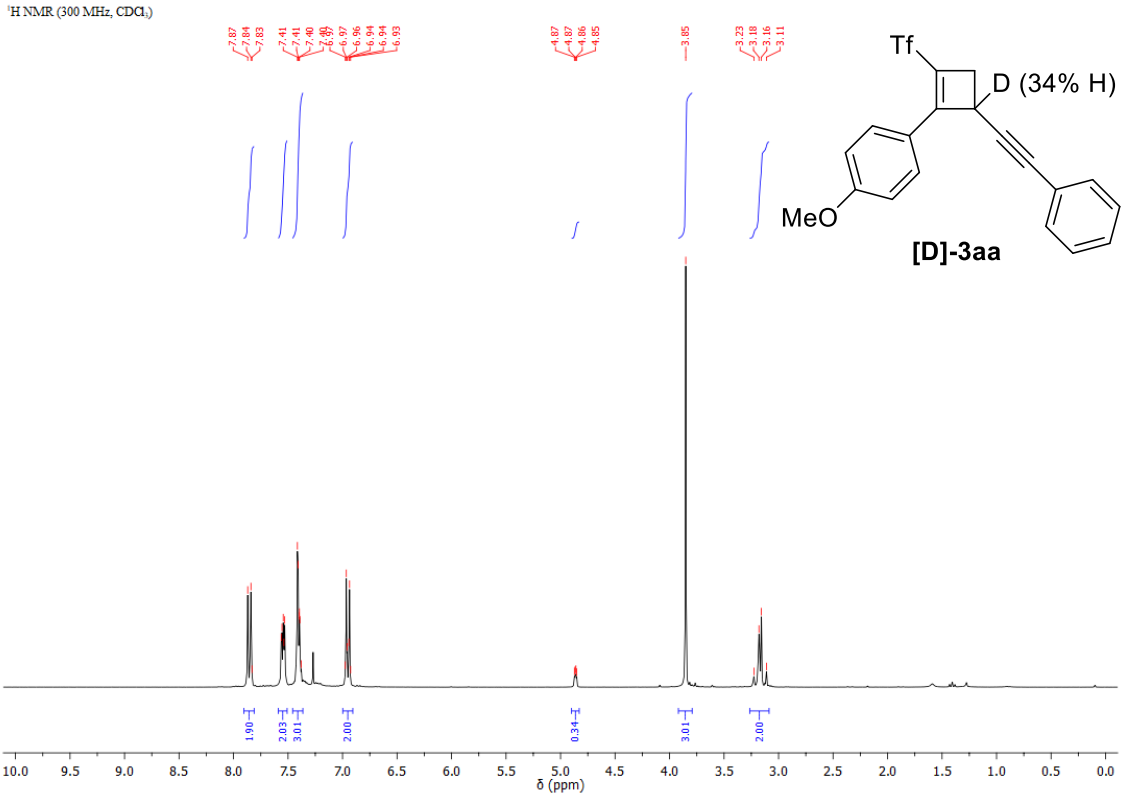


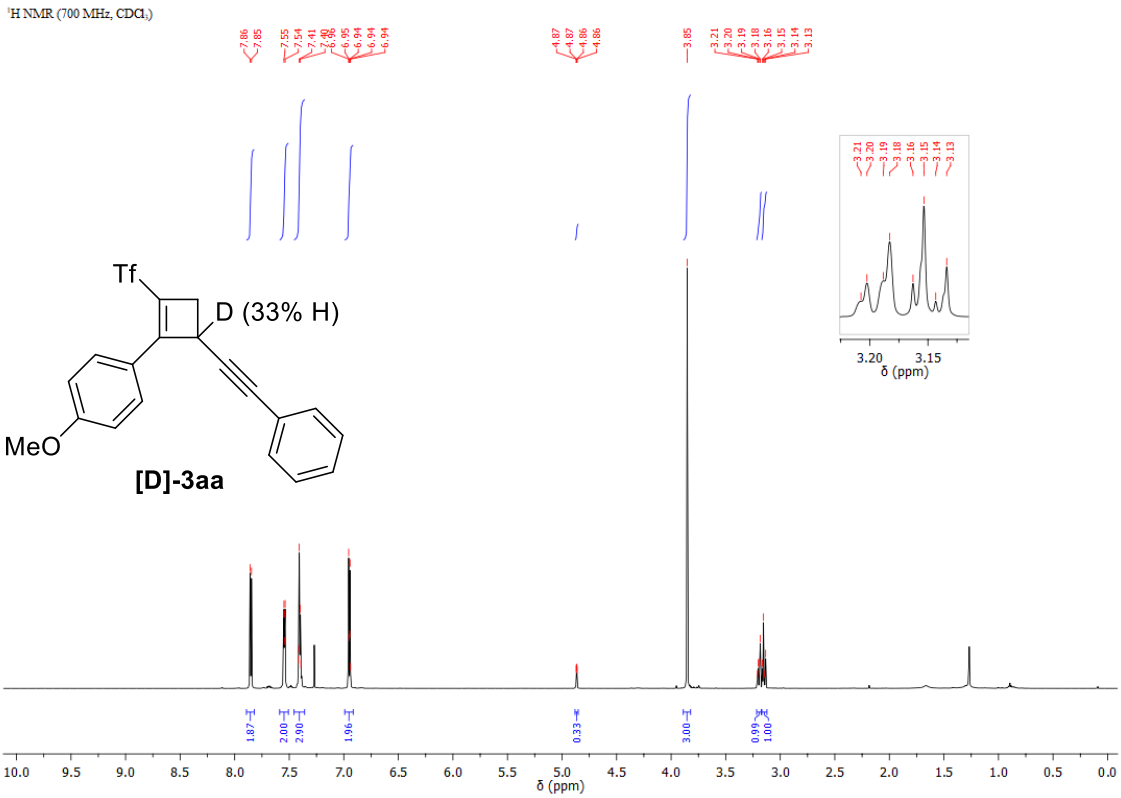
^{13}C NMR (75 MHz, $CDCl_3$)



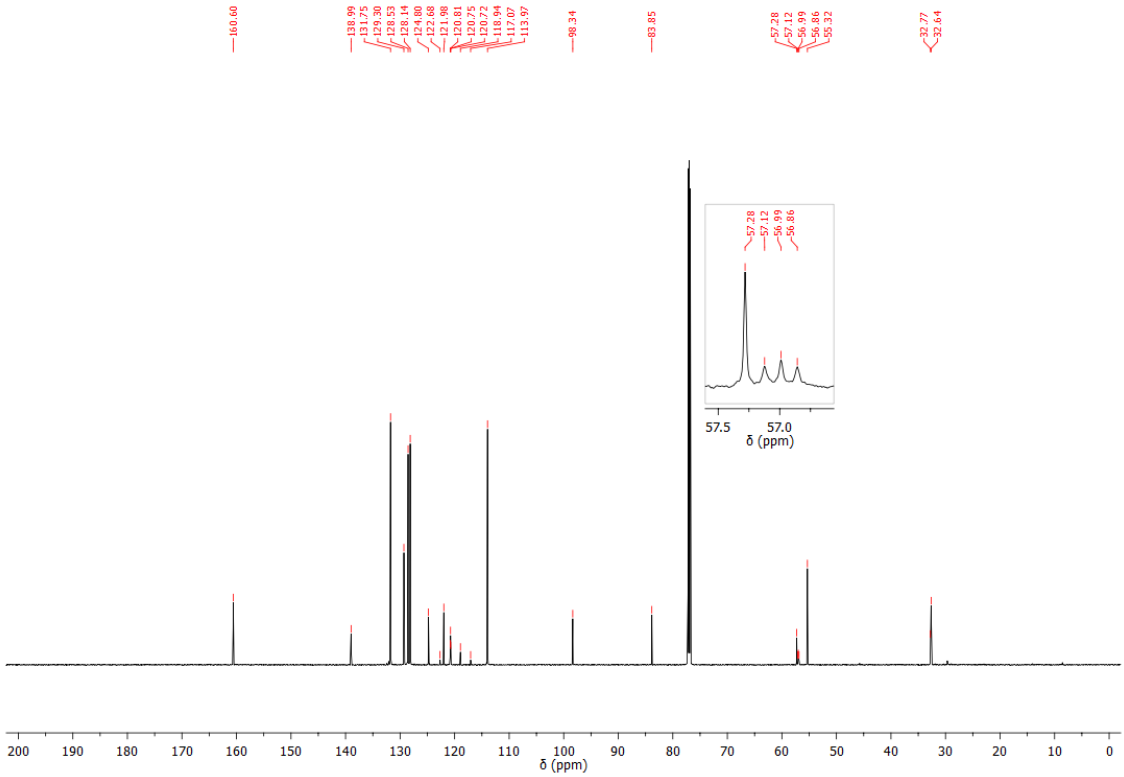
^{19}F NMR (282 MHz, $CDCl_3$)



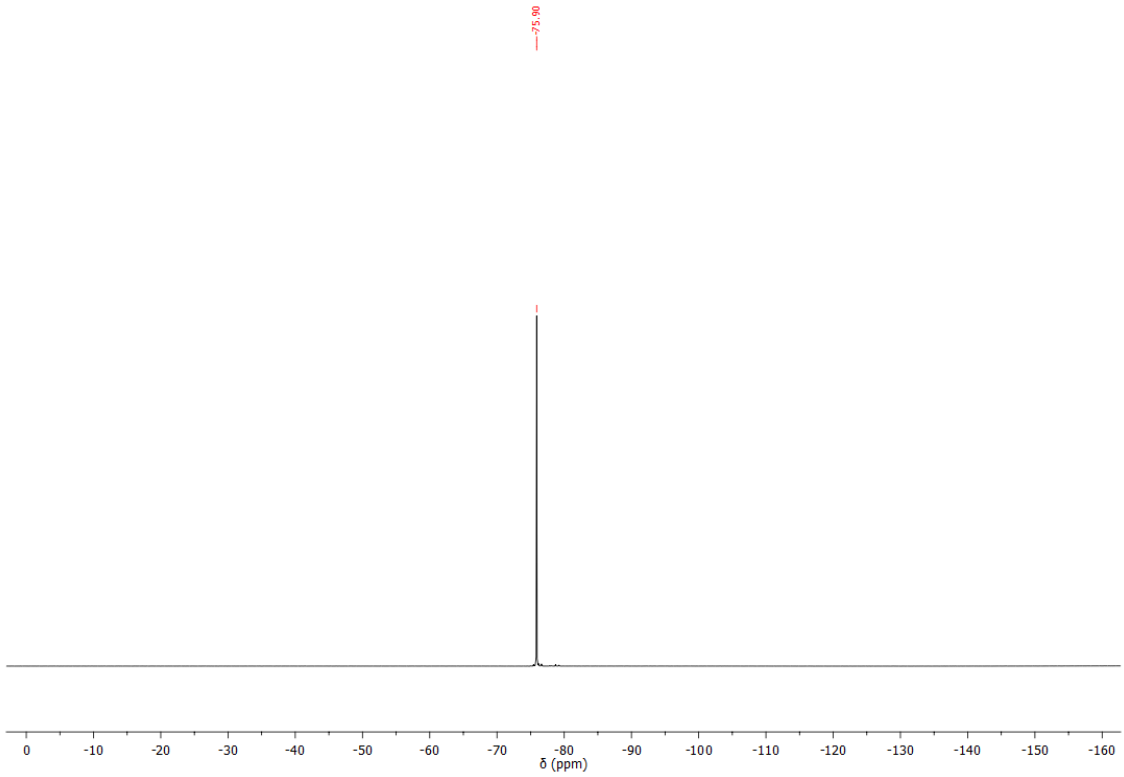

^{1}H NMR (300 MHz, CDCl$_3$)
Tf
D (34% H)
MeO
[D]-3aa
δ (ppm)

