Electronic supplementary materials *Mendeleev Commun.*, 2026, **36**, 37–40

Influence of N-heterocyclic carbene modification on the catalytic performance of Pd clusters and nanoparticles in the Mizoroki–Heck reaction

Alexander Yu. Kostyukovich, Evgeniya S. Shutovskaya and Darya O. Prima

Computational details

Quantum chemical calculations were carried out within the framework of density functional theory in the Gaussian 16 program.[S1] The PBE1PBE-GD3BJ/6-31G**&Def2TZVP (for Pd and I atoms) level of theory[S2-S5] was used to optimize the geometry and calculate the frequencies of molecular vibrations. The SMD continual model was chosen to consider the effect of the solvent.[S6] Tetrahydrofuran was used as the solvent (ε = 7.4257). Geometry optimization of Pd_2 and Pd_3 clusters was performed with a constraint on a fixed Pd-Pd distances to avoid destruction of the dimeric (trimeric) structure. Building and optimization of NHC-modified compounds was performed as follows: 1) two solvate molecules were removed from the NHC-free compound, and an NHC ligand was added instead; 2) the geometry of the NHC fragment was optimized with "freezing" the remaining atoms of the compound; 3) then the full optimization was performed. This approach was used to find structurally similar forms of NHC-containing and ligand-free catalytic systems.

General procedures

All the chemicals were purchased from commercial sources and used without additional purification. All synthetic manipulations were conducted under an argon atmosphere. Dry solvents were used for all manipulations.

The products detection and quantification was carried out with GC-MS and by NMR analysis of the reaction mixtures, using 1,4-dinitrobenzene as internal standard. The products were identified by comparison of products NMR spectral data with those reported in the literature and by comparison of mass spectra with NIST database. GC-MS measurements were done with Agilent Technologies 6890B gas chromatograph (HP-5 ms column) equipped with an MSD 5975 mass-selective detector. NMR spectra were recorded on a Bruker Fourier 300 HD spectrometer. ^{1}H NMR (300 MHz) chemical shifts were determined relative to the signal of tetramethylsilane.

The cross-coupling reaction procedure

To a screw-capped test-tube with a magnetic stir bar was loaded 1.3 mg of Pd/C 5% and 49.8 mg K_2CO_3, followed by 0.5 mL of the solution of IPr·HCl in NMP (*c* = 1mg/mL), alkene (0.45 mmol) and aryl halide (0.3 mmol). The reaction vessel was flushed with Ar for 10 seconds and the screw cap was closed tightly. The reaction was carried out at 120 °C for 4 h. Afterwards, 0.05 mL of solution of 1,4-dinitrobenzene in NMP was mixed with the reaction mixture and the test-tube was centrifuged. The product yield was evaluated by ^{1}H NMR spectra of the reaction mixture recorded in $CDCl_3$, using signal of 1,4-dinitrobenzene as internal standard.

Leaching test reaction procedure.

A test-tube containing a magnetic stir bar was loaded with 49.8 mg (0.36 mmol) of K_2CO_3, 6.4 mg of Pd/C 5% and 2.6 mg (0.0006 mmol) of IPr·HCl (if required). The reaction vessel was washed with 0.5 mL of NMP, afterwards 52 μL (0.45 mmol) of styrene, and 31 μL (0.3 mmol) of bromobenzene were added and the test-tube was immediately flushed with Ar and closed. Following the reaction at 120 °C for 1 h, the mixture was centrifuged at 3500 rpm. The resulting clear supernatant was carefully filtered through a 0.45 μm membrane filter via syringe and transferred to a new vessel containing a fresh portion of K_2CO_3. The reaction was then prolonged for an additional two hours.

The isolated solid was washed with acetone (2x3 mL), water (3x3 mL), acetone (1x3 mL) and left to dry on the air at room temperature overnight.

TEM experiment

The sample morphology was studied via a Hitachi HT7700 transmission electron microscope. The images were acquired in bright-field TEM mode at accelerating voltage of 100 kV accelerating voltage. The TEM magnification values given in the figures were adopted from original images provided by the electron microscope software.

TEM images of Pd/C catalyst before and after the reaction

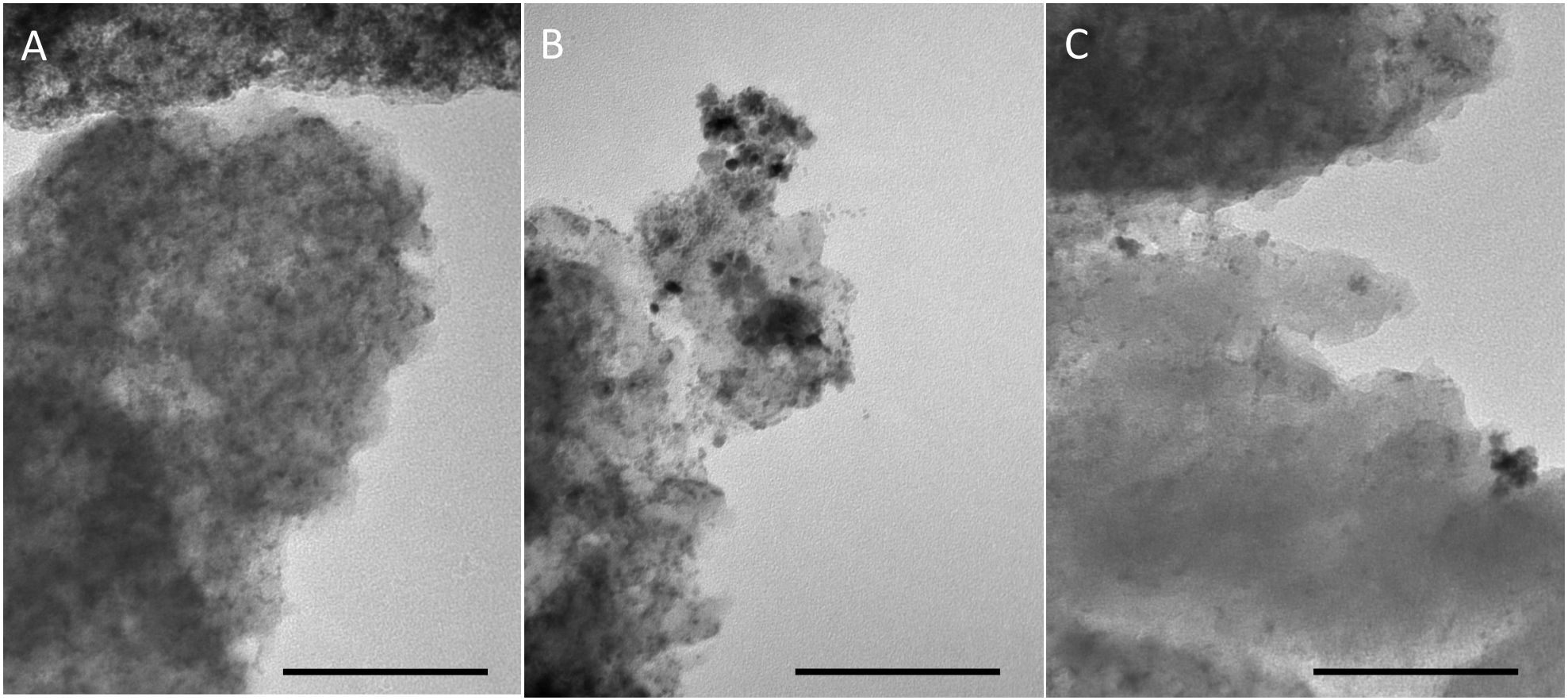


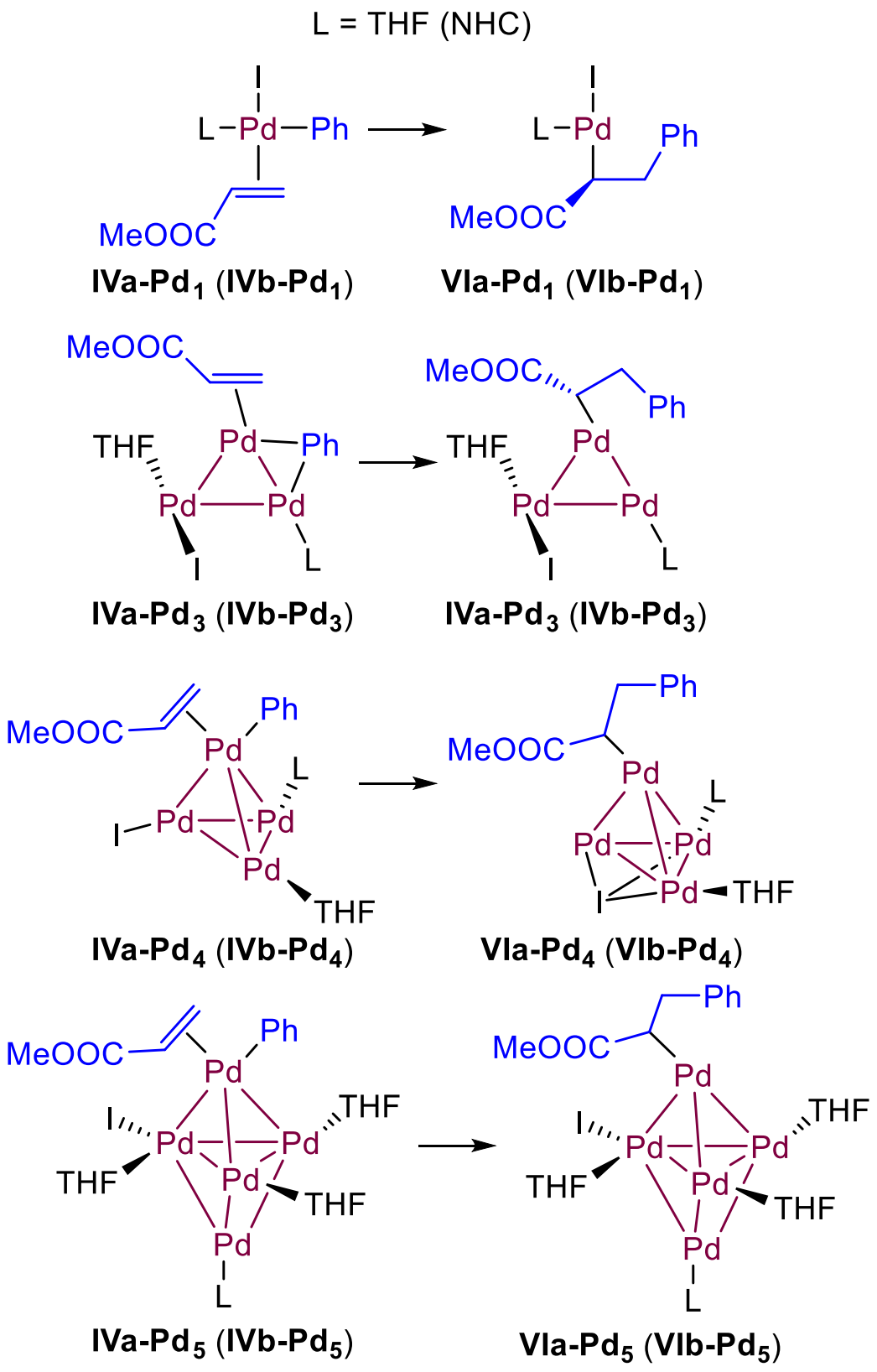
Figure S1. TEM images of Pd/C catalyst: Initial sample of Pd/C 5 % (A); Sample isolated after the coupling of bromobenzene and styrene with IPr·HCl additive (B) and without additive (C). Scale bar – 100 nm.

Computational modeling of alkene insertion stage of the Mizoroki–Heck reaction for metal complex Pd_1 and clusters Pd_3-Pd_5

The main challenge of computational modeling of catalytic reactions stems from the vast variability of active Pd species and the multitude of possible reaction pathways. Catalytically active species formed in situ from precatalyst can differ in nuclearity, ligand environment, and isomeric or conformational forms. Consequently, patterns identified in a single calculated reaction pathway may not always be applicable to real systems. To address this problem, we conducted additional calculations to assess the reproducibility of the observed effect across systems with varying nuclearity. The model range was expanded to include a mononuclear Pd complex and Pd_3 - Pd_5 clusters. Only the key step of alkene insertion was considered. The activation energy of the insertion stage for the modified compounds decreased by 0.7 - 6.5 kcal/mol (or by 9 - 42% in relative terms) compared to NHC-free systems (Table 2, Scheme 2). Therefore, the effect of NHC modification was consistently observed for all considered systems as a reduction of the reaction potential barrier.

Table S1. Potential barriers of the methyl acrylate insertion into the Pd-Ph bond in NHC-modified and NHC-free compounds Pd_1 - Pd_5.

	NHC-free	NHC-modified
Pd_1	15.3	8.8
Pd_2	17.7	13.6
Pd_3	21.6	16.7
Pd_4	13.1	11.7
Pd_5	8.1	7.5



Scheme S1. Insertion of methyl acrylate into the Pd-Ph bond
in model unmodified (L = THF) and modified (L = NHC) compounds Pd_1, Pd_3 - Pd_5.

^{1}H NMR spectra of Pd/C$_{IPr\cdot HCl}$ catalyzed Heck reaction

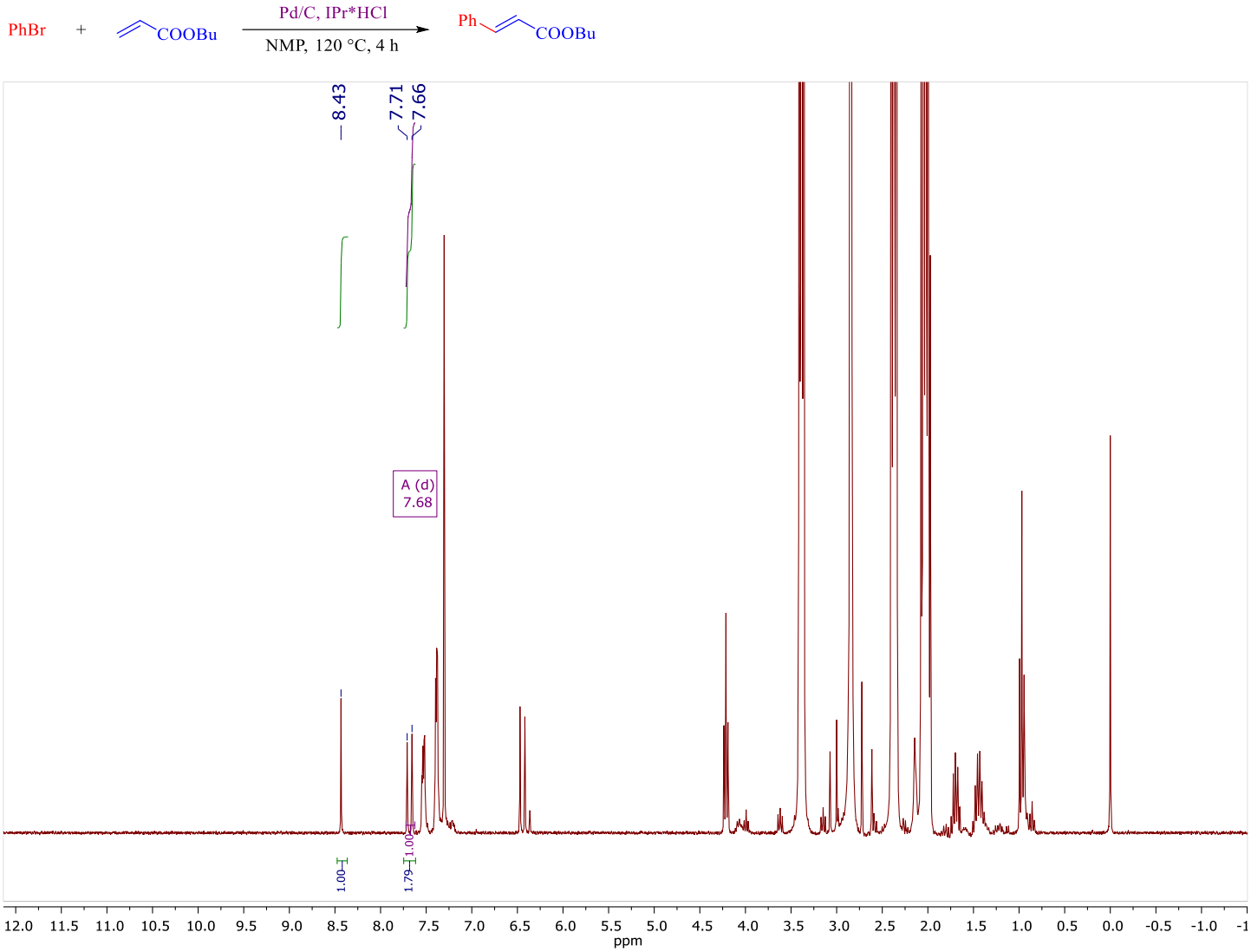
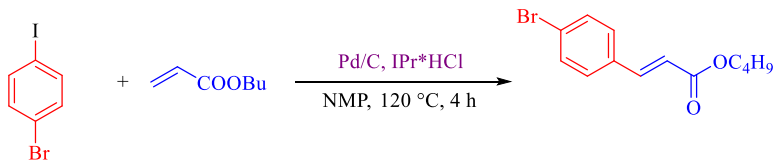


Figure S2. ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing butyl cinnamate. Characteristic signal: 7.68 (d, *J* = 16.0 Hz, 1H, =CH). Signal of *p*-dinitrobenzene: 8.43 ppm (s, 4H), n = 0.03125 mmol.



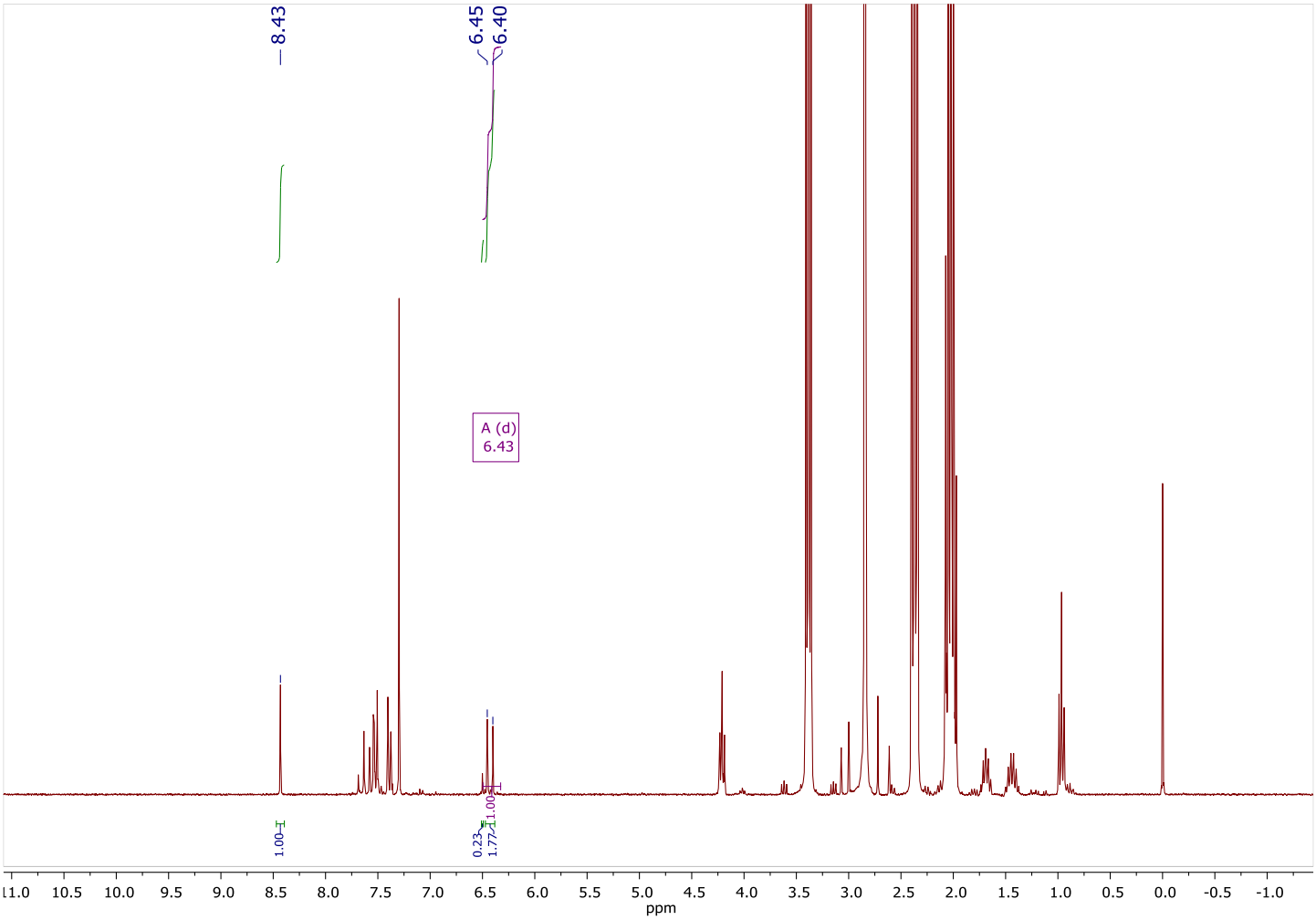
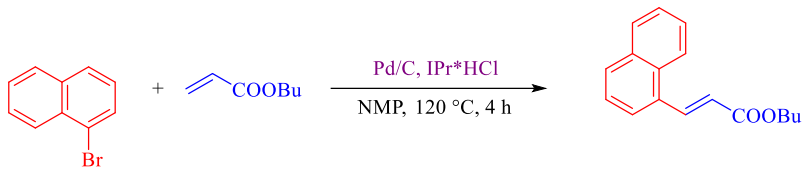


Figure S3. ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing butyl (*E*)-3-(4-bromophenyl)acrylate. Characteristic product signal: 6.43 ppm (d, *J* = 16.0 Hz, 1H, =CH). Signal of *p*-dinitrobenzene: 8.43 ppm (s, 4H), n = 0.03125 mmol.



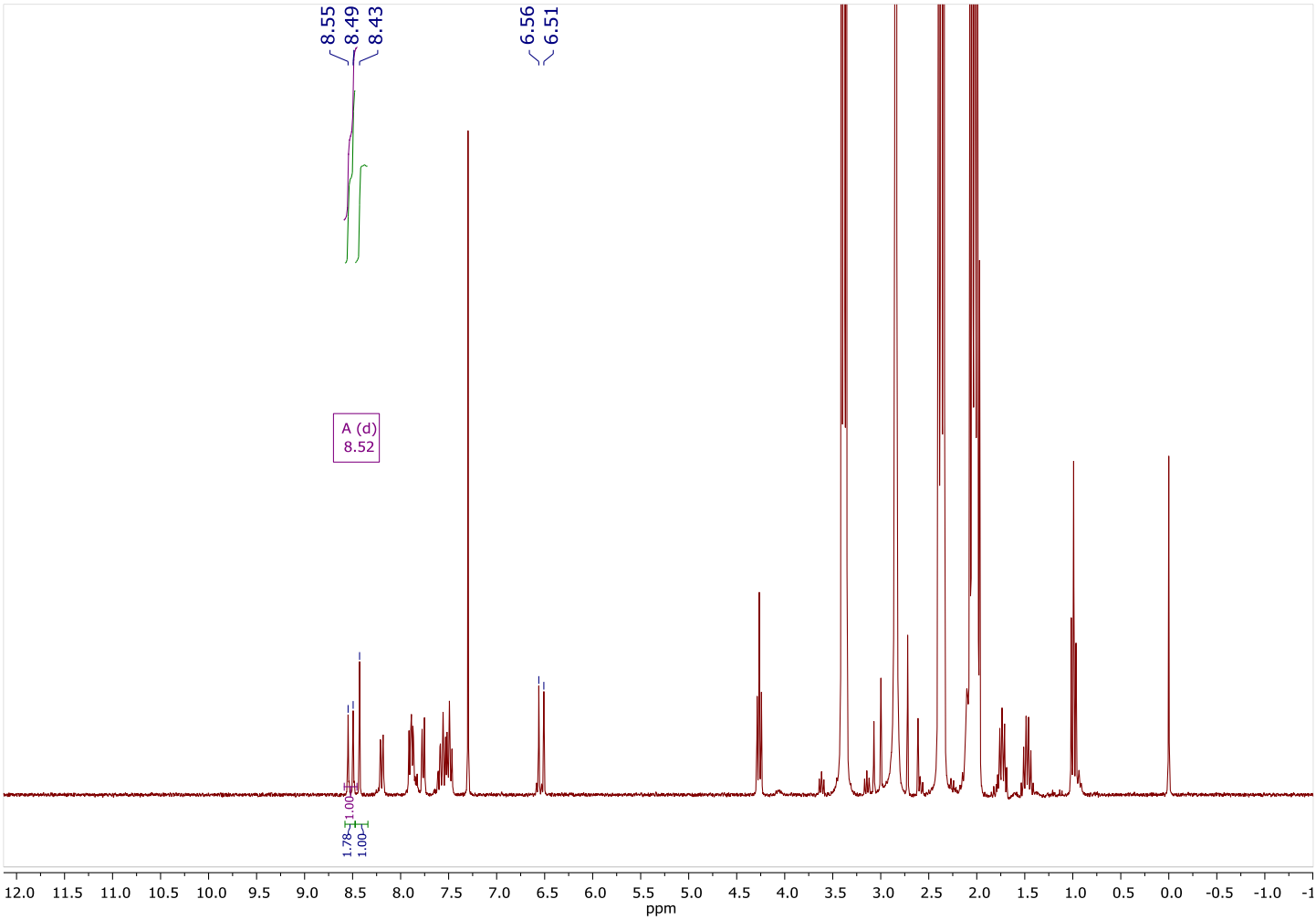
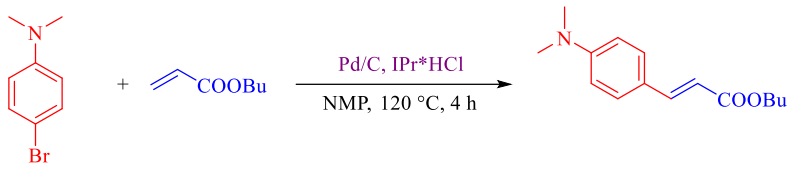


Figure S4. ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing butyl (*E*)-3-(naphthalen-1-yl)acrylate. Characteristic product signal: 6.43 ppm (d, *J* = 16.0 Hz, 1H, =CH). Signal of *p*-dinitrobenzene: 8.43 ppm (s, 4H), n = 0.03125 mmol.