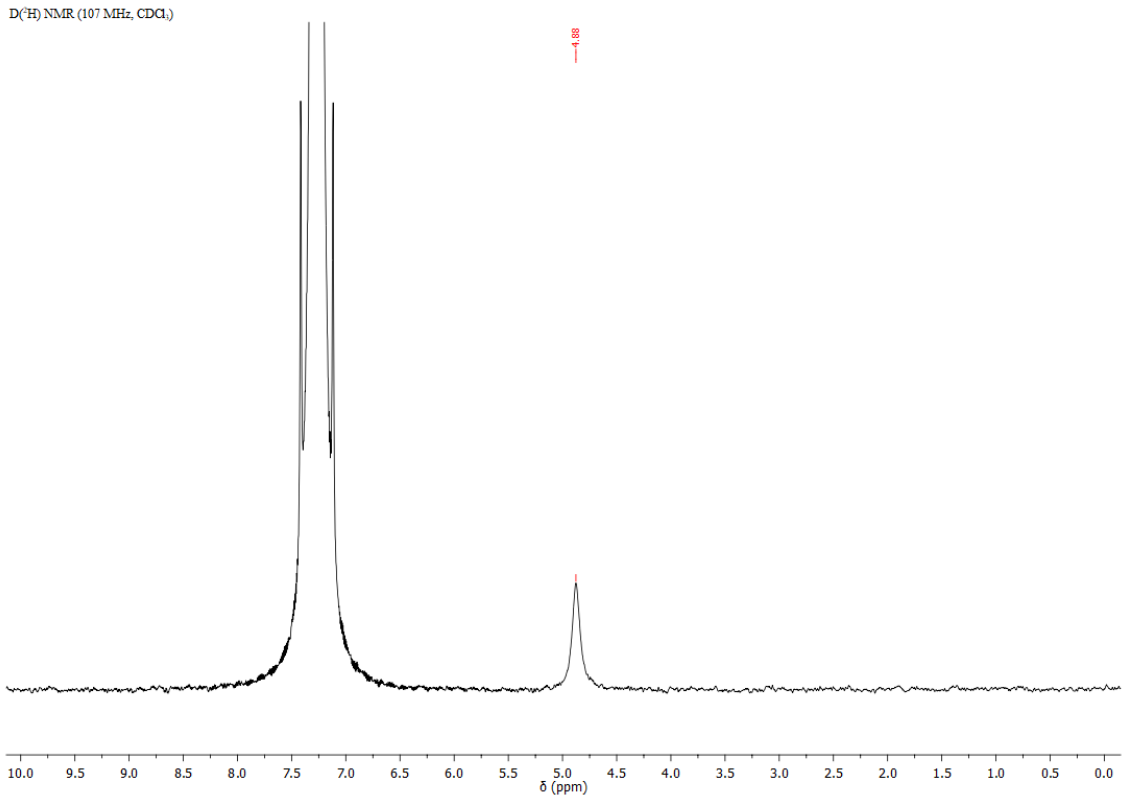

^{1}H NMR (700 MHz, CDCl$_3$)
Tf
D (33% H)
MeO
[D]-3aa
δ (ppm)

^{13}C NMR (175 MHz, $CDCl_3$)

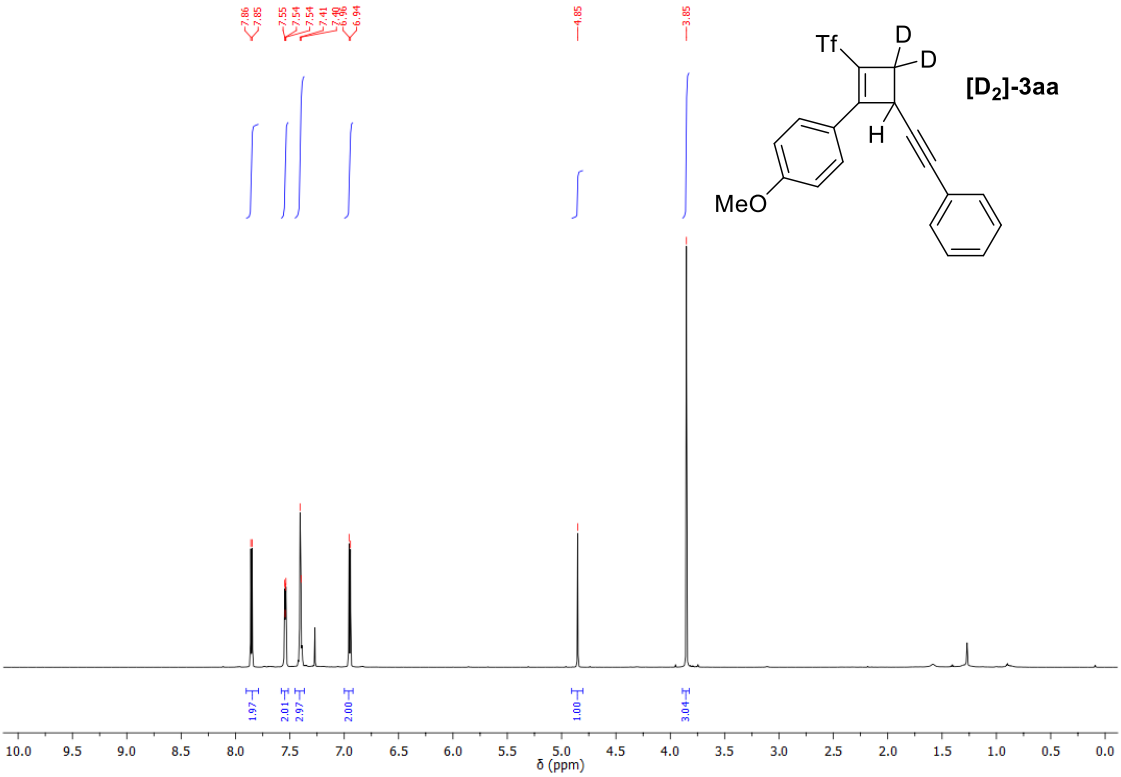


^{19}F NMR (282 MHz, $CDCl_3$)

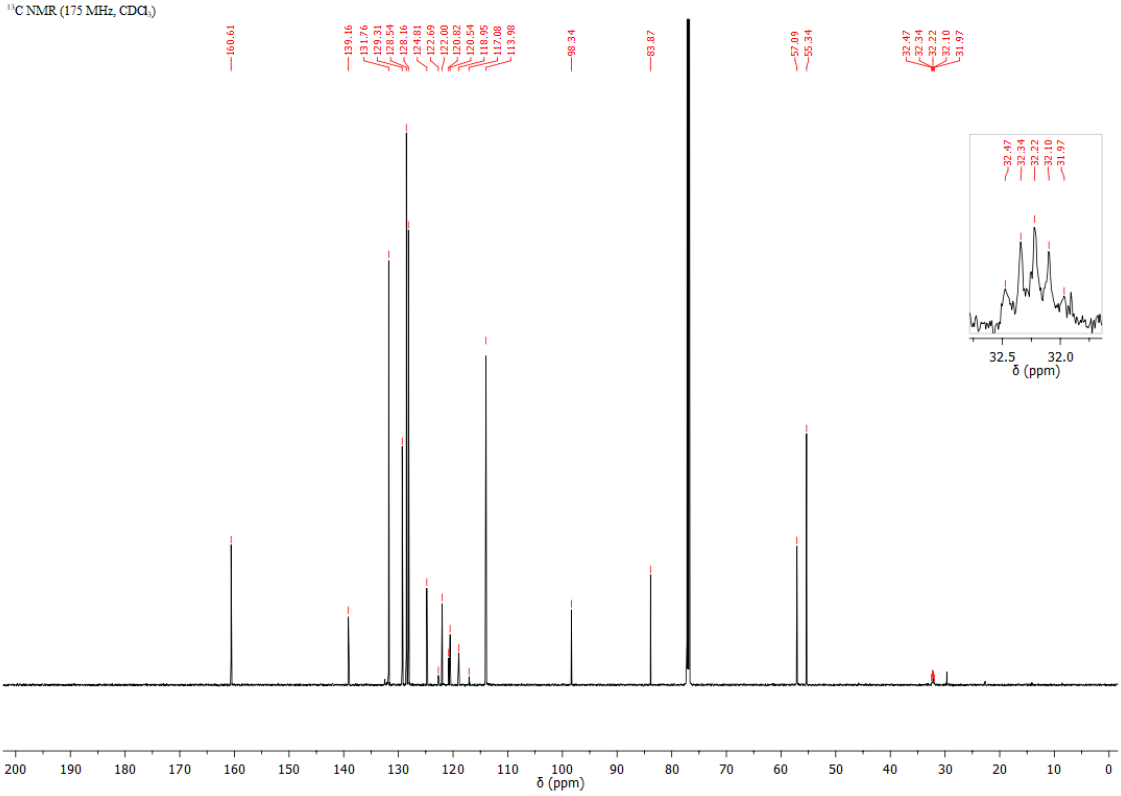



D(²H) NMR (107 MHz, CDCl₃)
4.88
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ (ppm)

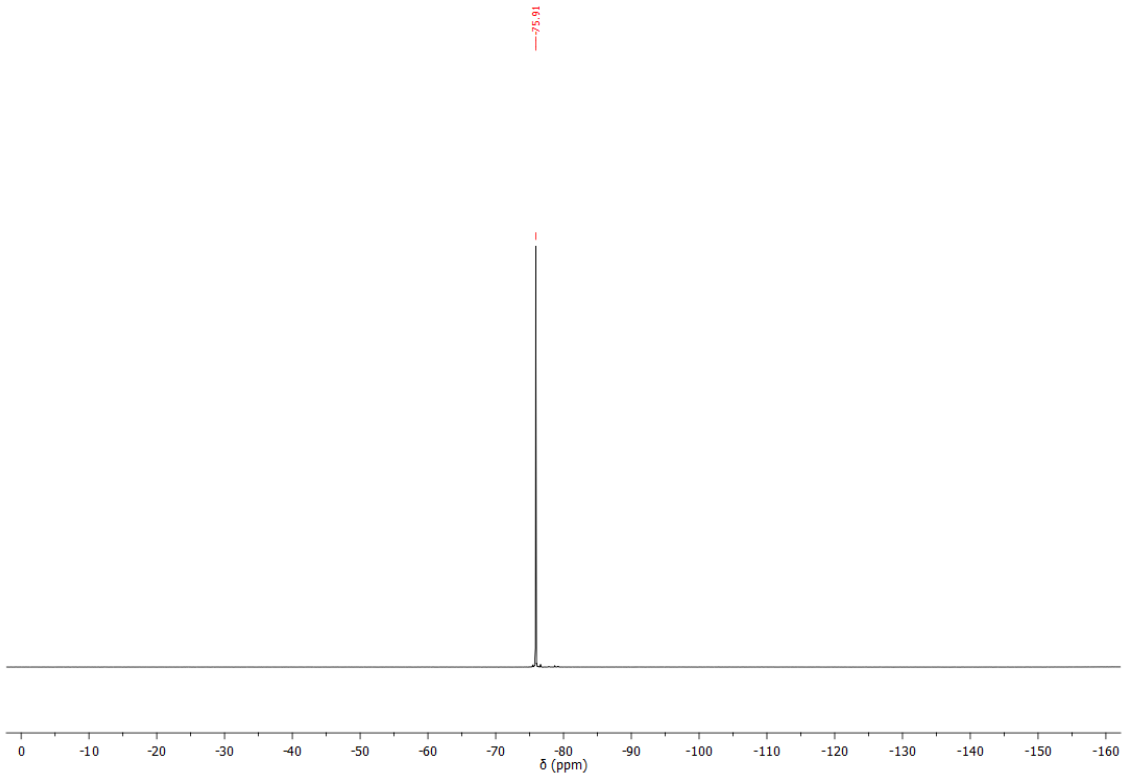
^{1}H NMR (700 MHz, $CDCl_3$)