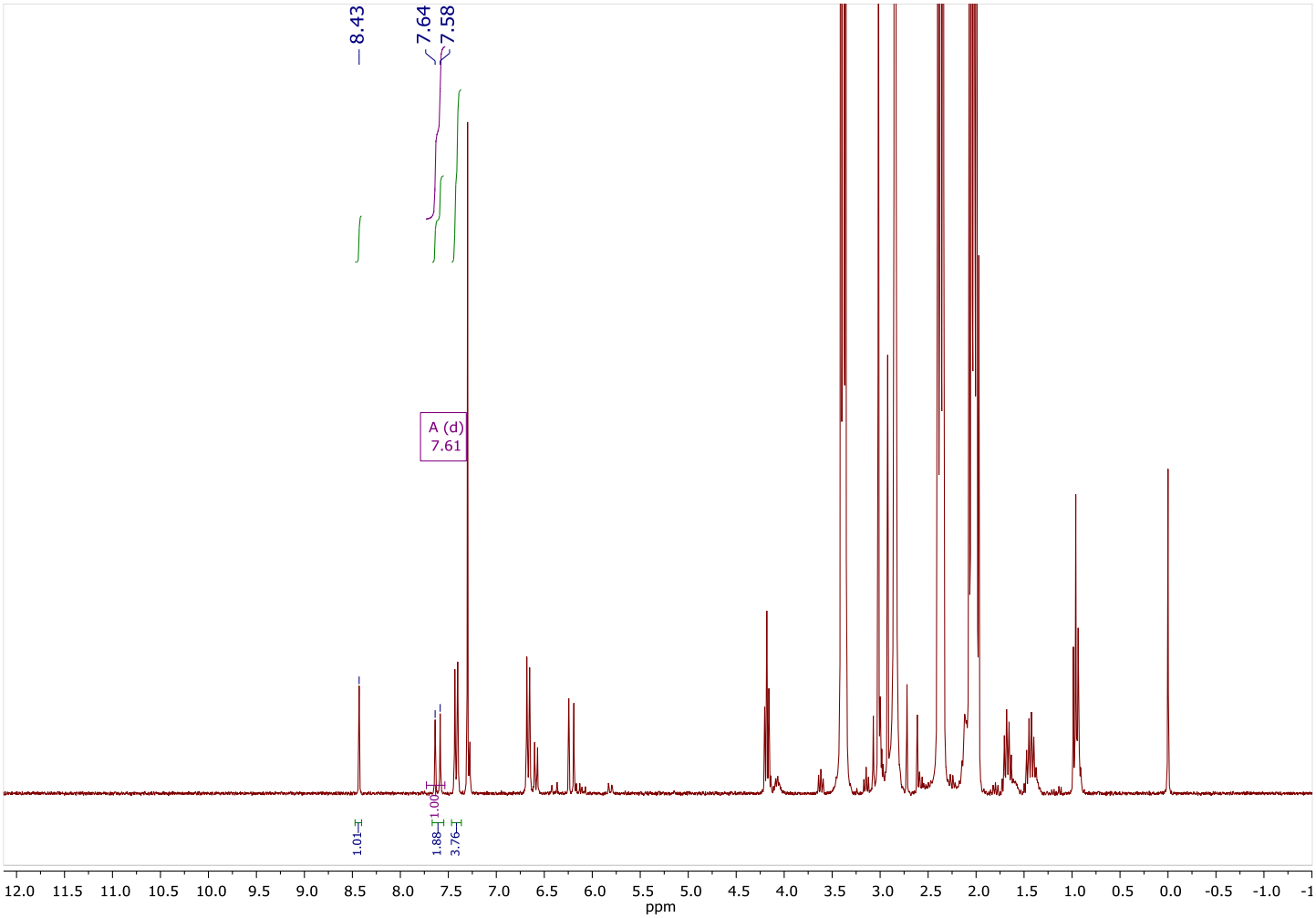


Figure S5. ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing butyl (*E*)-3-(4-dimethylaminophenyl)acrylate. Characteristic product signal: 7.61 (d, J = 15.9 Hz, 1H, =CH). Signal of *p*-dinitrobenzene: 8.43 ppm (s, 4H), n = 0.03125 mmol.

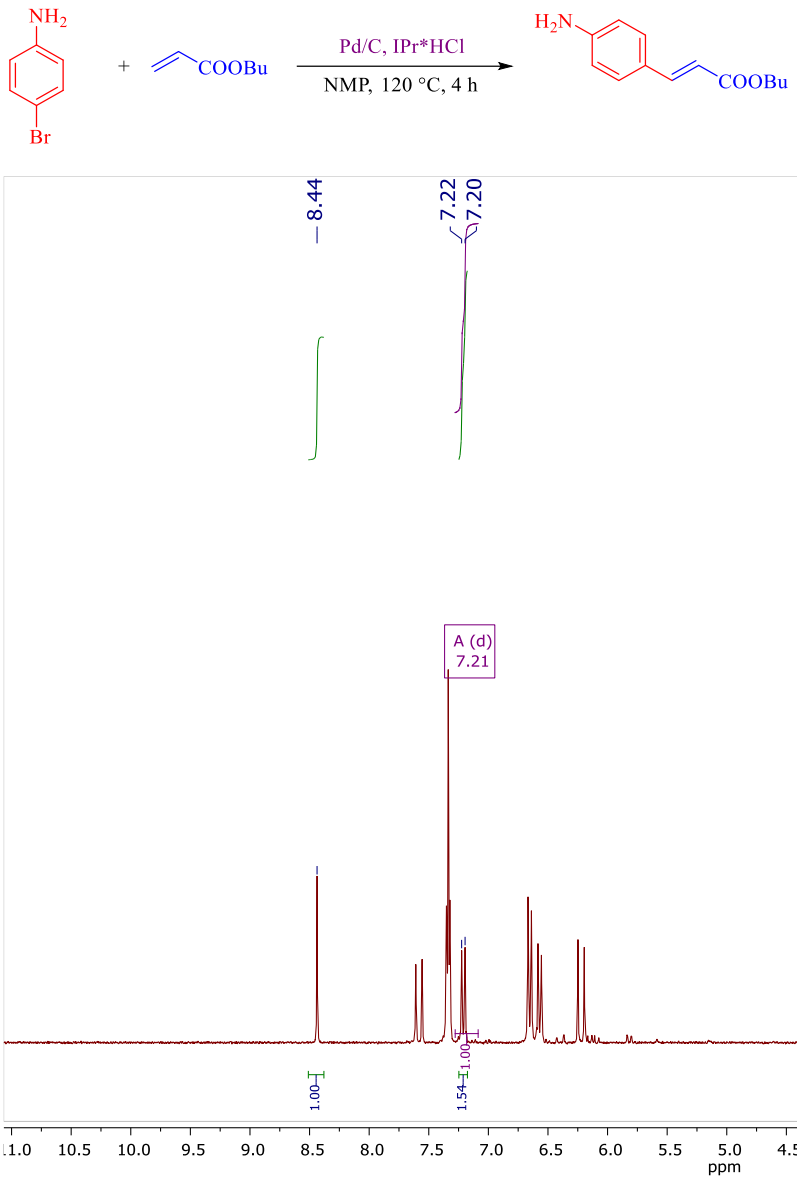


Figure S6. ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing butyl (*E*)-3-(4-aminophenyl)acrylate. Characteristic product signal: 7.21 (d, J = 8.7 Hz, 1H, =CH). Signal of *p*-dinitrobenzene: 8.44 ppm (s, 4H), n = 0.03125 mmol.

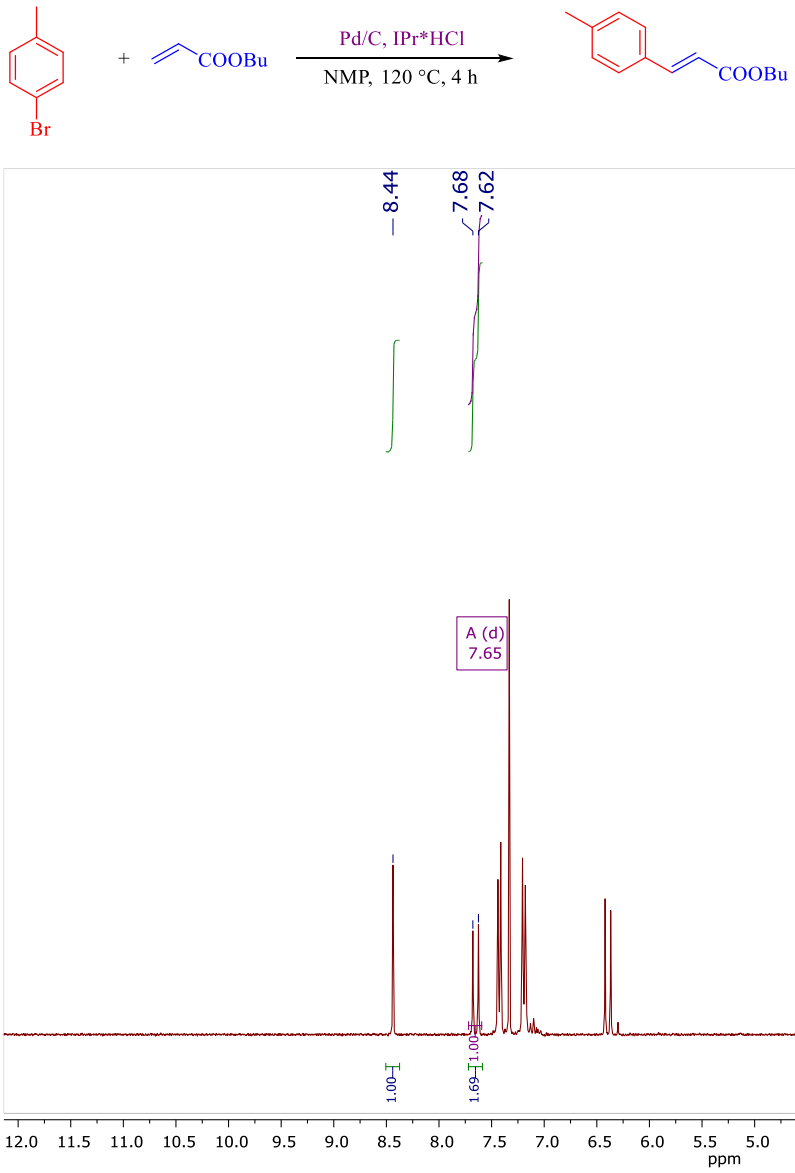
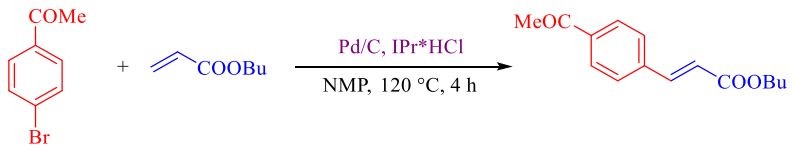


Figure S7. ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing butyl (*E*)-3-(*p*-tolyl)acrylate. Characteristic product signal: 7.65 (d, J = 16.0 Hz, 1H). Signal of *p*-dinitrobenzene: 8.44 ppm (s, 4H), n = 0.03125 mmol.