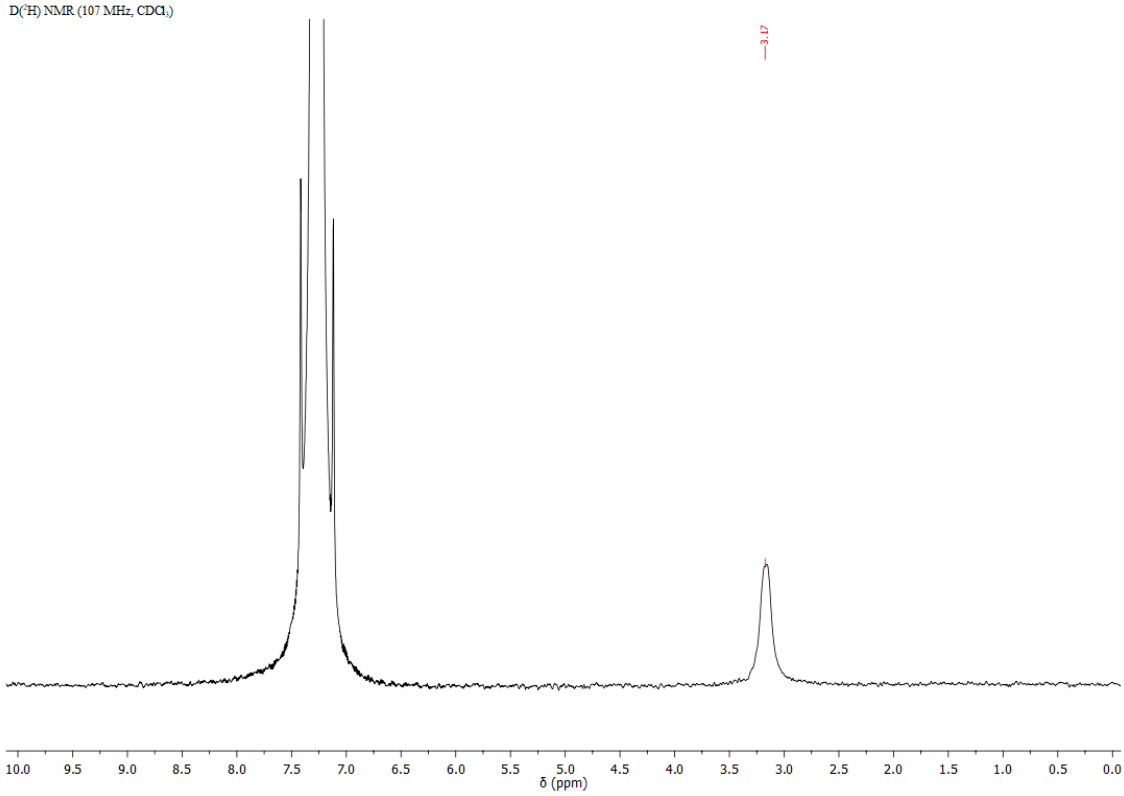
^{13}C NMR (175 MHz, $CDCl_3$)



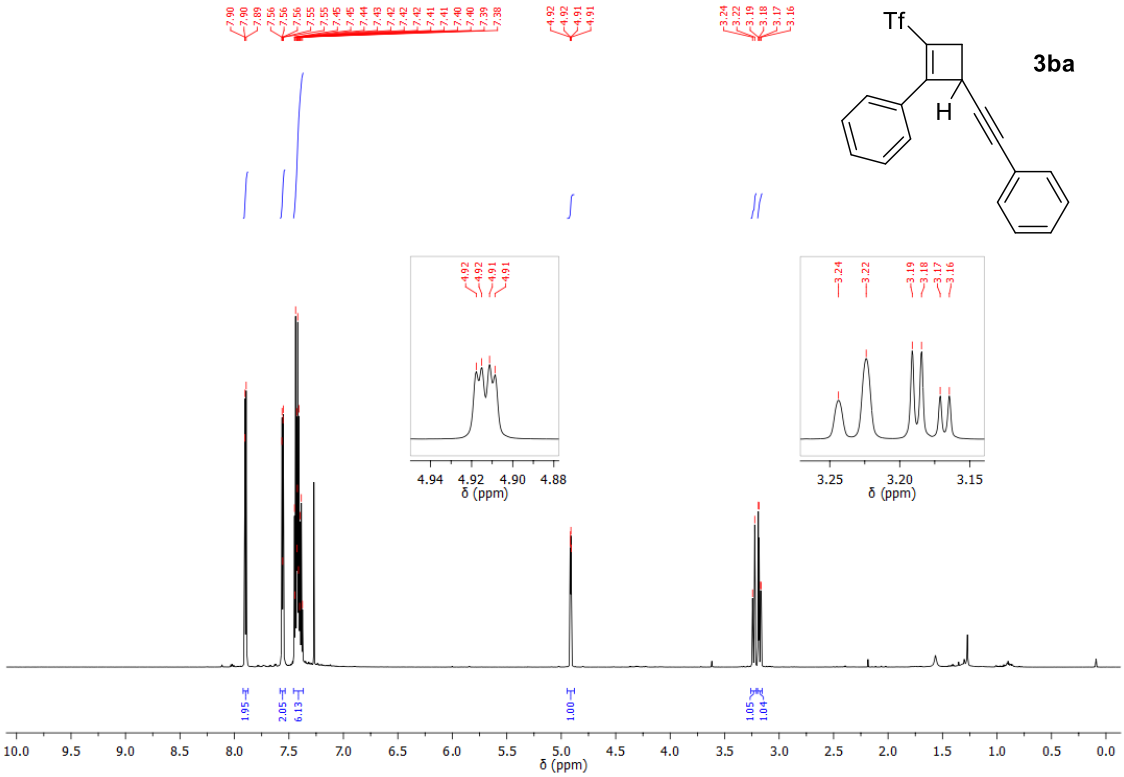
^{19}F NMR (282 MHz, $CDCl_3$)



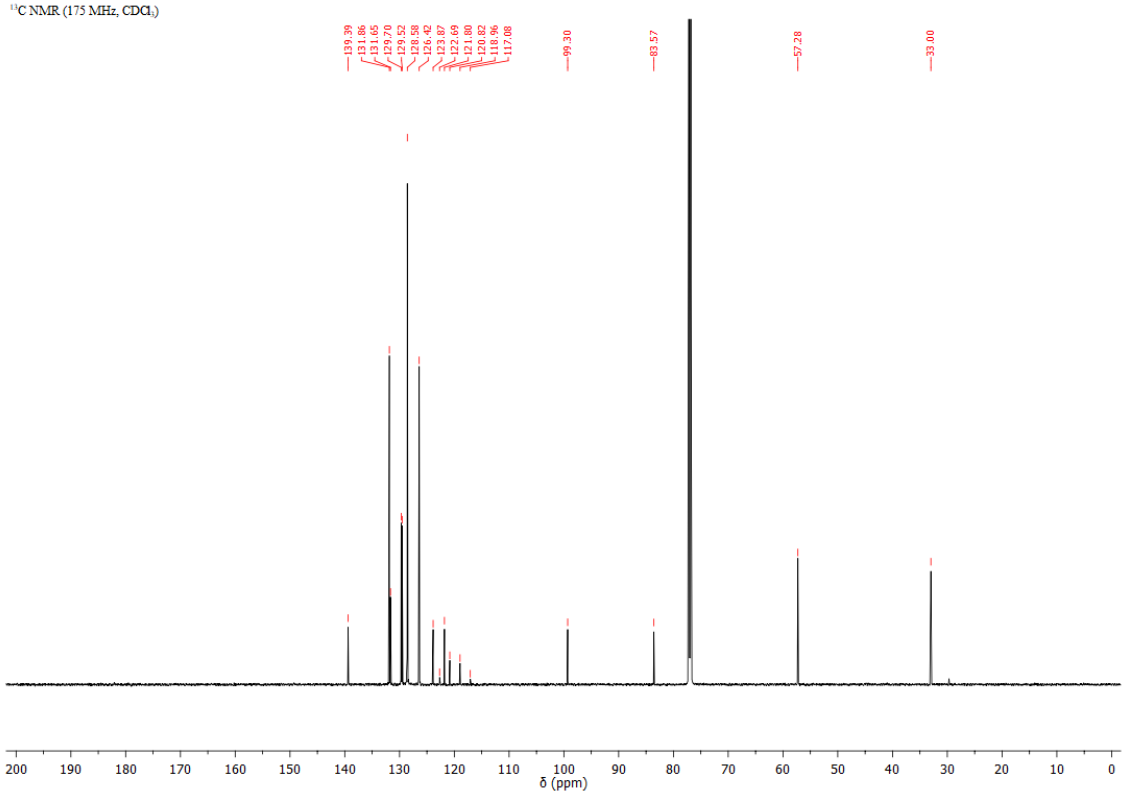
D(^{2}H) NMR (107 MHz, $CDCl_3$)



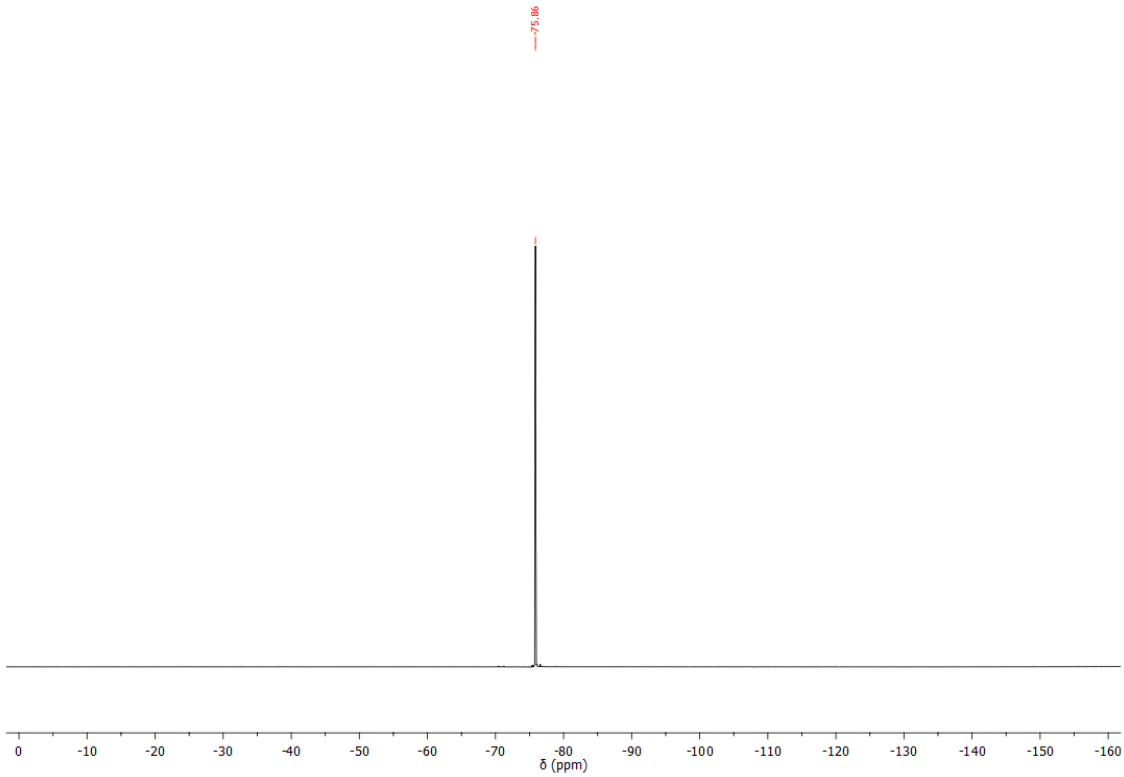
^{1}H NMR (700 MHz, $CDCl_3$)