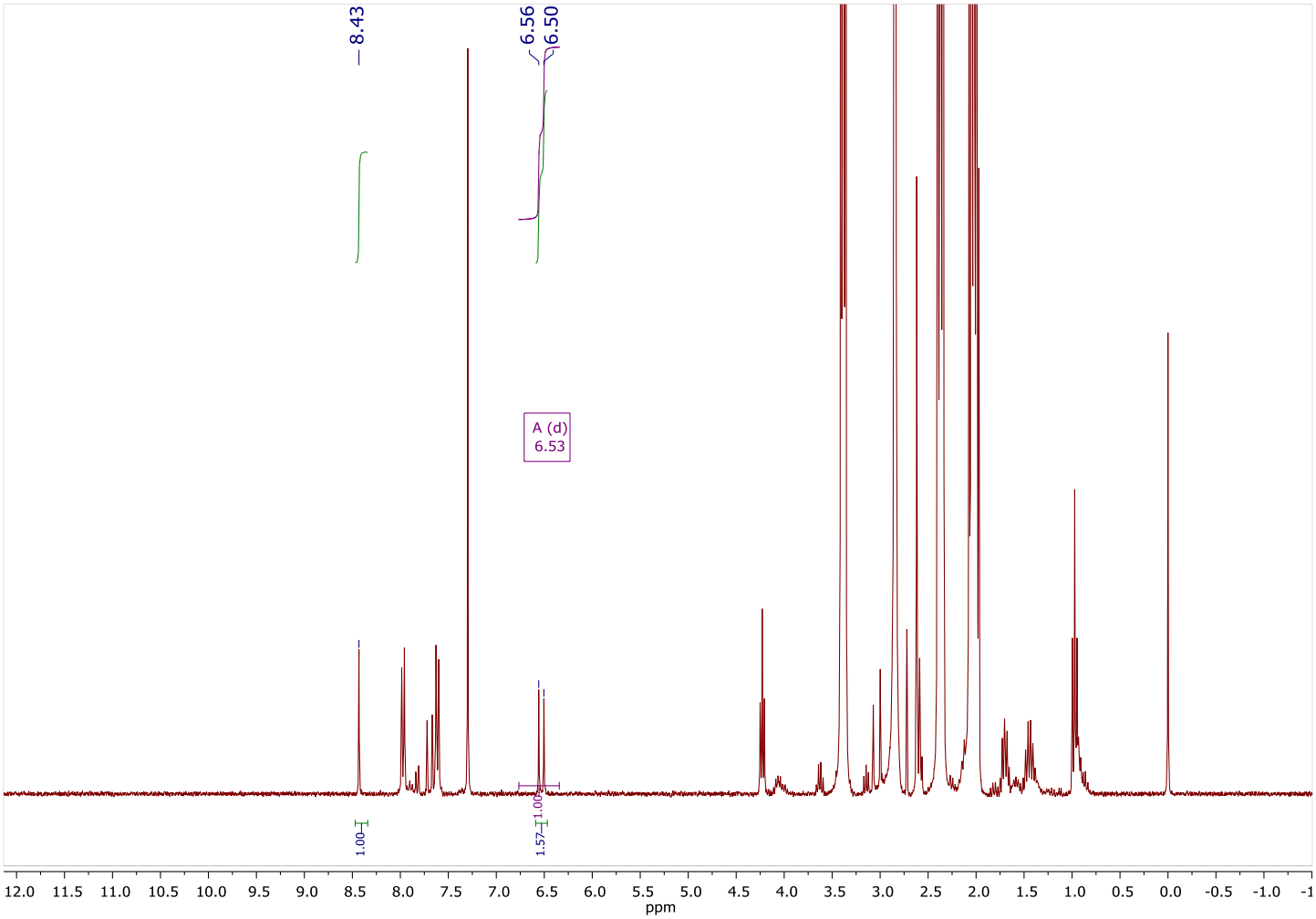
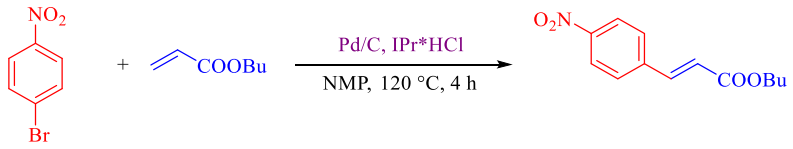


Figure S8. ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing butyl (i)-3-(4-acetylphenyl)acrylate. Characteristic product signal: 6.53 (d, J = 16.0 Hz, 1H). Signal of *p*-dinitrobenzene: 8.43 ppm (s, 4H), n = 0.03125 mmol.



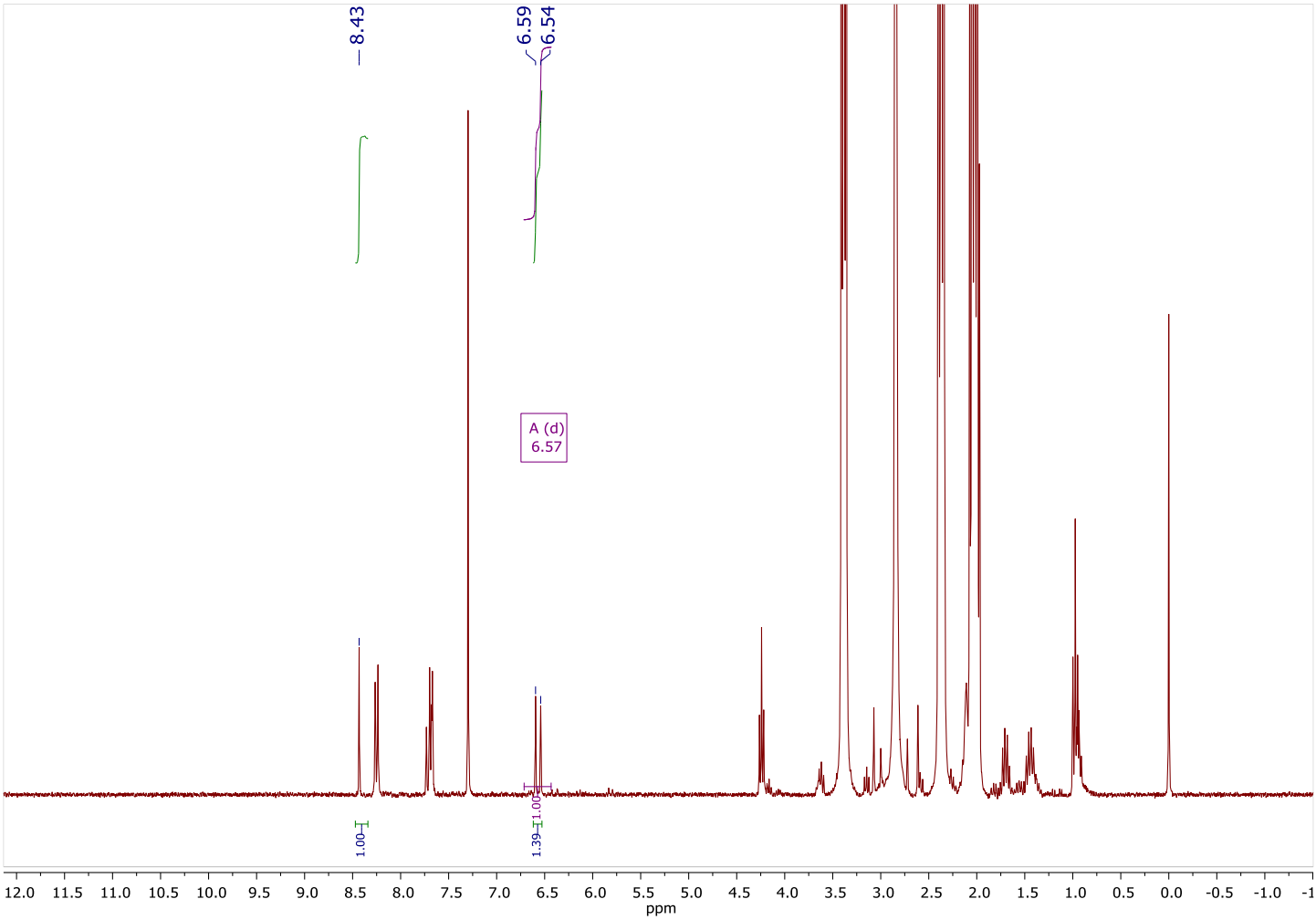
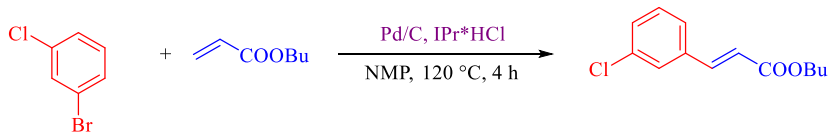


Figure S9. ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing butyl (*E*)-3-(4-nitrophenyl)acrylate. Characteristic product signal: 6.57 (d, *J* = 16.0 Hz, 1H). Signal of *p*-dinitrobenzene: 8.43 ppm (s, 4H), n = 0.03125 mmol.



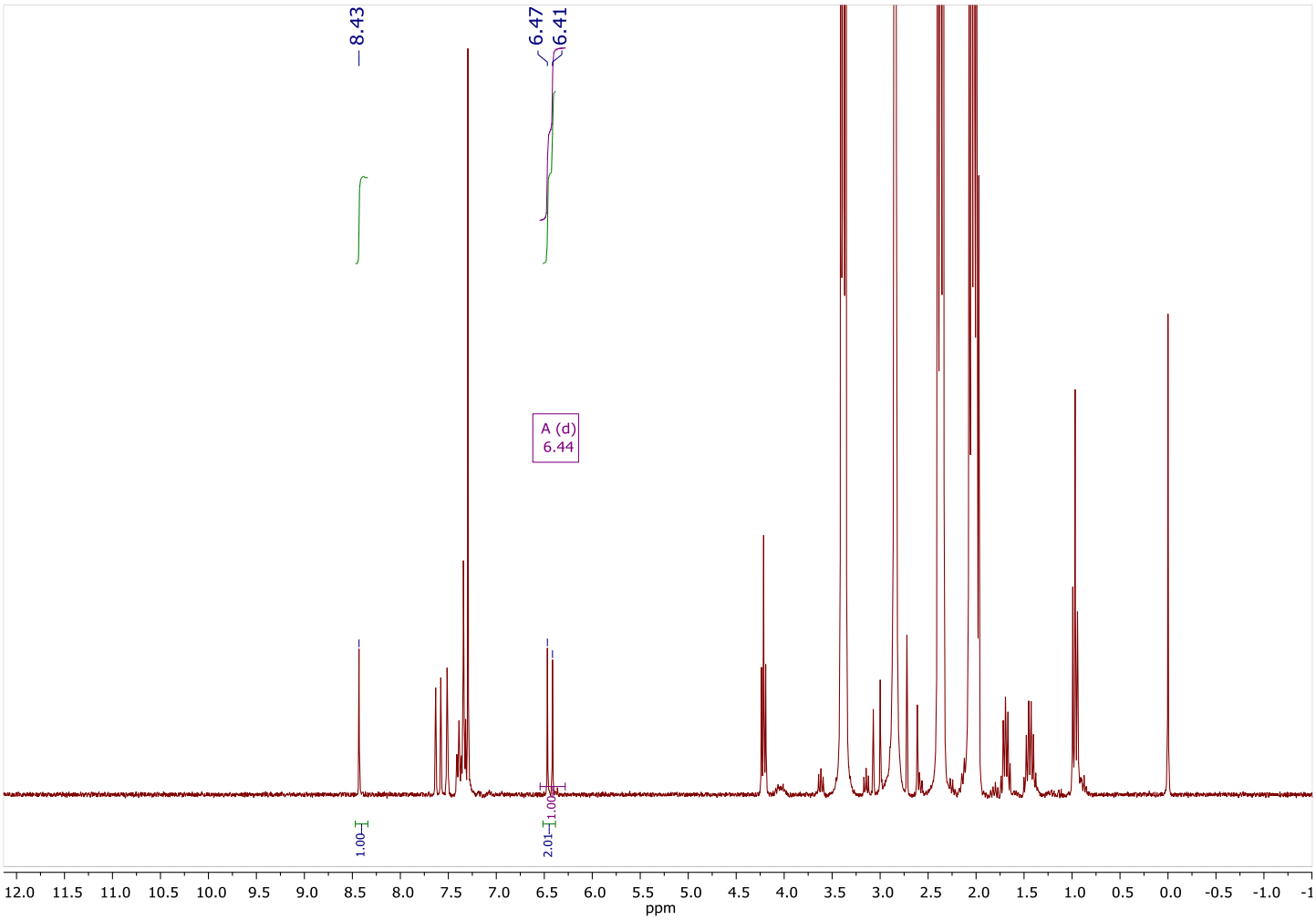


Figure S10. ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing butyl (*E*)-3-(3-chlorophenyl)acrylate. Characteristic product signal: 6.44 (d, *J* = 16.0 Hz, 1H). Signal of *p*-dinitrobenzene: 8.43 ppm (s, 4H), n = 0.03125 mmol.

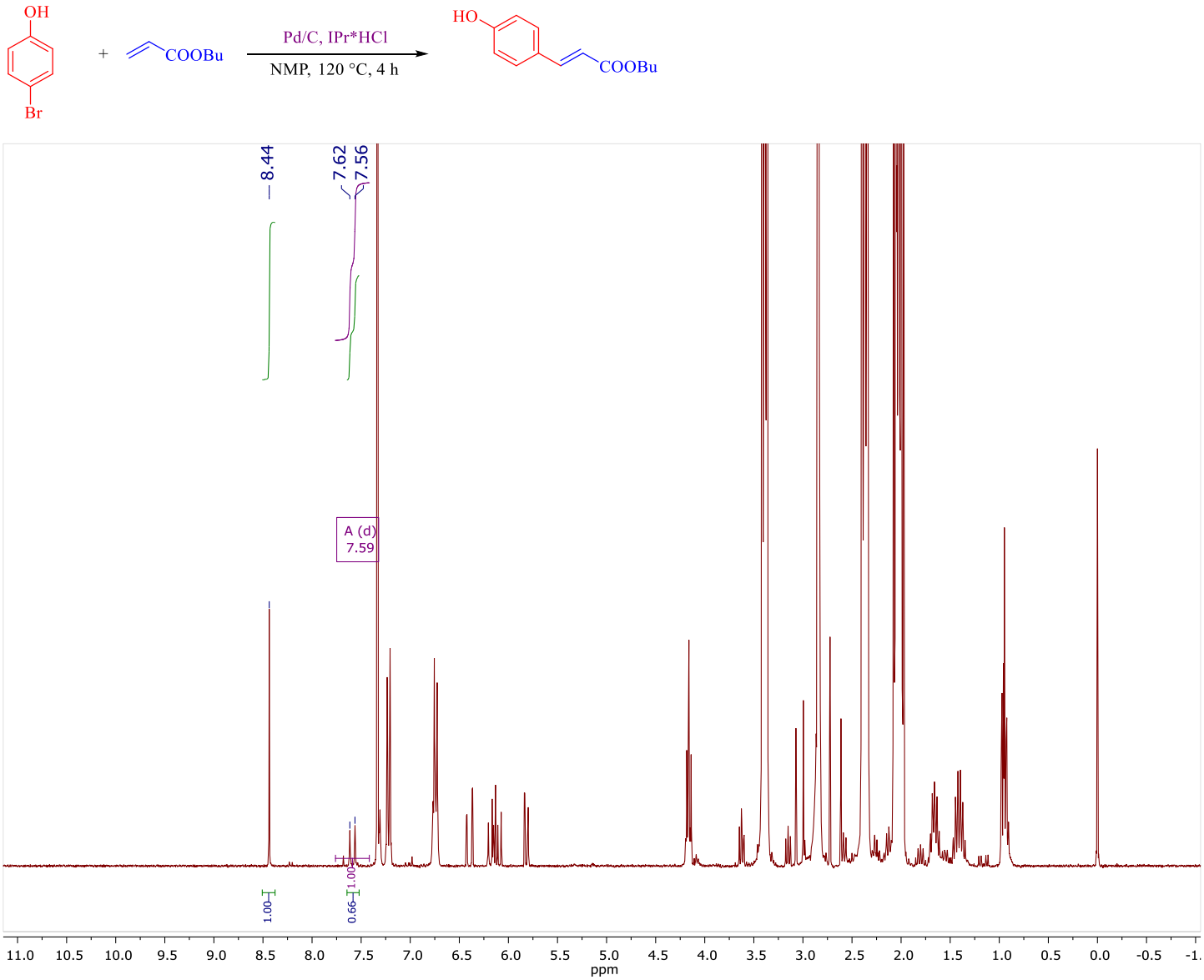


Figure S11. ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing butyl (*E*)-3-(4-hydroxyphenyl)acrylate. Characteristic product signal: 7.59 (d, *J* = 15.8 Hz, 1H). Signal of *p*-dinitrobenzene: 8.44 ppm (s, 4H), n = 0.03125 mmol.

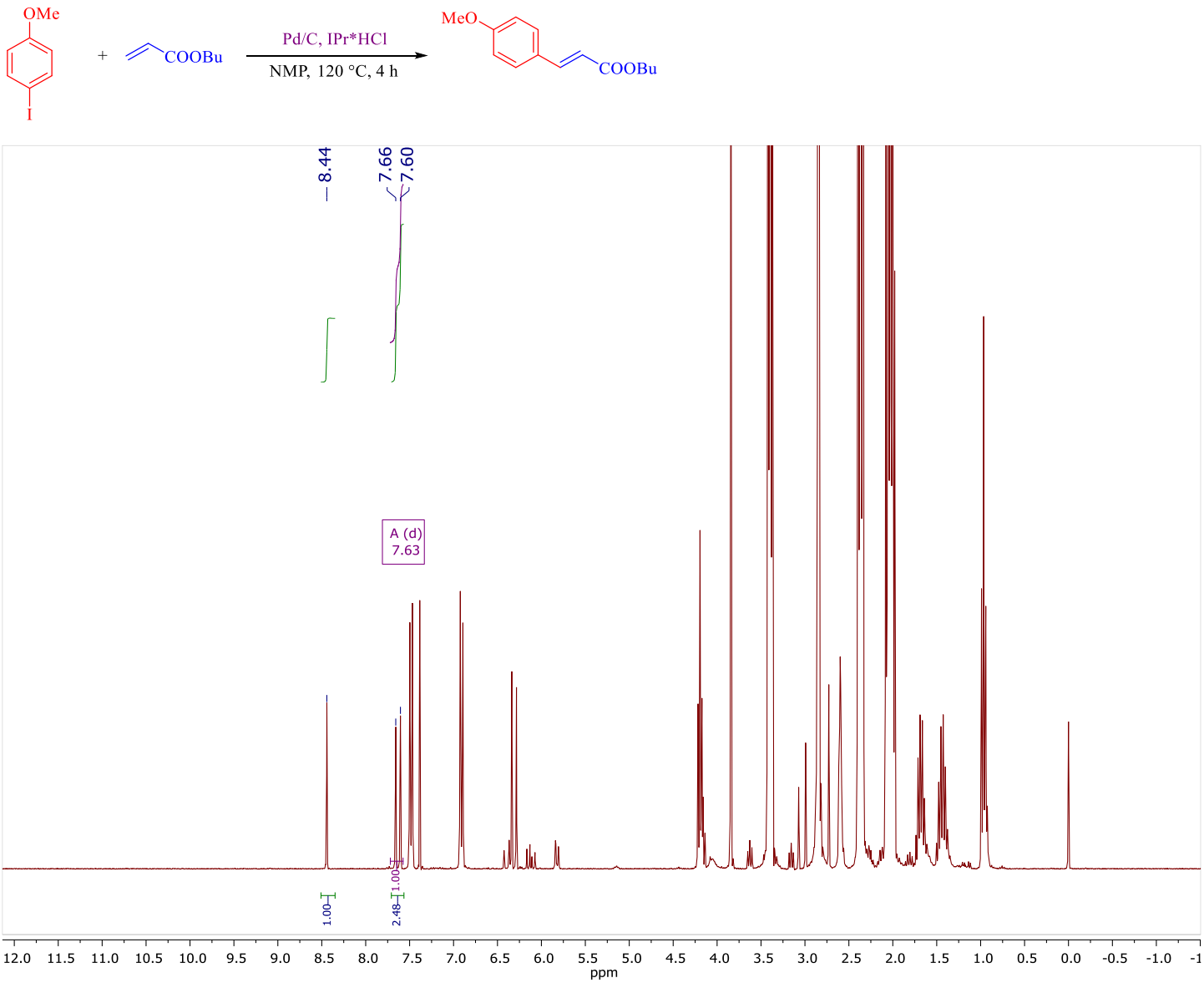


Figure S12. ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing butyl (*E*)-3-(4-methoxyphenyl)acrylate. Characteristic product signal: 7.63 (d, *J* = 16.0 Hz, 1H). Signal of *p*-dinitrobenzene: 8.44 ppm (s, 4H), n = 0.0375 mmol.

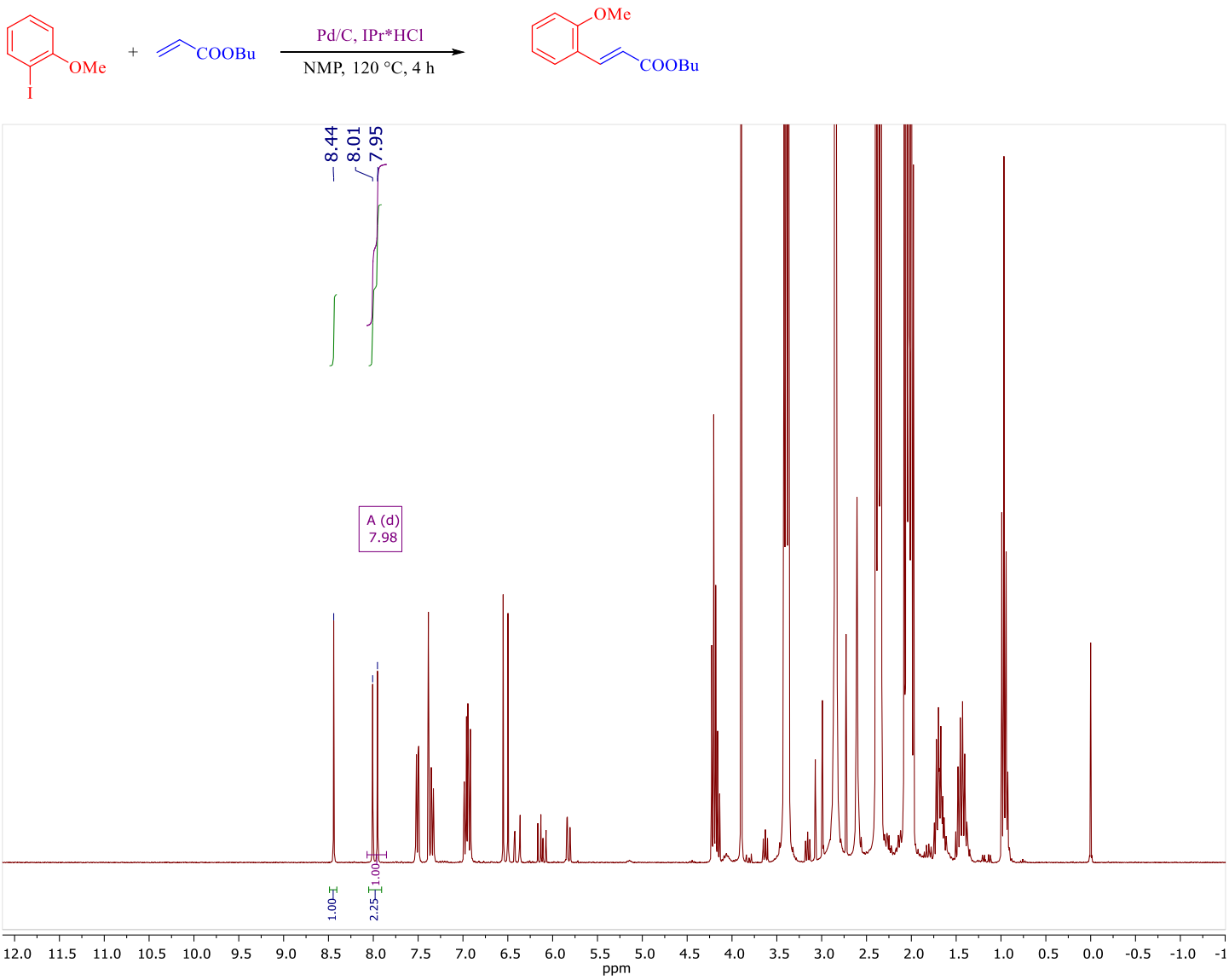
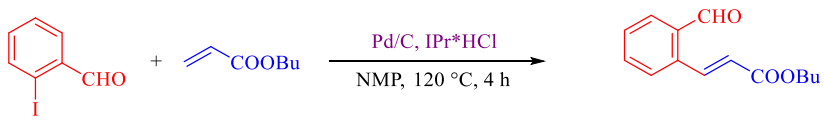


Figure S13. ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing butyl (*E*)-3-(2-methoxyphenyl)acrylate. Characteristic product signal: 7.98 (d, *J* = 16.2 Hz, 1H). Signal of *p*-dinitrobenzene: 8.43 ppm (s, 4H), n = 0.0375 mmol.



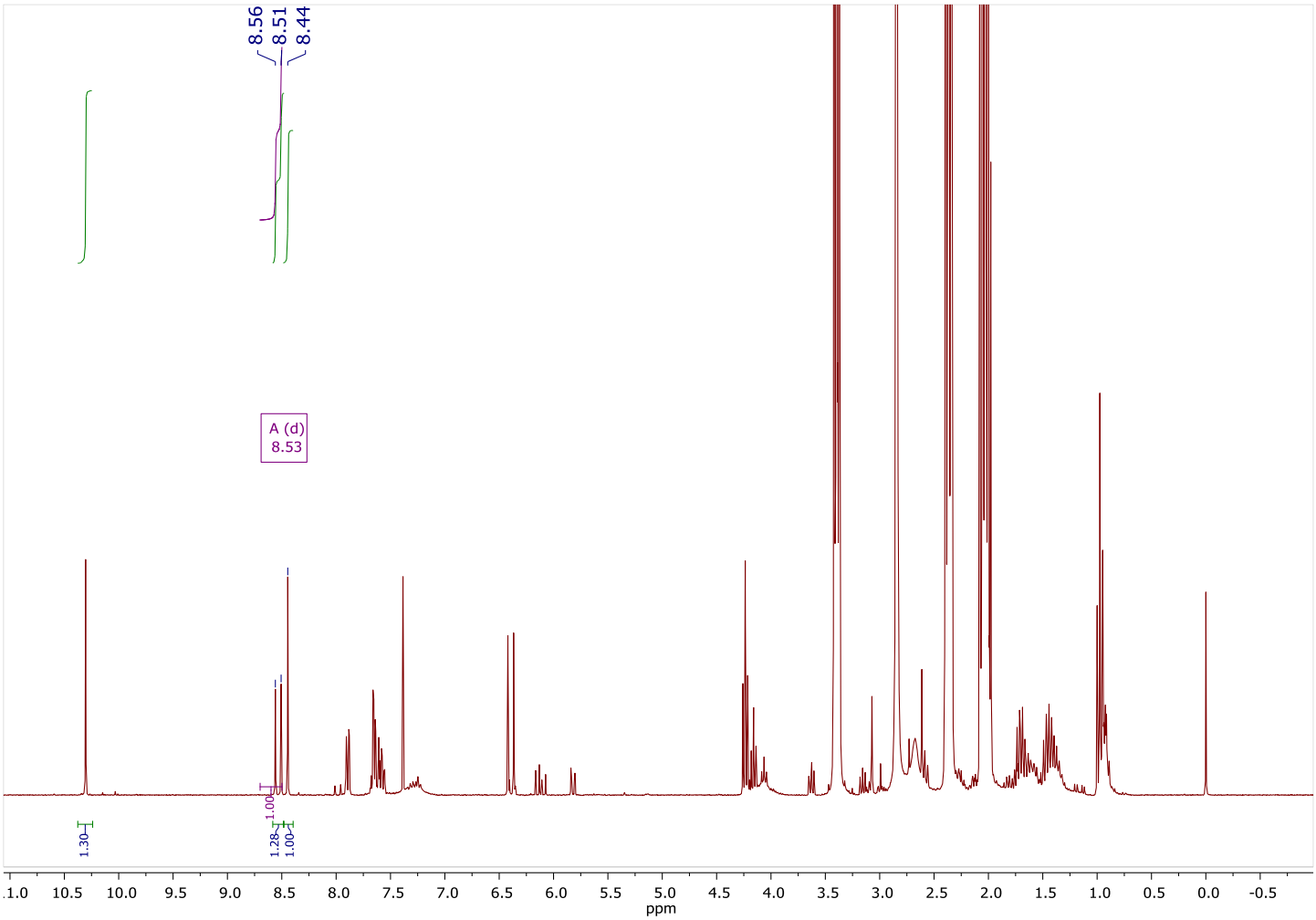


Figure S14. ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing butyl (*E*)-3-(2-formylphenyl)acrylate. Characteristic product signal: 8.53 (d, *J* = 15.9 Hz, 1H). Signal of *p*-dinitrobenzene: 8.44 ppm (s, 4H), n = 0.0375 mmol.