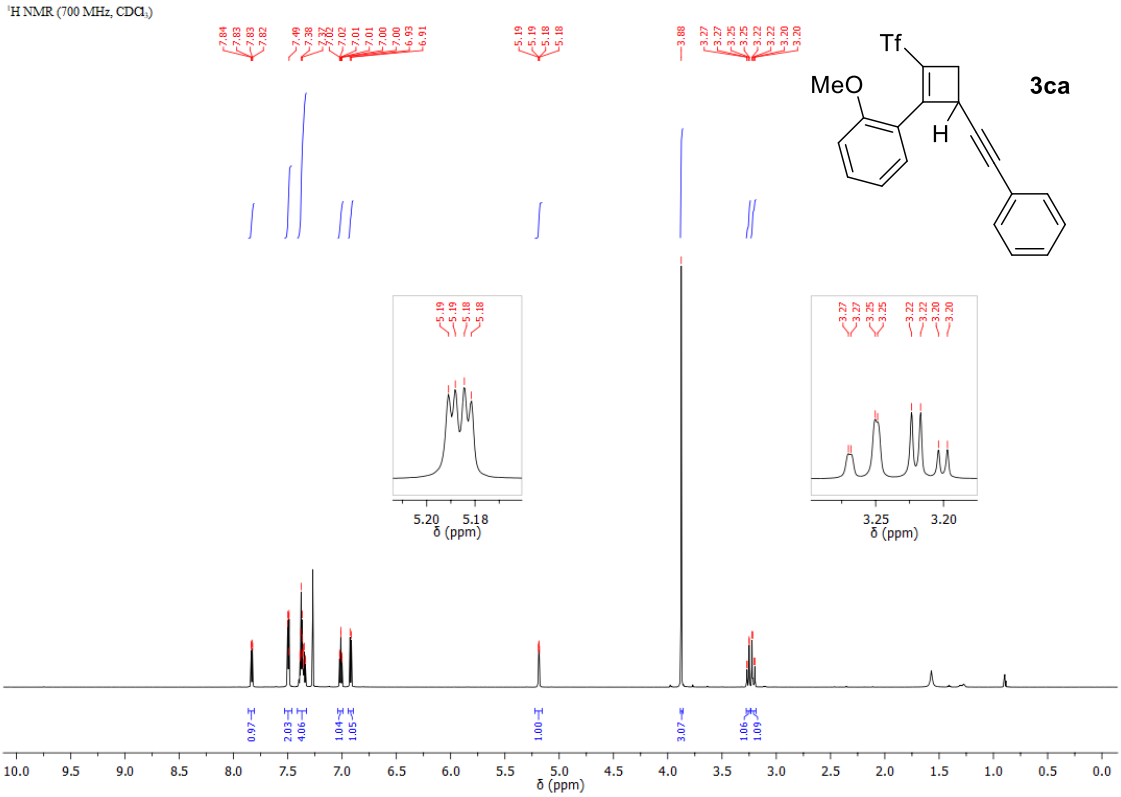


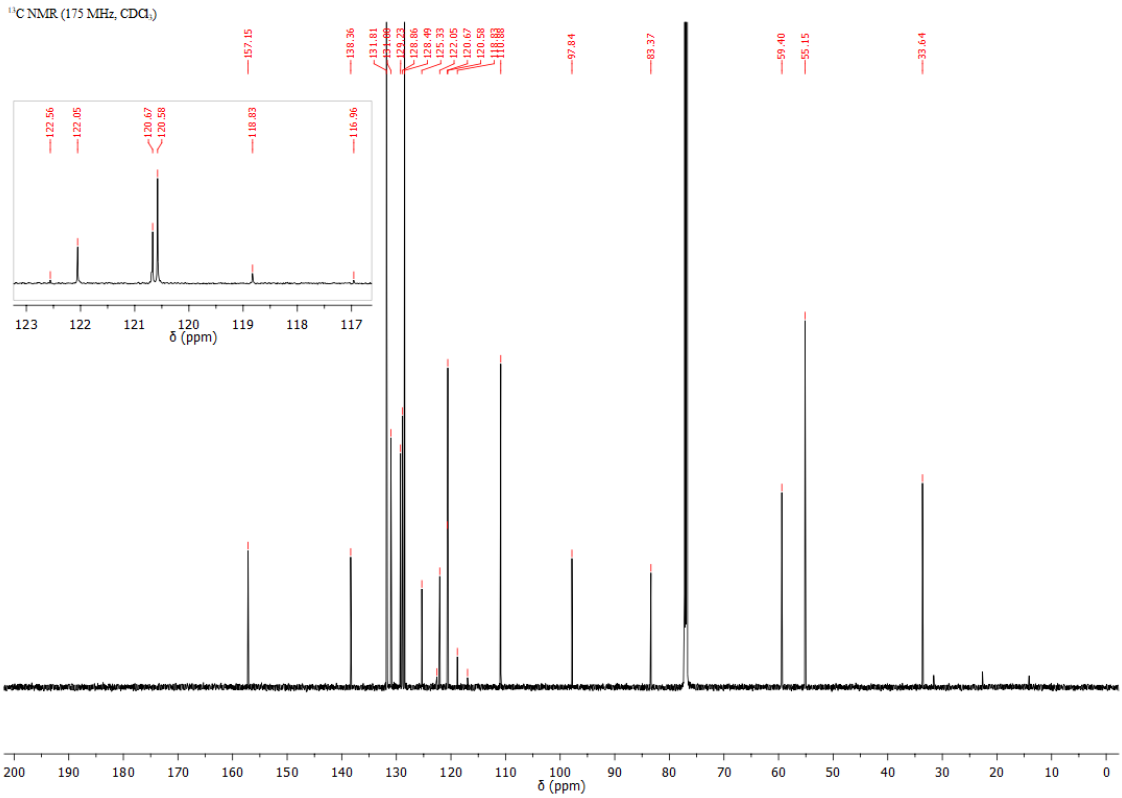
^{13}C NMR (175 MHz, $CDCl_3$)



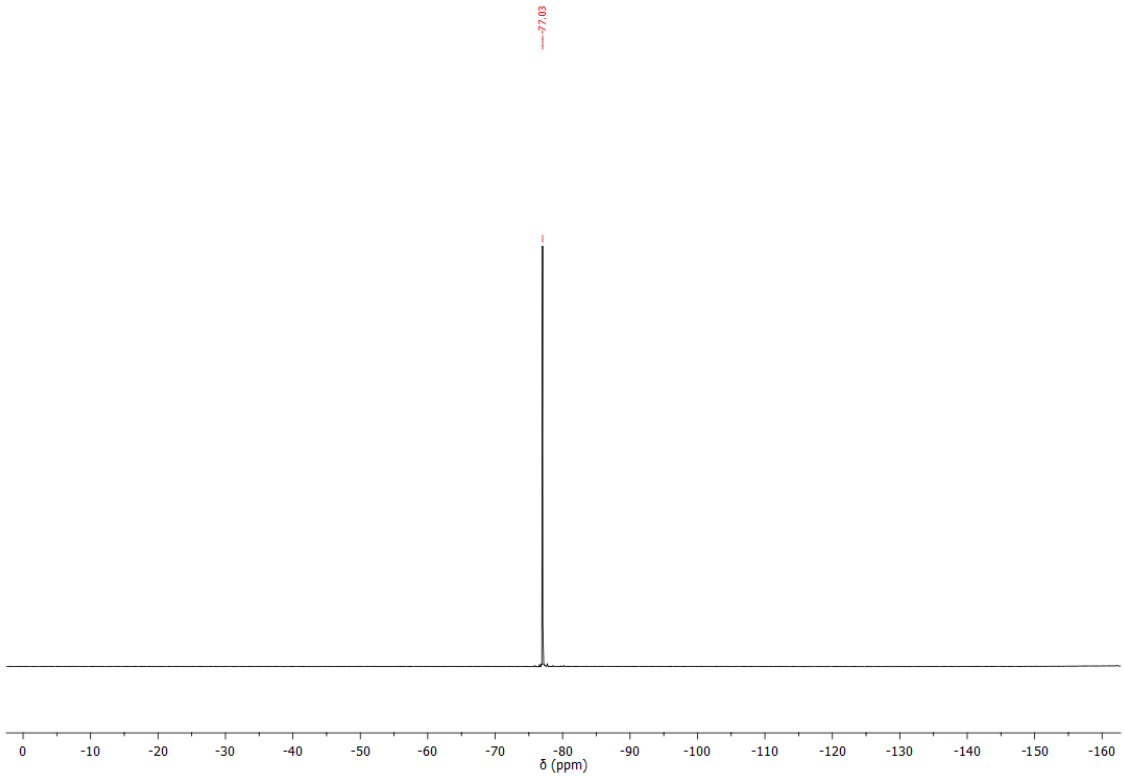
^{19}F NMR (282 MHz, $CDCl_3$)

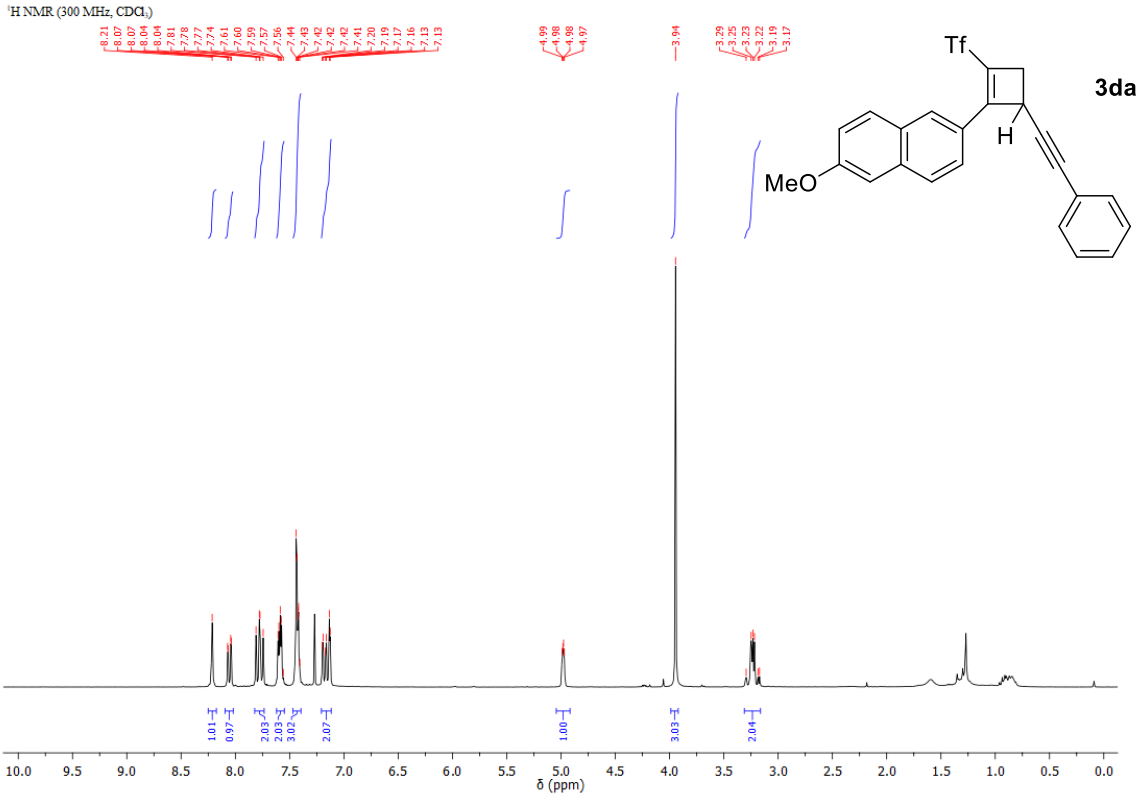


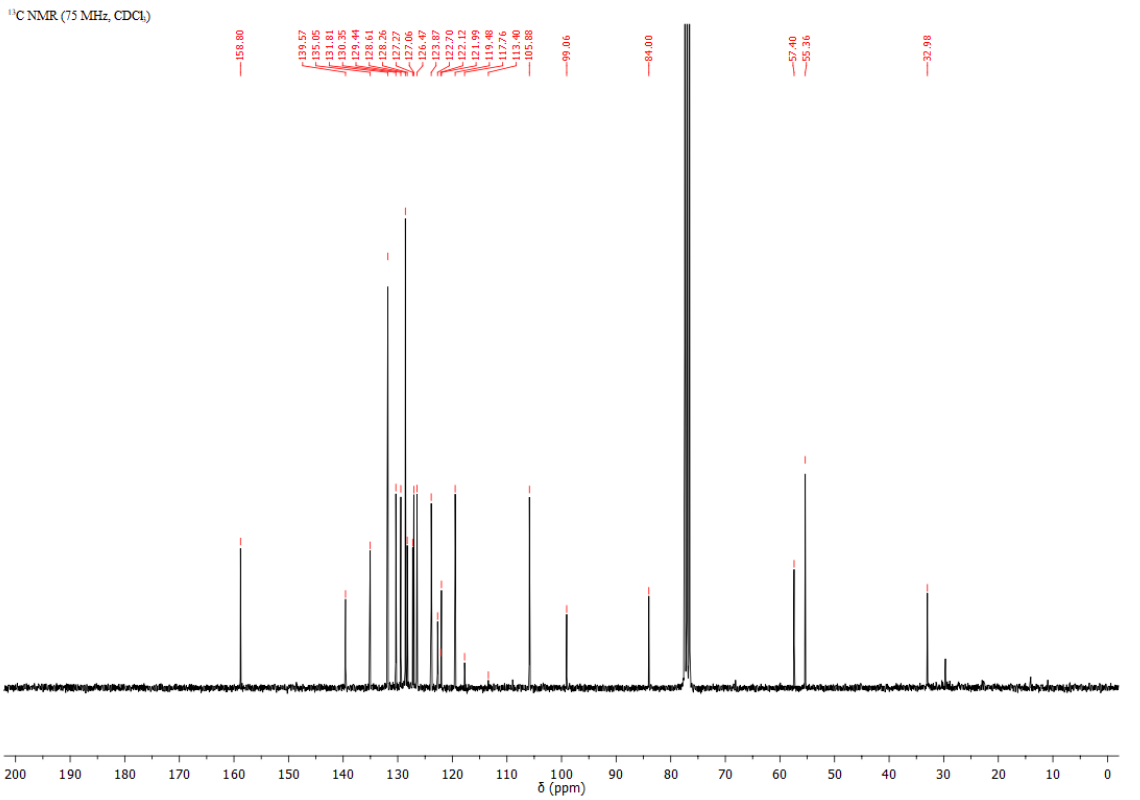

^{1}H NMR (700 MHz, CDCl$_3$)
Tf
MeO
H
3ca
δ (ppm)