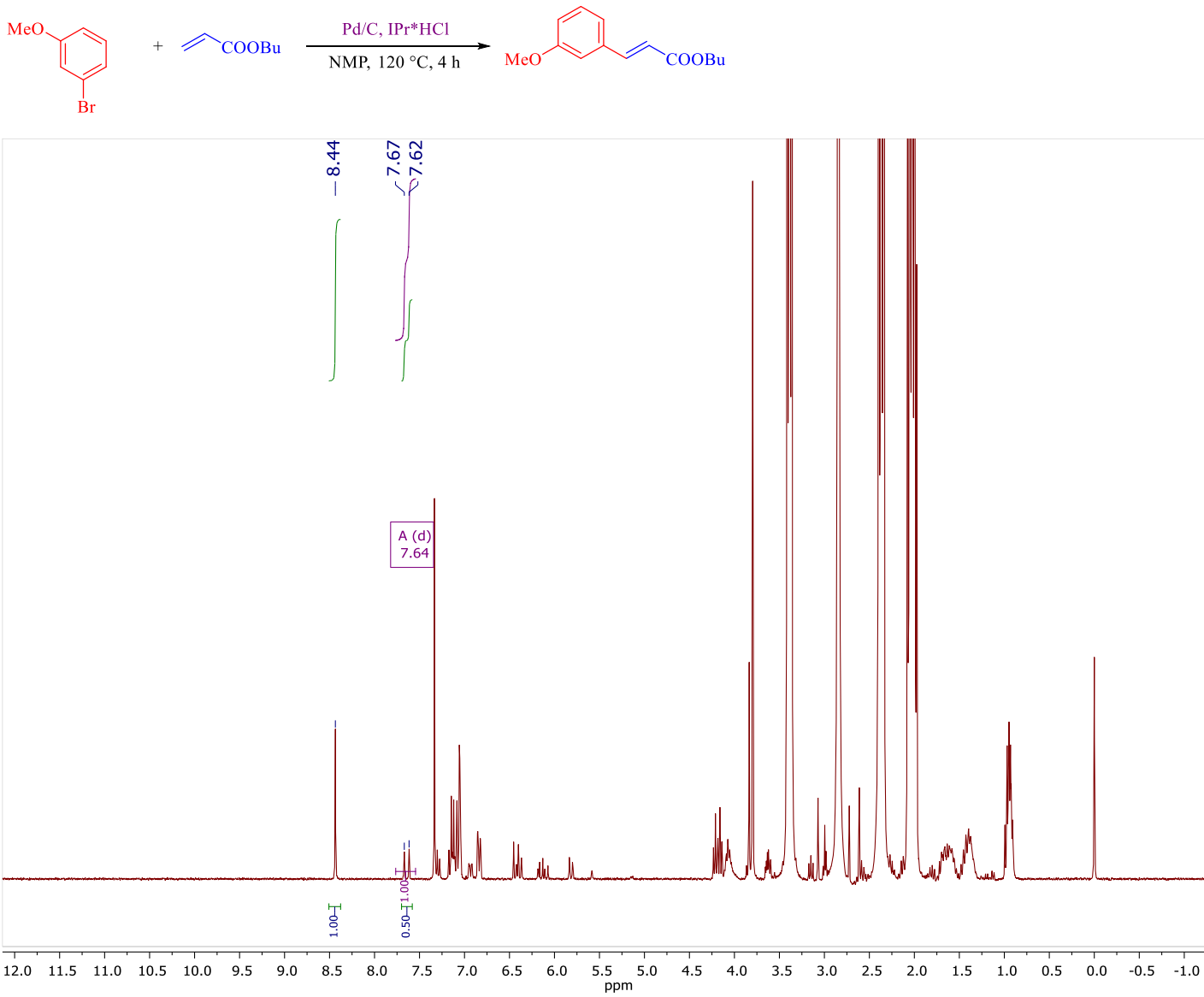


Figure S15. ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing butyl (*E*)-3-(3-methoxyphenyl)acrylate. Characteristic product signal: 7.64 (d, J = 16.0 Hz, 1H). Signal of *p*-dinitrobenzene: 8.43 ppm (s, 4H), n = 0.03125 mmol.

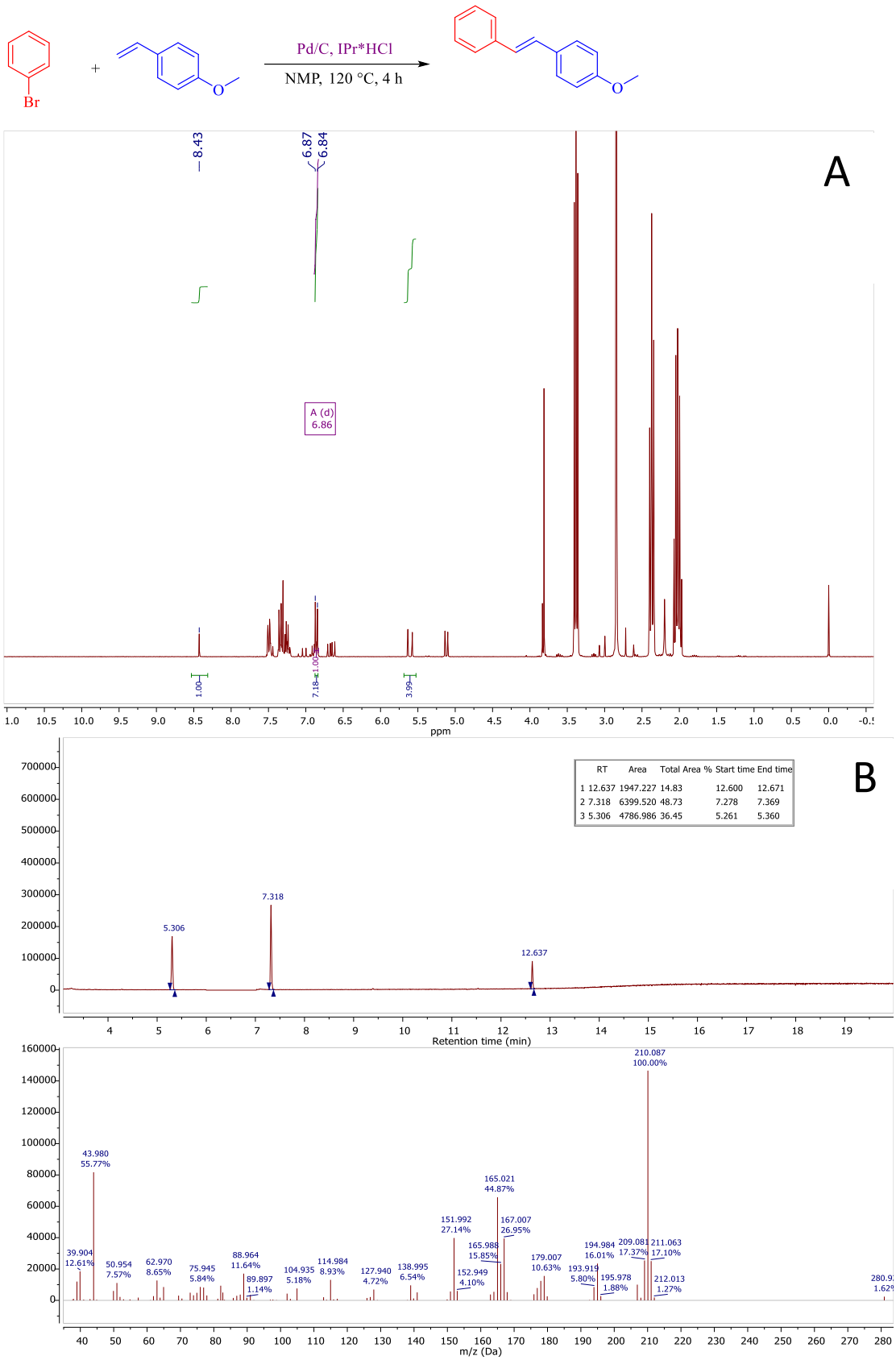


Figure S16. (A)^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing (*E*)-1-methoxy-4-styrylbenzene. Signal of *p*-dinitrobenzene: 8.43 ppm (s, 4H), n = 0.0375 mmol. (B) GC-MS spectrum of the reaction mixture. RT(1-methoxy-4-styrylbenzene) = 12.6 min, RT (1-methoxy-4-vinylbenzene) = 7.3 min, RT (BrPh) = 5.3 min.

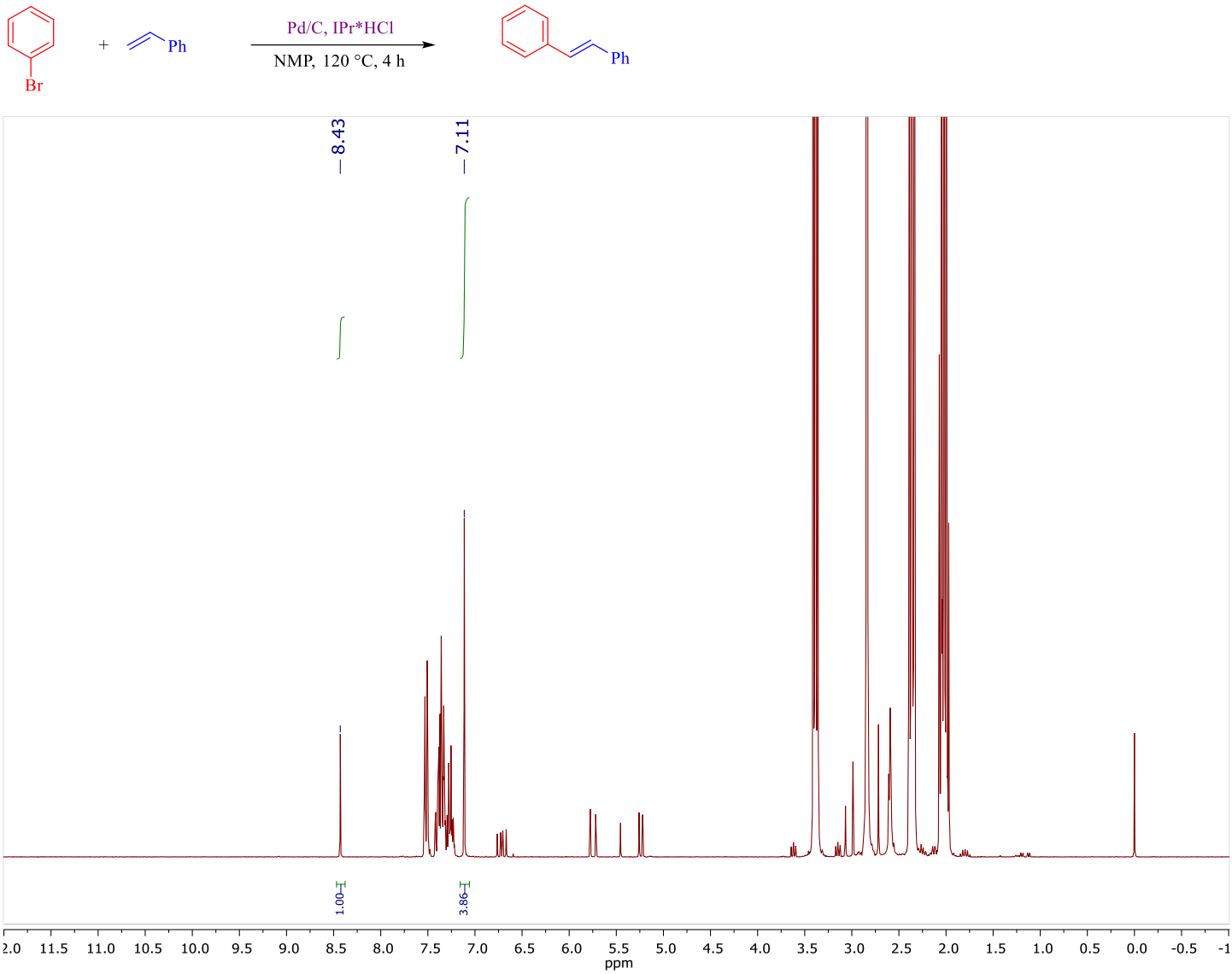


Figure S17. ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing (*E*)-stilbene. Characteristic product signal: 7.11 (s, 2H). Signal of *p*-dinitrobenzene: 8.43 ppm (s, 4H), n = 0.0375 mmol.