^{13}C NMR (175 MHz, CDCl$_3$)
δ (ppm)

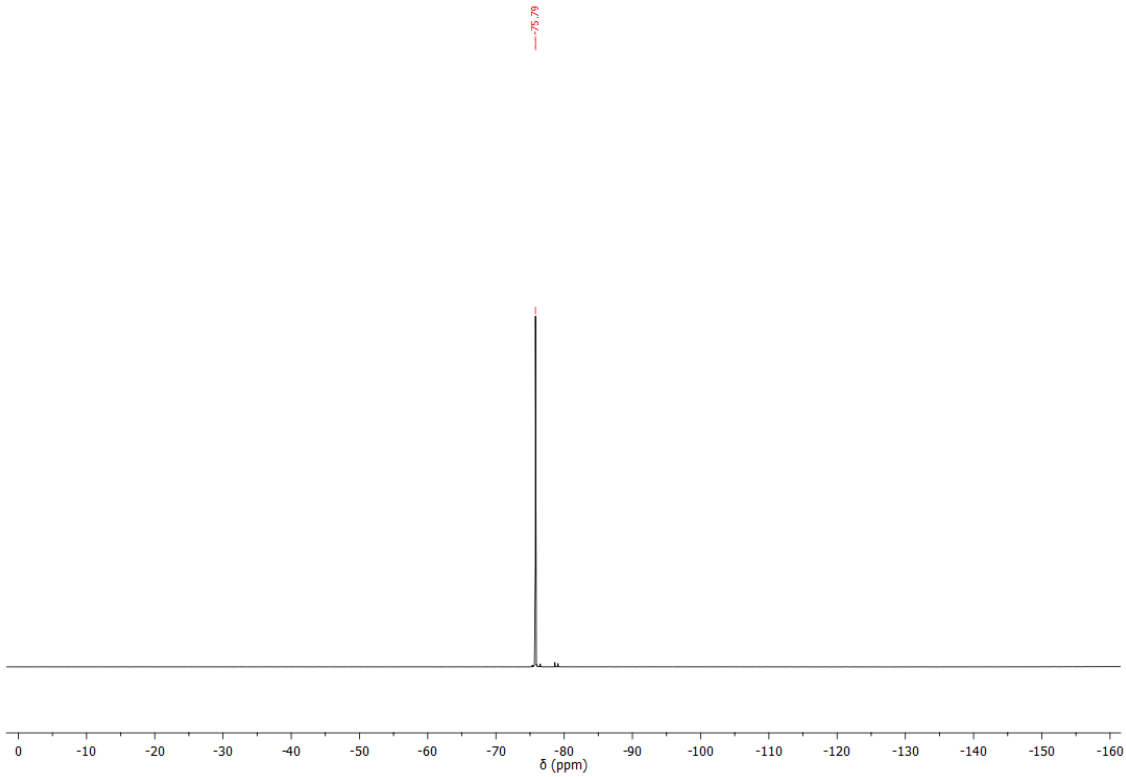
^{19}F NMR (282 MHz, $CDCl_3$)



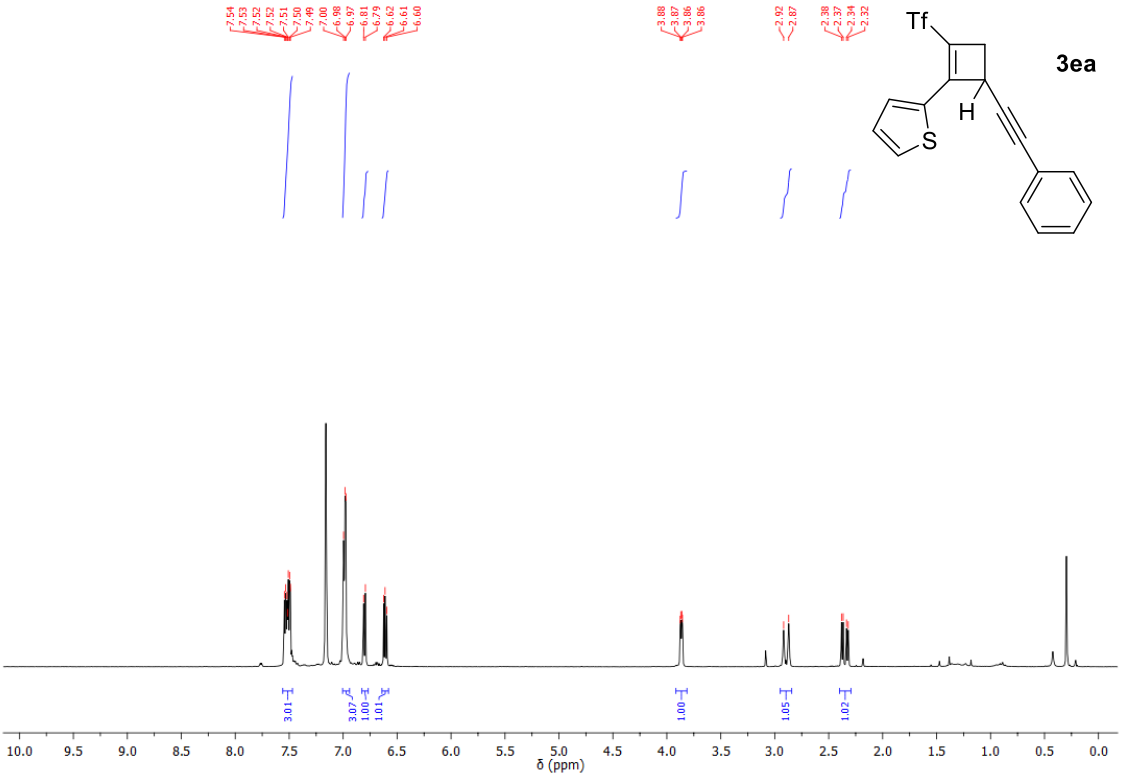

^{1}H NMR (300 MHz, CDCl$_3$)
Tf
H
MeO
3da
δ (ppm)


^{13}C NMR (75 MHz, CDCl$_3$)
δ (ppm)

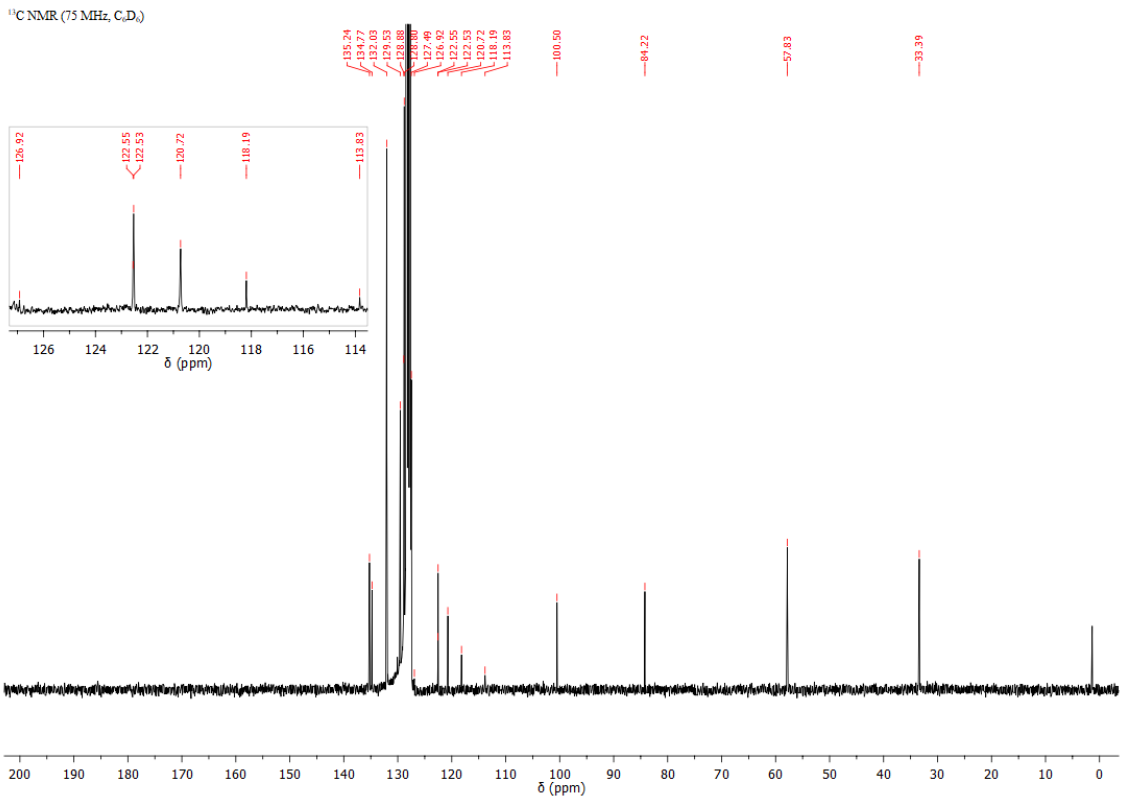
^{19}F NMR (282 MHz, $CDCl_3$)



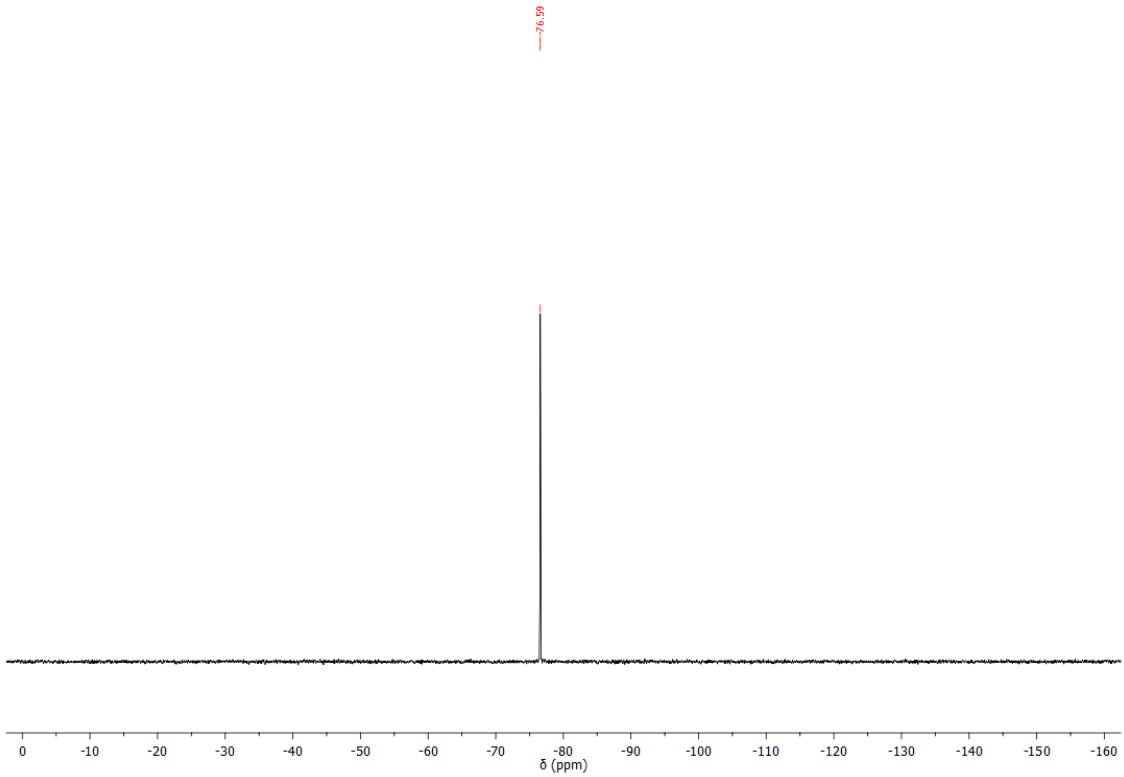
^{1}H NMR (300 MHz, C_6D_6)



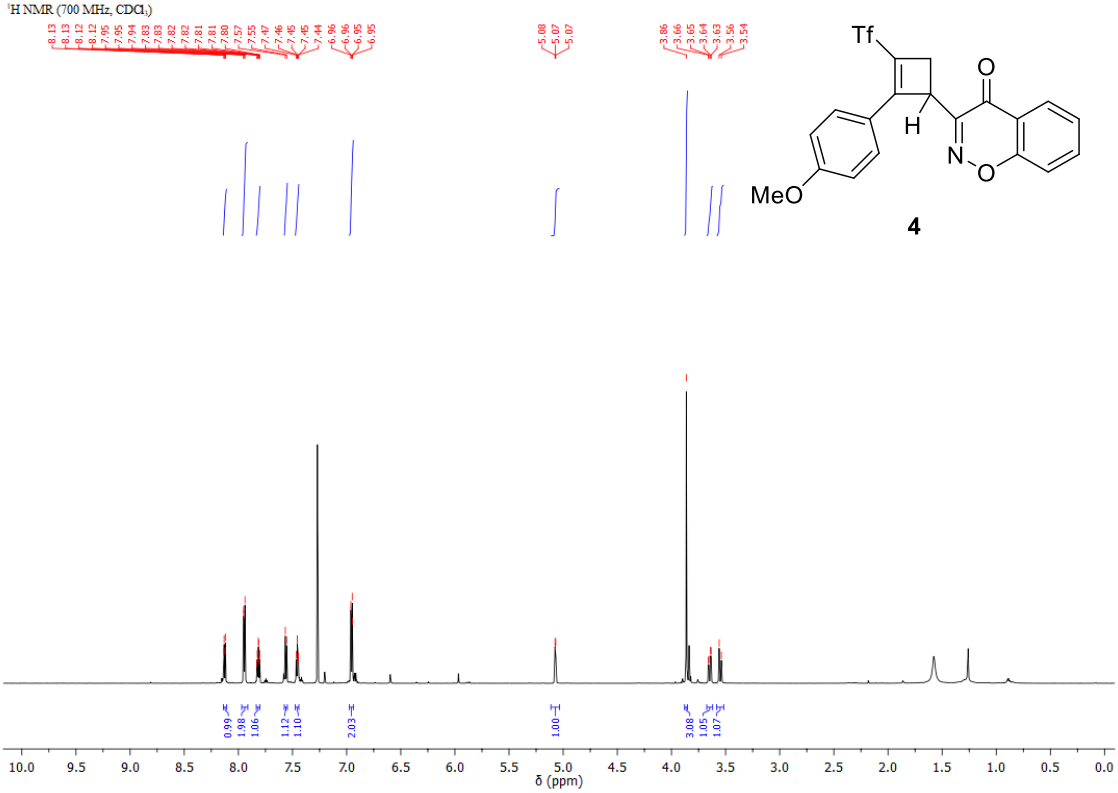
^{13}C NMR (75 MHz, C_6D_6)



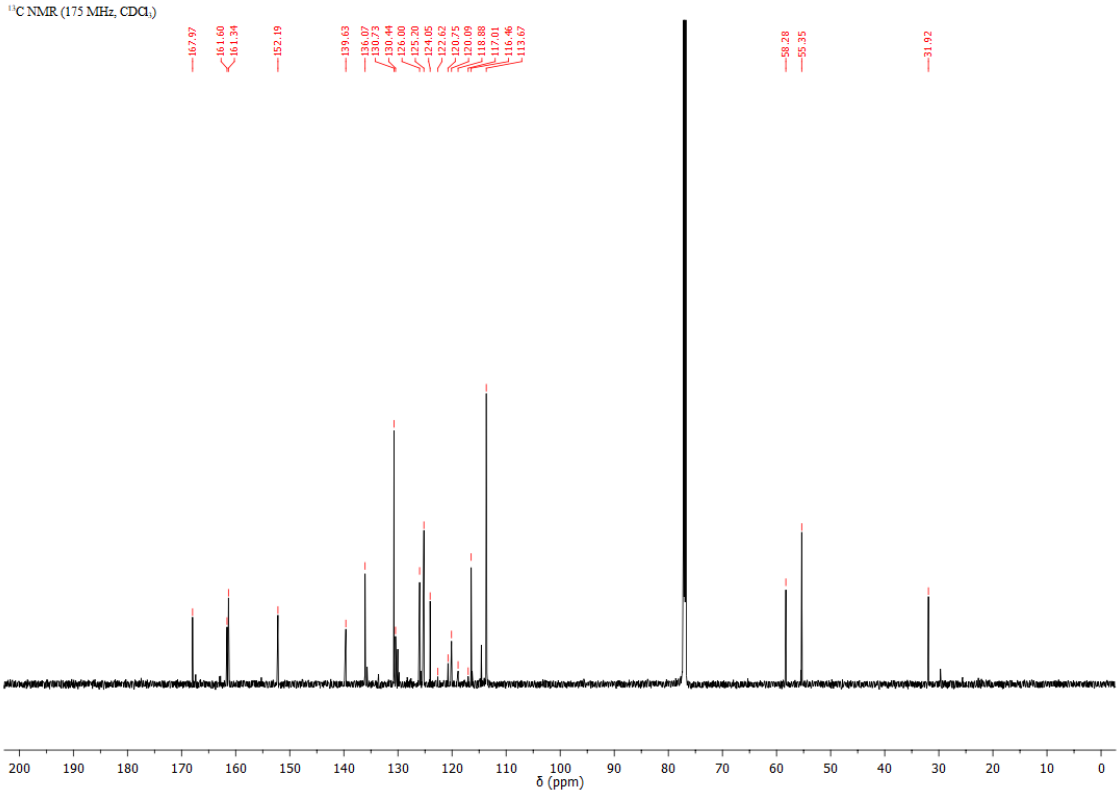
^{19}F NMR (282 MHz, C_6D_6)



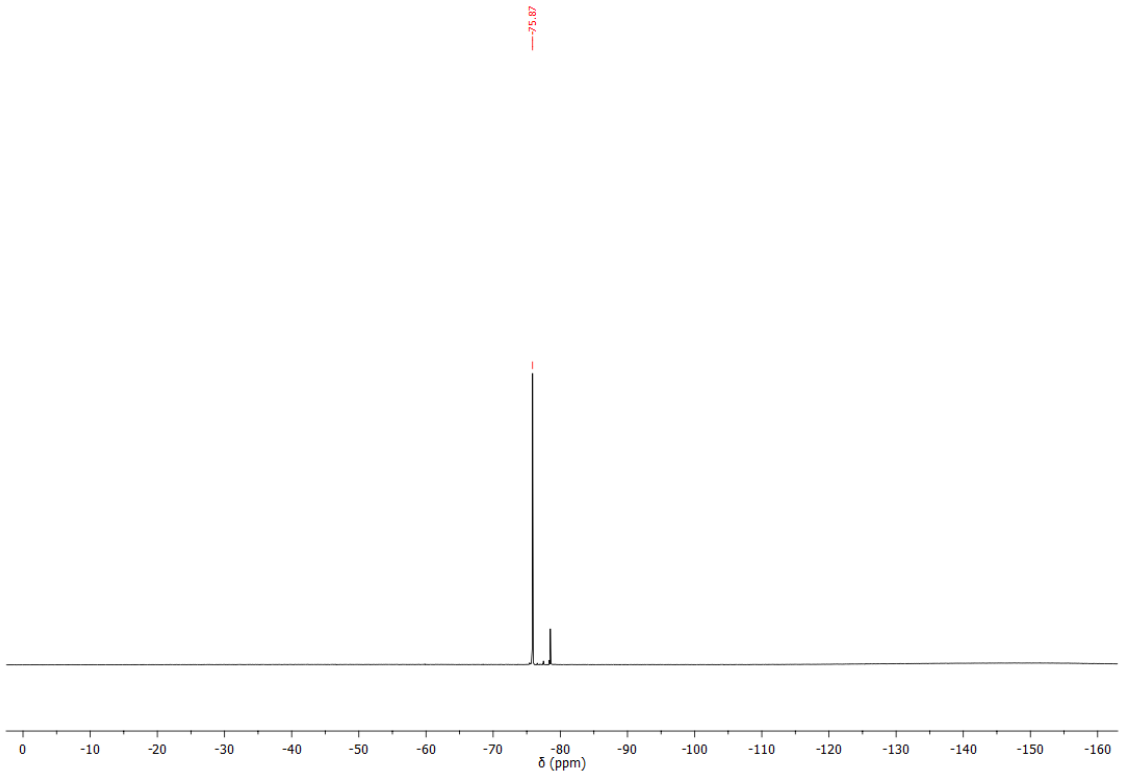
^{1}H NMR (700 MHz, $CDCl_3$)



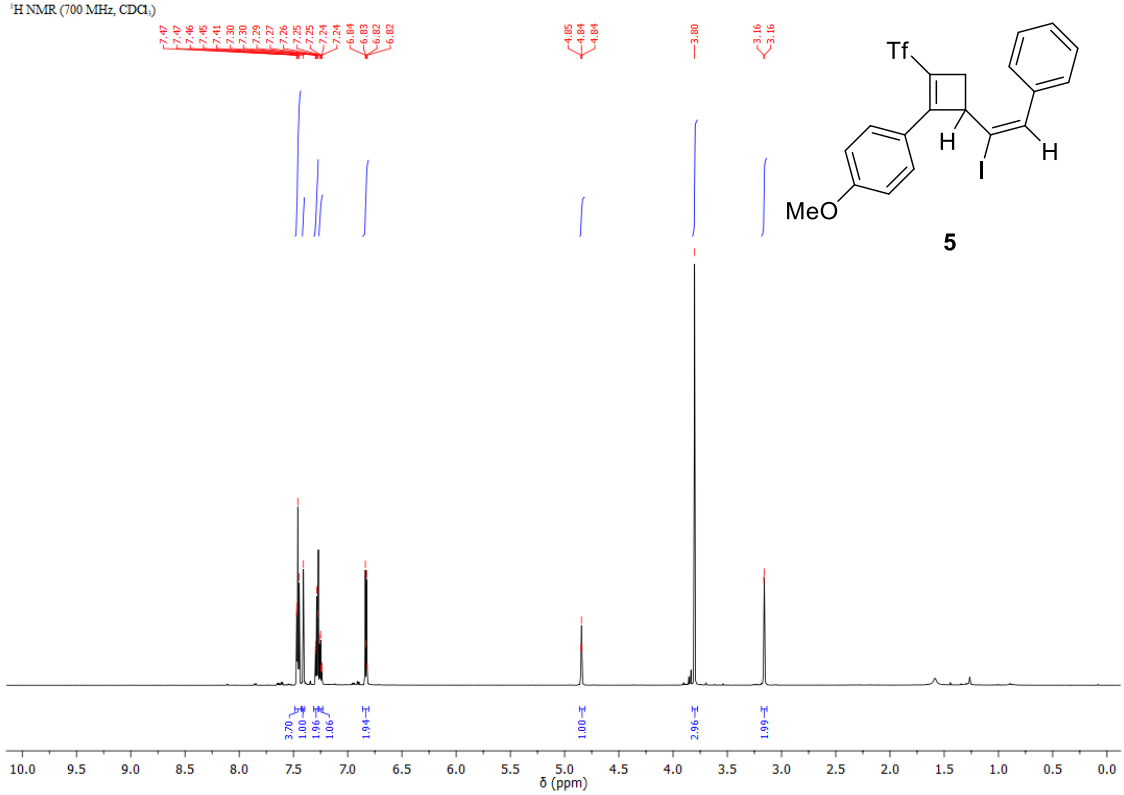
^{13}C NMR (175 MHz, $CDCl_3$)