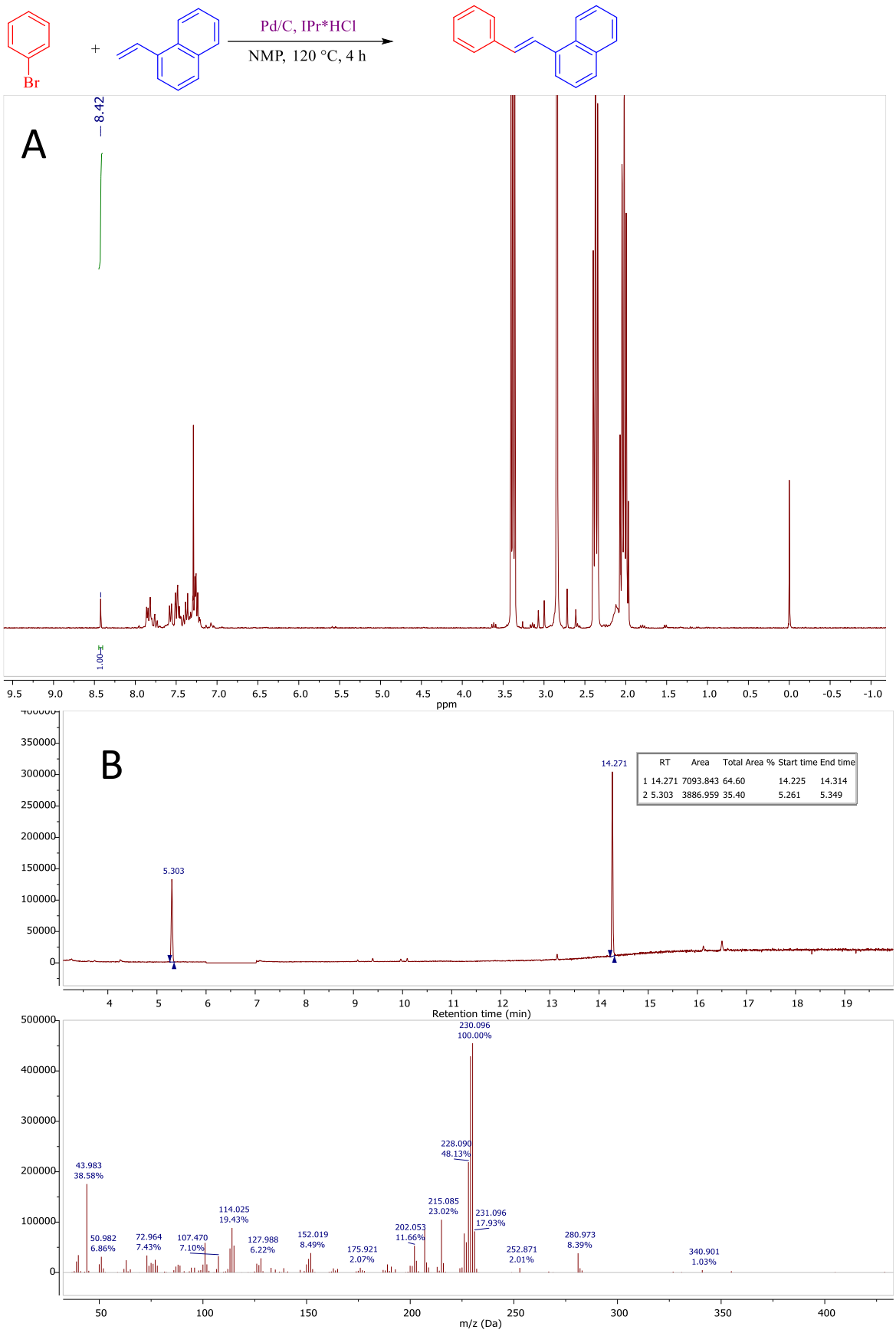
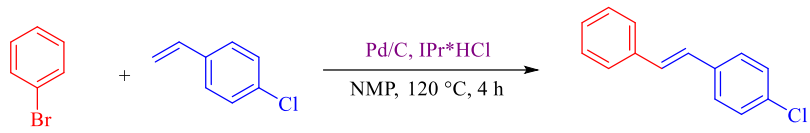


Figure S18. (A) ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing (*E*)-1-styrylnaphthalene. Signal of *p*-dinitrobenzene: 8.43 ppm (s, 4H), n = 0.0375 mmol. (B) GC-MS spectrum of the reaction mixture. RT(1-styrylnaphthale) = 14.3 min, RT (BrPh) = 5.3 min.



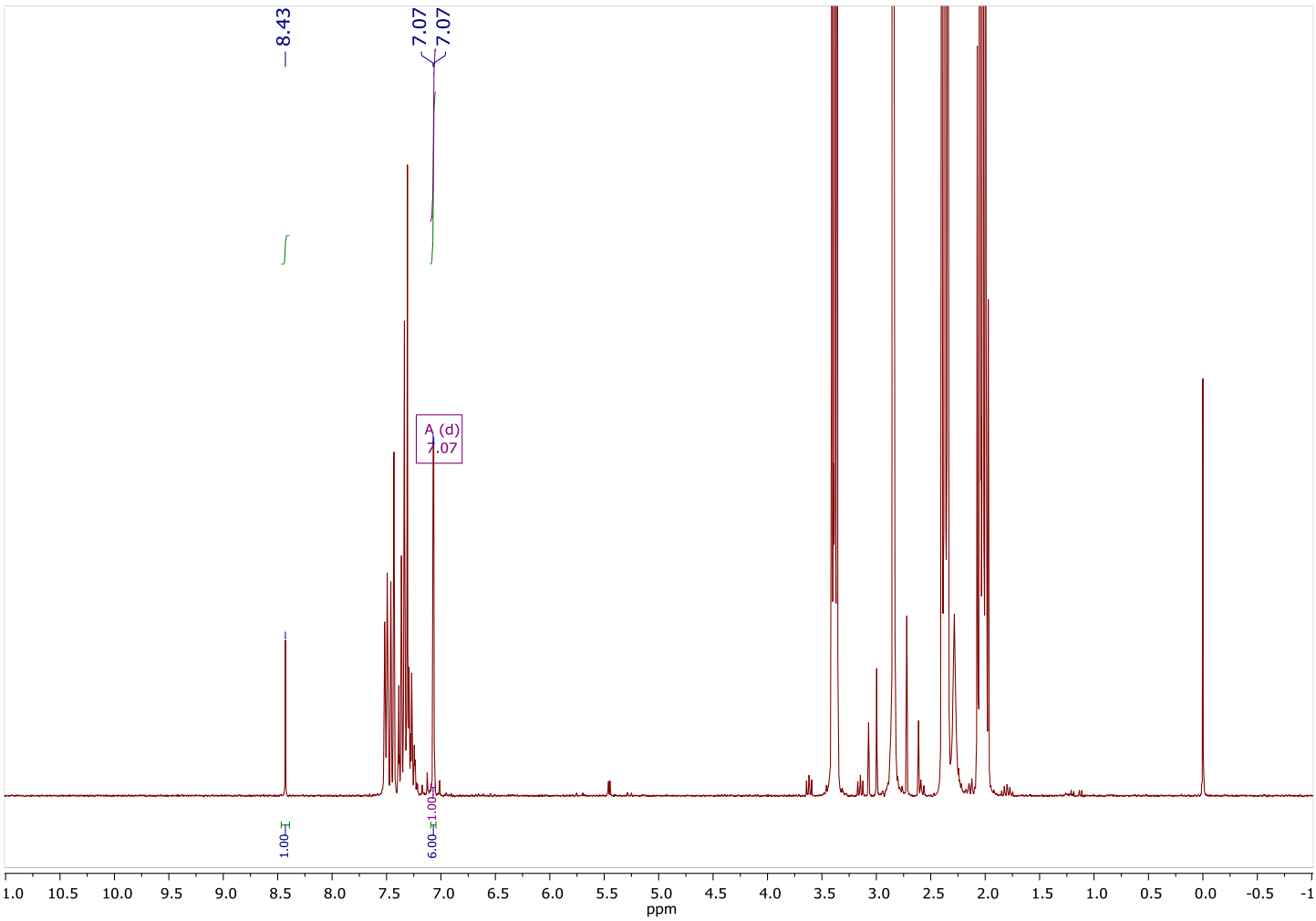


Figure S19. ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing (*E*)-1-chloro-4-styrylbenzene. Characteristic product signal: 7.07 (d, *J* = 1.7 Hz, 2H). Signal of *p*-dinitrobenzene: 8.43 ppm (s, 4H), n = 0.0375 mmol.

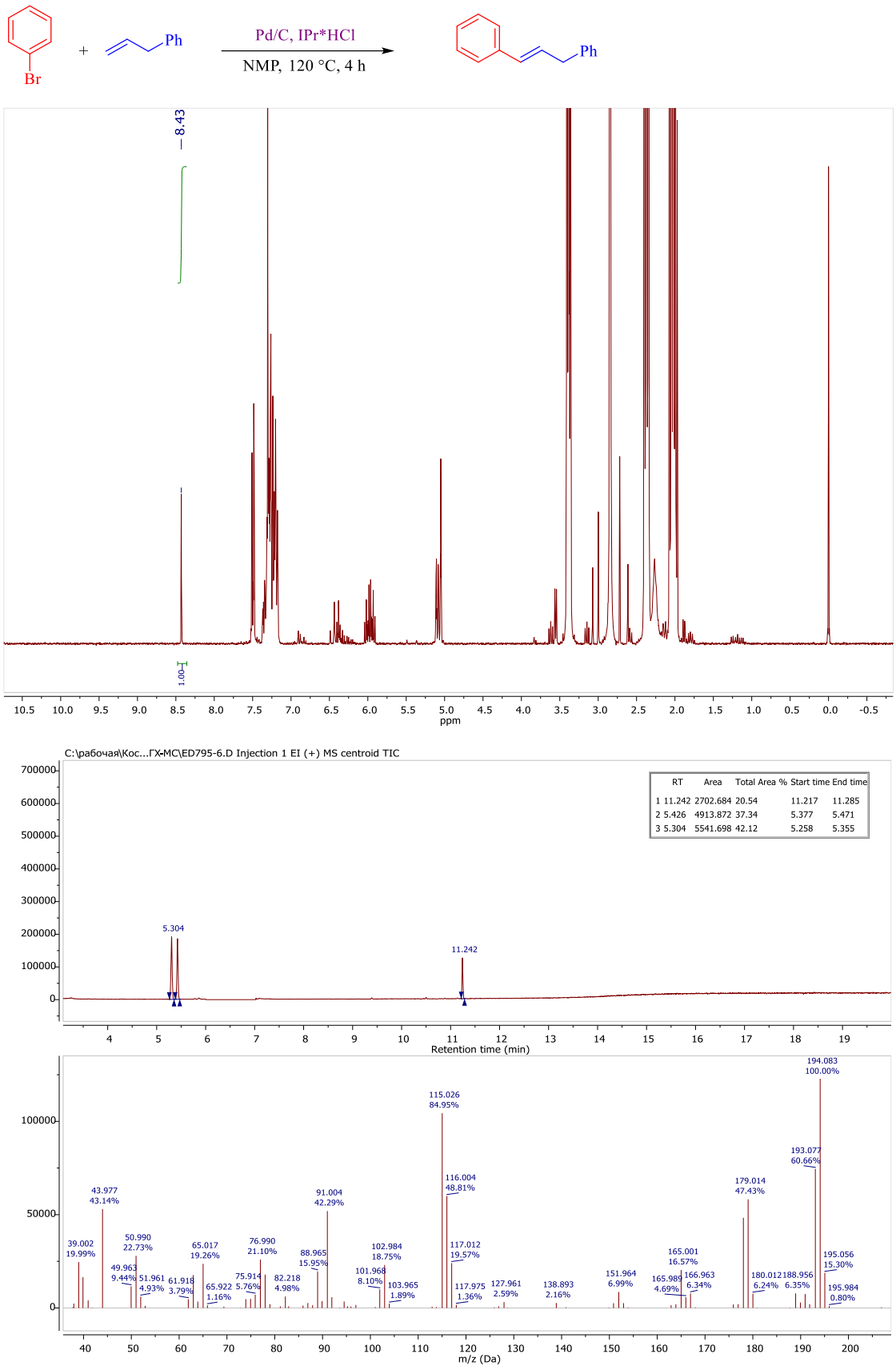
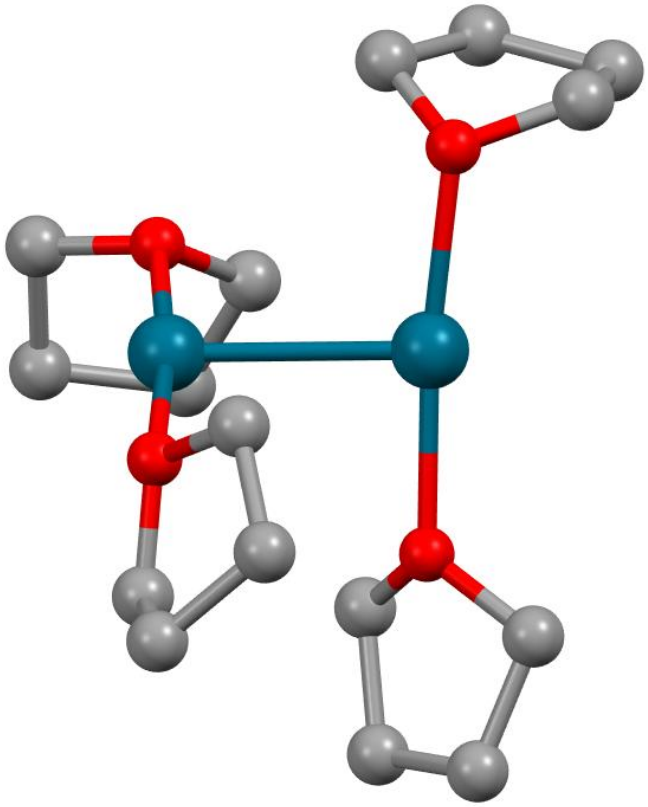


Figure S20. (A) ^{1}H NMR spectrum of the reaction mixture in $CDCl_3$ containing (*E*)-prop-1-ene-1,3-diyldibenzene. Signal of *p*-dinitrobenzene: 8.43 ppm (s, 4H), n = 0.0375 mmol. (B) GC-MS spectrum of the reaction mixture. RT(prop-1-ene-1,3-diyldibenzene) = 11.2 min, RT (allylbenzene) = 5.4 min, RT (BrPh) = 5.3 min.