^{19}F NMR (282 MHz, $CDCl_3$)

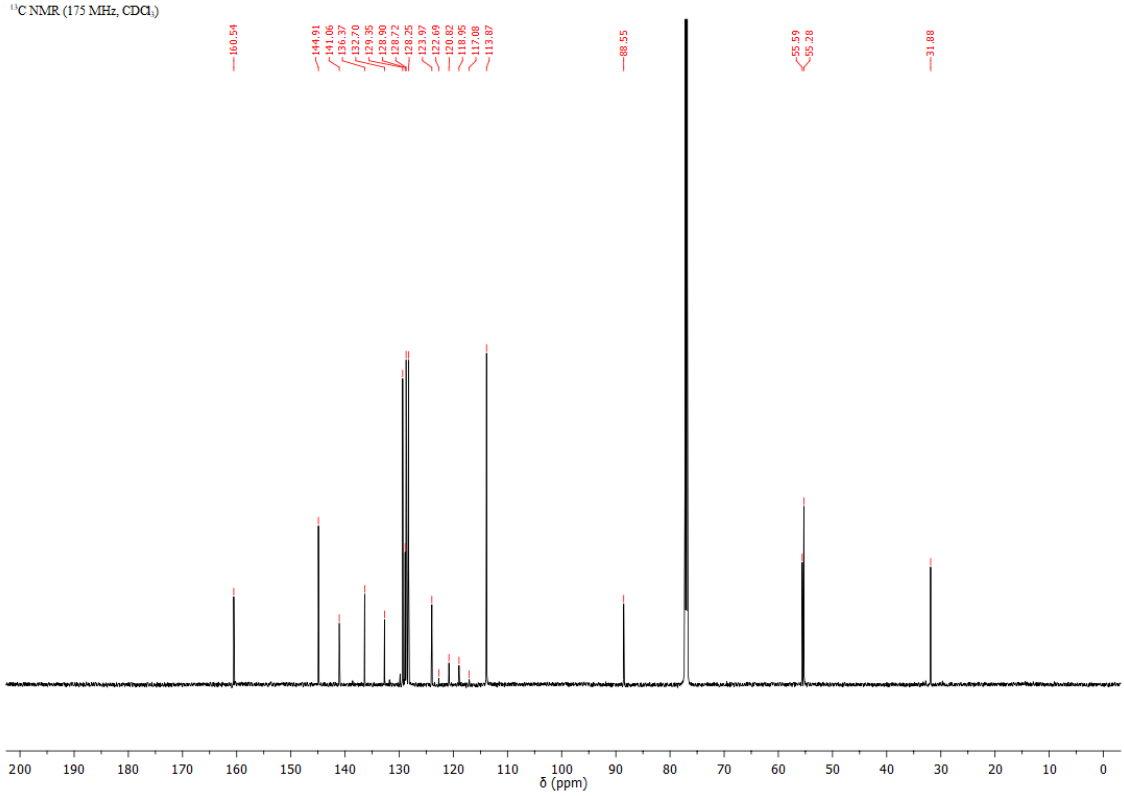


^{1}H NMR (700 MHz, $CDCl_3$)

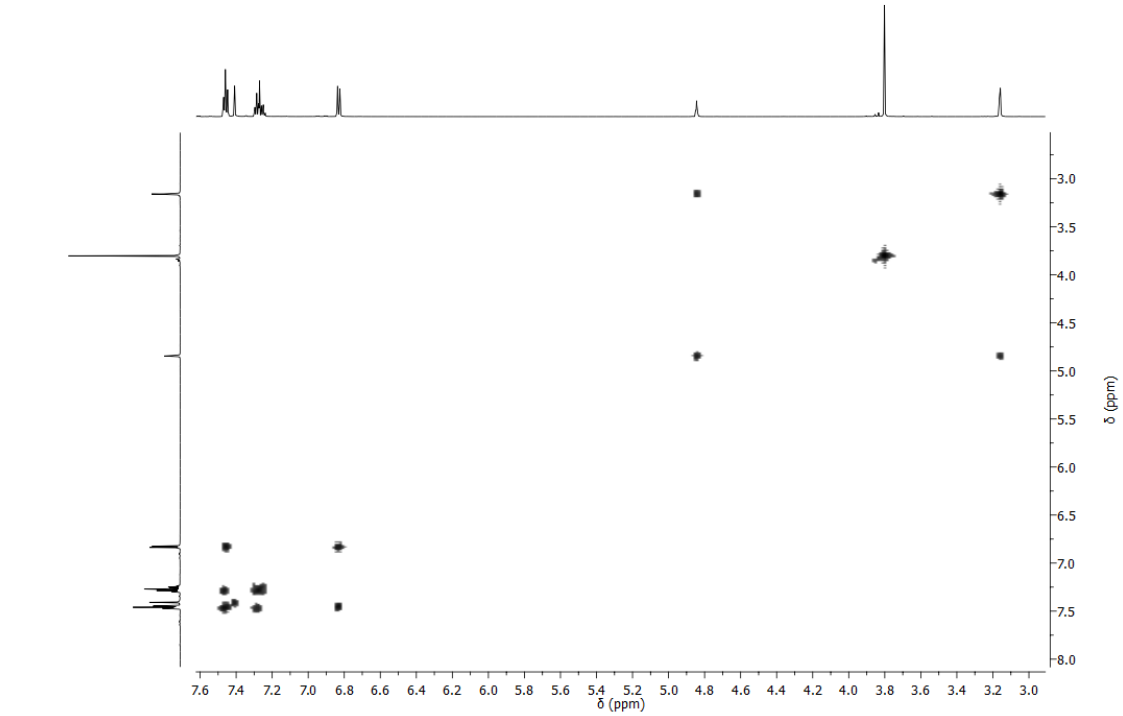


5

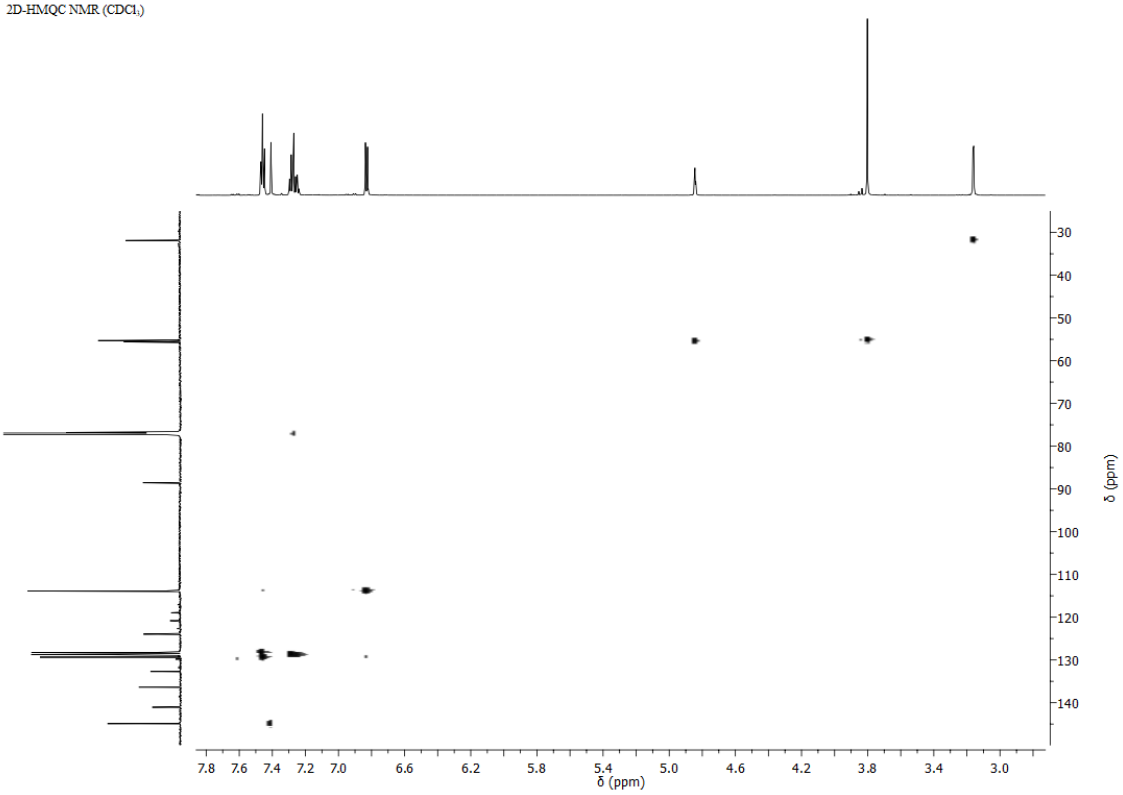
^{13}C NMR (175 MHz, $CDCl_3$)



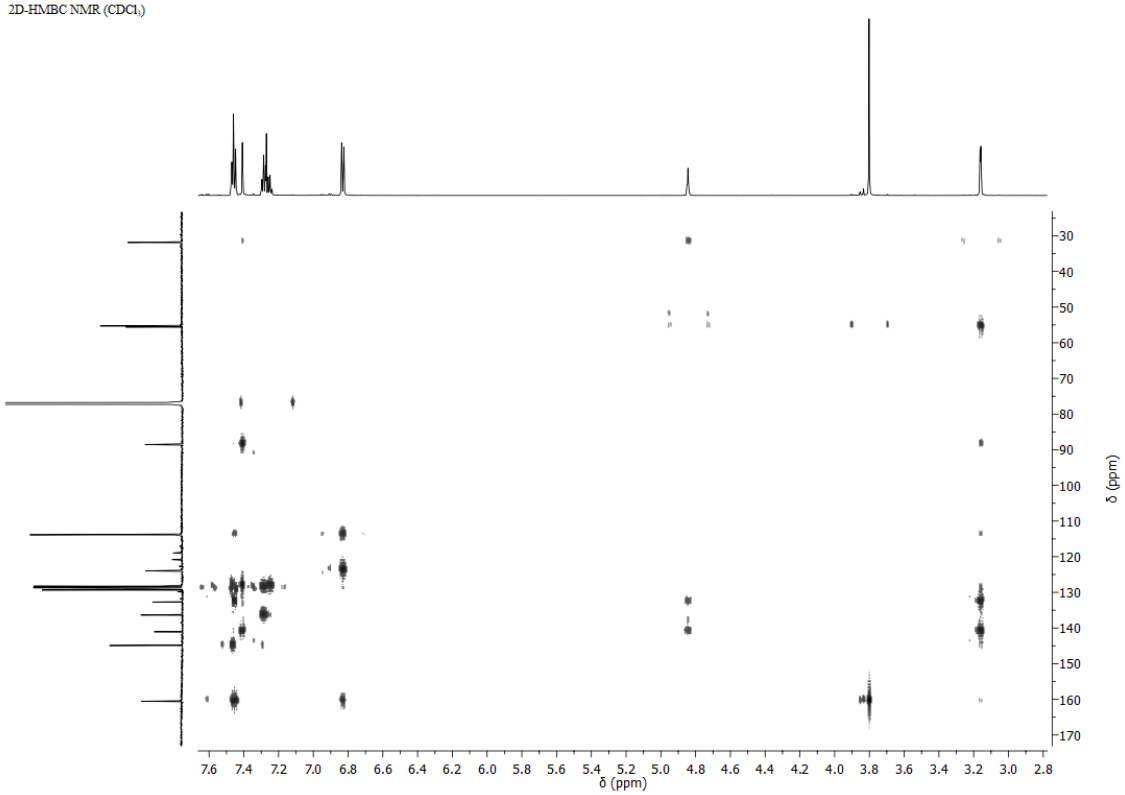
2D-COSY NMR ($CDCl_3$)



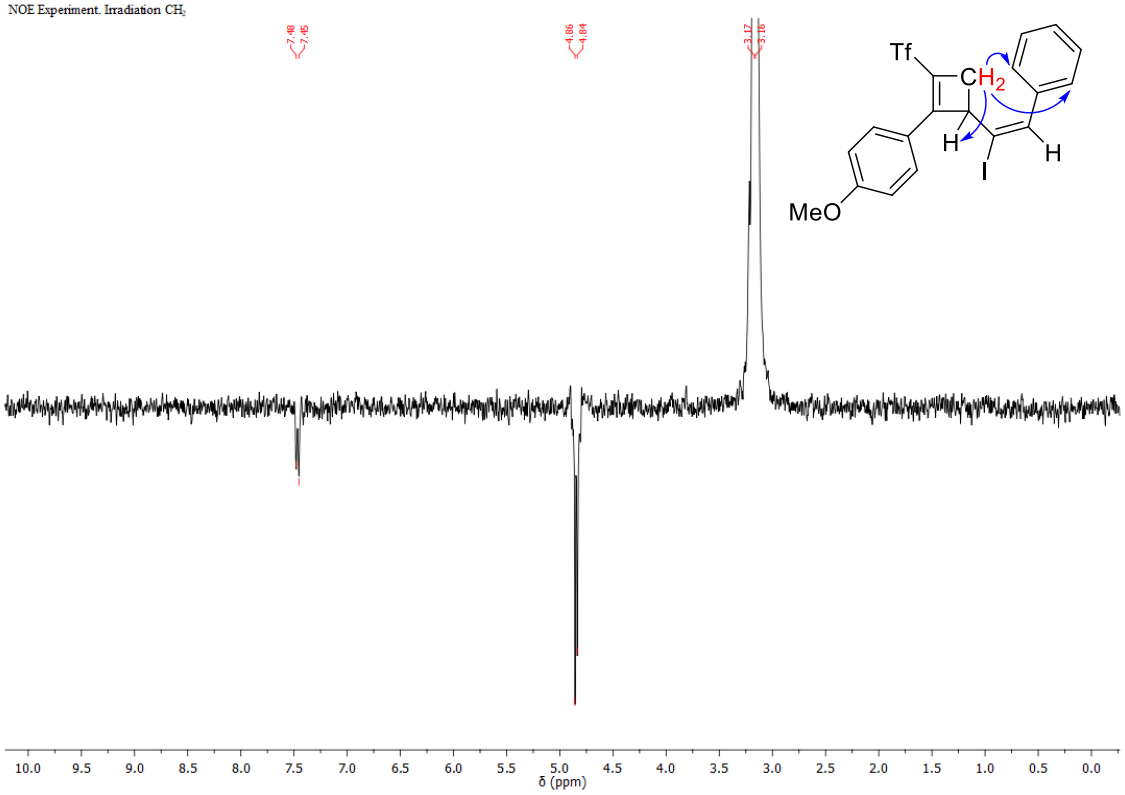
2D-HMQC NMR ($CDCl_3$)

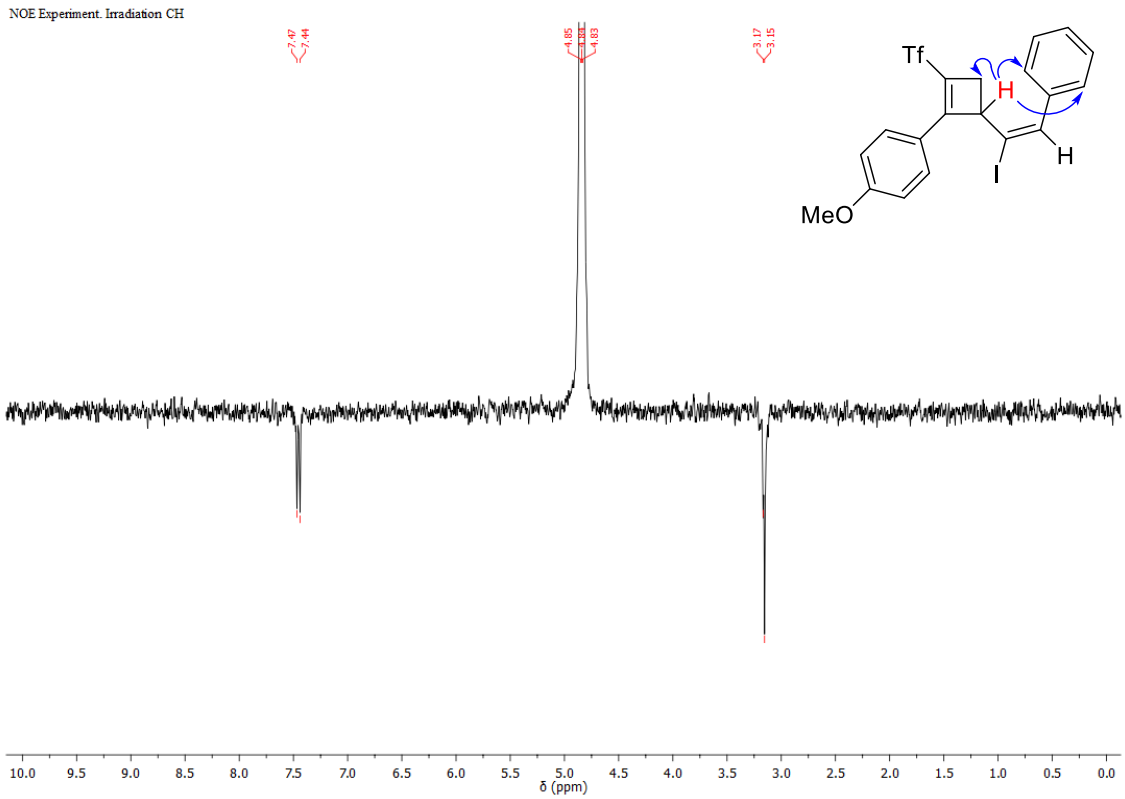


2D-HMBC NMR ($CDCl_3$)

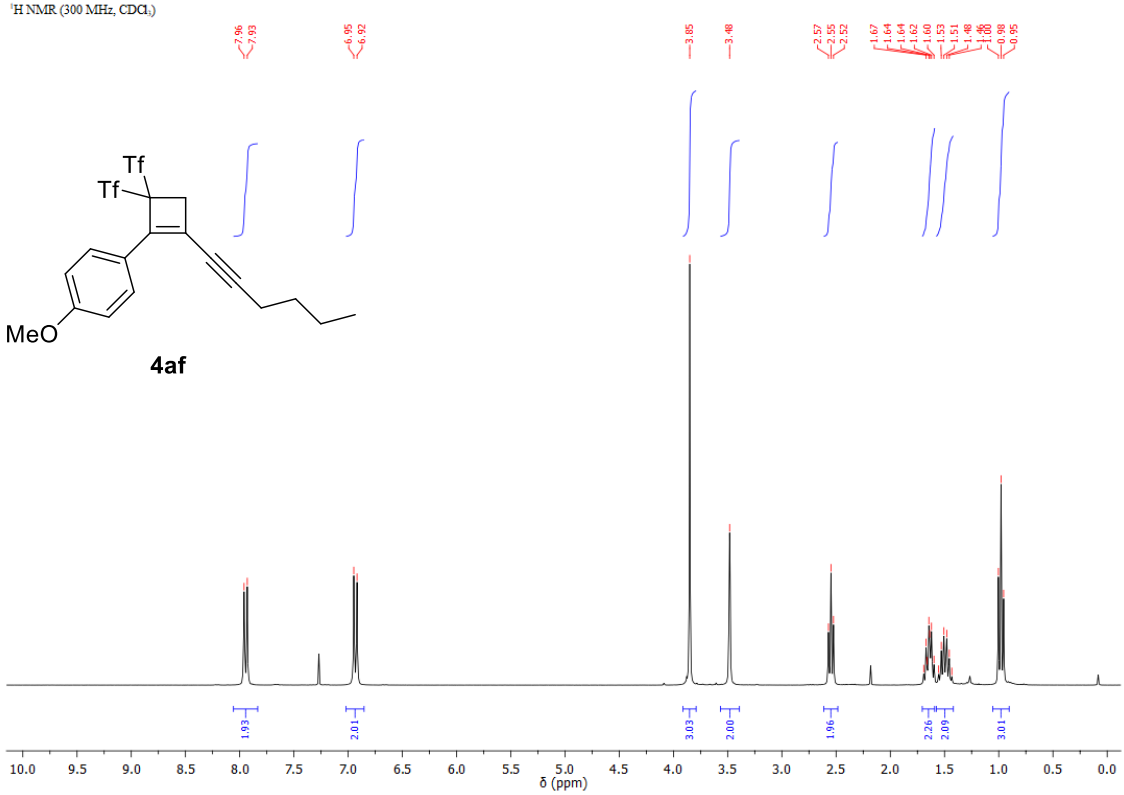


NOE Experiment. Irradiation CH_2

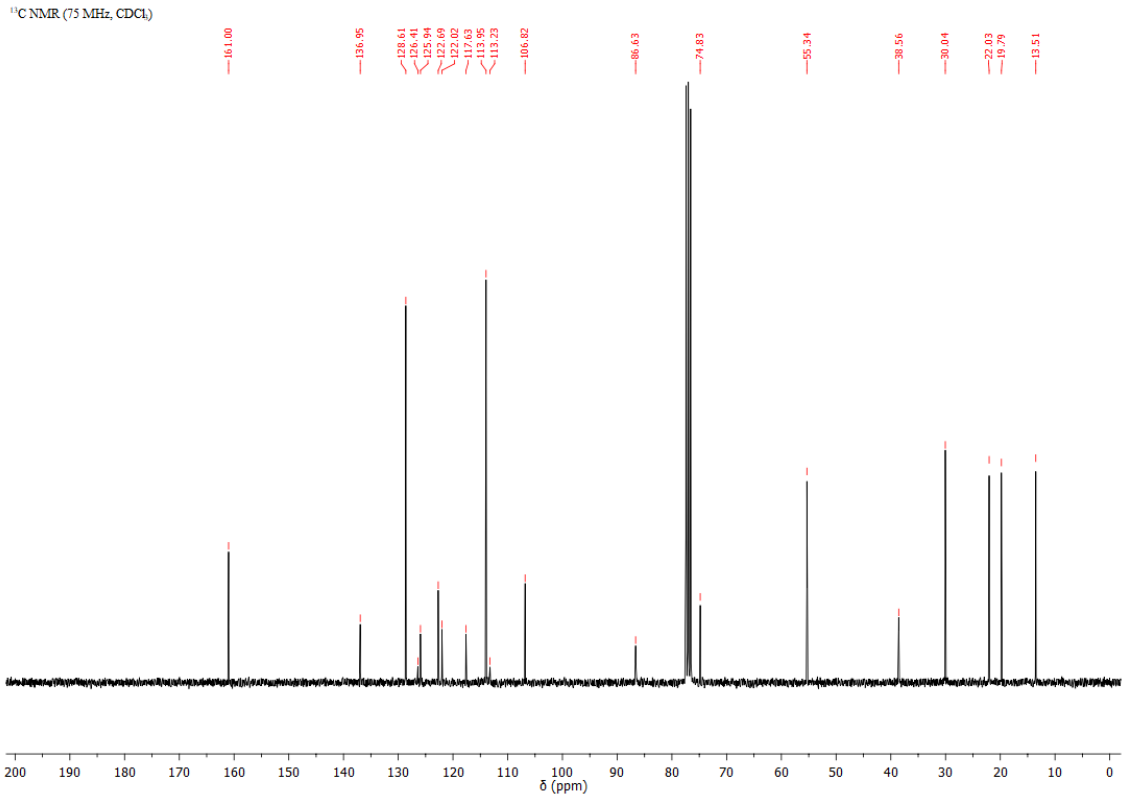



NOE Experiment. Irradiation CH
7.47
7.44
4.85
4.83
3.17
3.15
Tf
H
H
I
MeO
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ (ppm)

^{1}H NMR (300 MHz, $CDCl_3$)



^{13}C NMR (75 MHz, $CDCl_3$)



^{19}F NMR (282 MHz, $CDCl_3$)