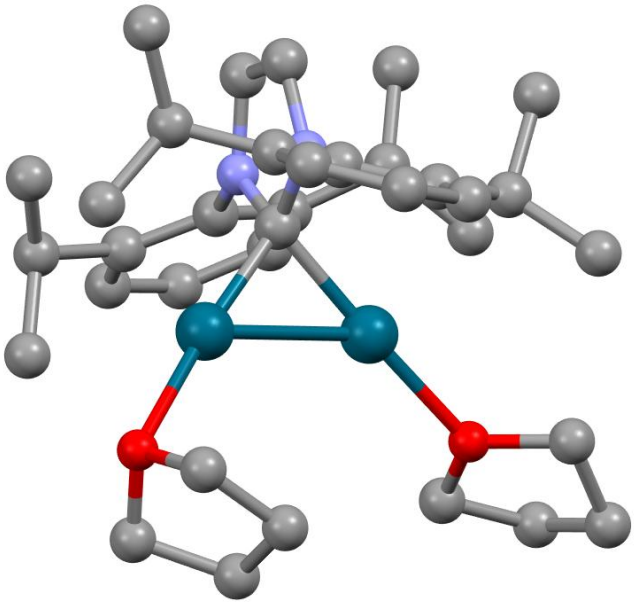
Structures, *XYZ coordinates and thermodynamic parameters of calculated compounds*

Ia E = -1184.652291, E+ZPE = -1184.173901, H = -1184.144967, G = -1184.240755

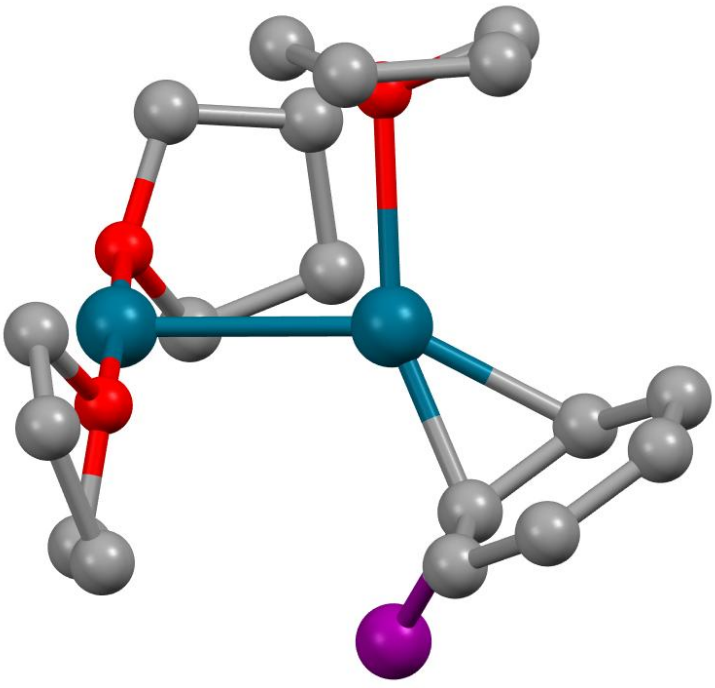


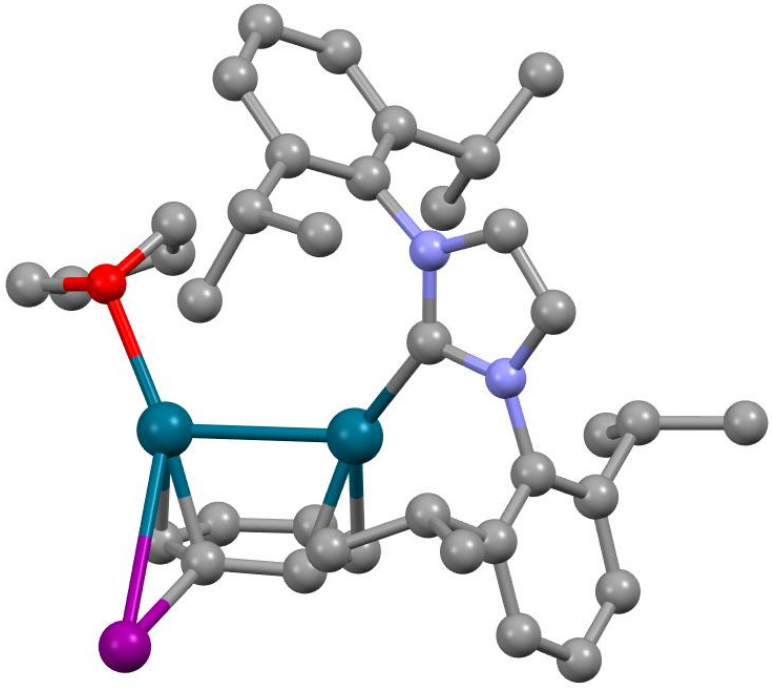
O	1.86440	0.43070	-1.80450
C	3.07650	0.79680	-1.13150
C	4.14250	-0.02910	-1.82260
C	3.41340	-1.36000	-2.00590
C	1.96720	-0.93840	-2.25900
H	2.99940	0.53610	-0.06940
H	3.19250	1.87830	-1.23500
H	5.05520	-0.11650	-1.22720
H	4.39730	0.41520	-2.79090
H	3.47740	-1.95070	-1.08580
H	3.81470	-1.96270	-2.82450
H	1.24440	-1.54320	-1.69390
H	1.69750	-0.94130	-3.32010
Pd	0.01660	1.13990	-0.99990
O	-1.82370	2.04050	-0.31760
C	-1.95220	3.45740	-0.50590
C	-1.25260	4.06960	0.69930
C	-1.47720	3.02000	1.80960
C	-2.12200	1.84060	1.07490
H	-3.02420	3.70530	-0.51240
H	-1.51320	3.70710	-1.47180
H	-1.66200	5.05170	0.95000
H	-0.18530	4.18360	0.48900
H	-2.13470	3.38770	2.60190
H	-0.52930	2.72810	2.26720
H	-3.21490	1.85320	1.19080
H	-1.73310	0.85400	1.34560
O	1.39730	-0.74980	1.48460
C	1.42340	0.48730	2.20490
C	2.79470	0.52780	2.89330
C	3.33140	-0.91150	2.75200
C	2.11370	-1.69410	2.28150
H	0.60460	0.49280	2.93630
H	1.24830	1.27600	1.46540
H	2.68950	0.82080	3.94110
H	3.46200	1.24750	2.41220
H	3.73740	-1.30810	3.68580
H	4.11800	-0.95790	1.99290
H	1.48510	-2.01870	3.12290
H	2.33840	-2.55540	1.65000
Pd	-0.30570	-1.25420	0.29540
O	-1.96150	-2.01000	-0.87370
C	-3.05440	-1.09650	-1.06670
C	-3.98320	-1.31230	0.13120
C	-3.59710	-2.71500	0.65080
C	-2.58730	-3.20300	-0.37980
H	-2.63250	-0.09400	-1.15160
H	-3.55460	-1.36590	-2.00770
H	-5.03150	-1.25330	-0.17340
H	-3.81220	-0.55540	0.90030
H	-4.45180	-3.39190	0.72980
H	-3.12180	-2.64320	1.63320
H	-3.08970	-3.69880	-1.22380
H	-1.80500	-3.85350	0.01170

Ib E = -1879.133427, E+ZPE = -1878.320760, H = -1878.273128, G = -1878.407753

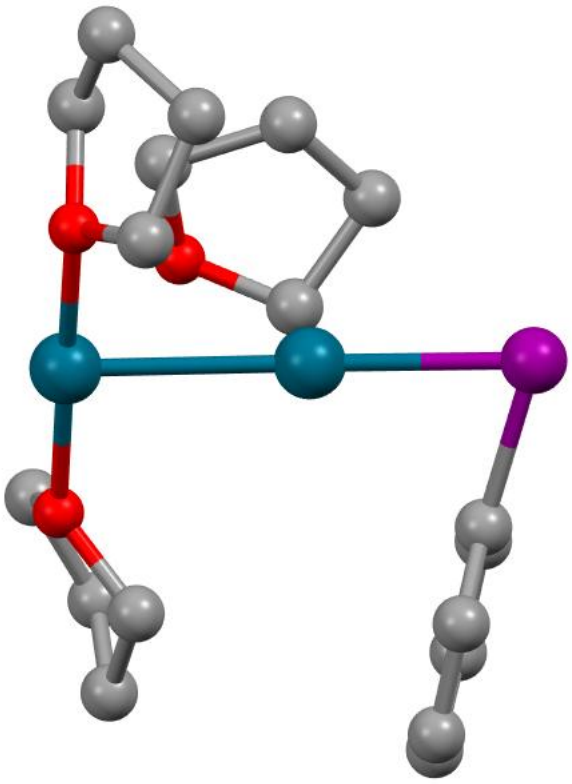


O	-2.59570	-2.00940	1.20310
C	-3.65670	-1.42520	1.98260
C	-4.83190	-2.37780	1.83850
C	-4.13150	-3.72260	1.65430
C	-2.94870	-3.33640	0.78400
H	-3.85220	-0.41990	1.59950
H	-3.31340	-1.34690	3.02130
H	-5.41590	-2.12880	0.94530
H	-5.49680	-2.34790	2.70520
H	-4.76260	-4.48040	1.18320
H	-3.78500	-4.10910	2.61900
H	-3.22180	-3.31490	-0.27930
H	-2.07110	-3.97510	0.91240
Pd	1.19300	0.64760	1.08580
C	0.23600	0.49860	-0.69010
N	-0.39350	1.58920	-1.31610
C	0.04870	1.77260	-2.61300
C	0.98240	0.82750	-2.85810
N	1.08940	0.05410	-1.71640
C	-1.56590	2.24250	-0.82760
C	-2.81120	1.73740	-1.26400
C	-3.97620	2.36160	-0.81930
C	-3.91510	3.46150	0.02870
C	-2.68140	3.96100	0.41650
C	-1.47820	3.37840	-0.00530
C	2.09900	-0.94310	-1.55450
C	1.75460	-2.30650	-1.65560
C	2.77440	-3.24530	-1.48760
C	4.08840	-2.85170	-1.25390
C	4.40960	-1.50290	-1.19360
C	3.42360	-0.52330	-1.34390
H	-0.34160	2.55760	-3.24200
H	1.58710	0.64080	-3.73250
C	-2.91550	0.57810	-2.23920
H	-4.94160	1.98520	-1.14650
H	-4.82890	3.94040	0.37020
H	-2.63400	4.83740	1.05910
C	-0.21210	4.05000	0.51190
C	0.33290	-2.73560	-1.95300
H	2.54070	-4.30350	-1.54390
H	4.86410	-3.60250	-1.12750
H	5.43920	-1.19960	-1.02290
C	3.81270	0.94100	-1.28340
C	4.79840	1.29510	-2.39800
C	4.36870	1.31860	0.08880
C	0.02050	-4.16440	-1.52620
C	-0.01280	-2.53100	-3.42960
C	-3.33430	1.08000	-3.62320
C	-3.86260	-0.51480	-1.74630
C	0.07830	3.58930	1.94240
C	1.04890	3.94850	-0.34190
H	-1.92510	0.12100	-2.32730
H	-0.46990	5.11700	0.56230
H	-0.32090	-2.06880	-1.35390
H	2.90900	1.53680	-1.43760
H	5.01970	2.36800	-2.38370
H	5.74680	0.75860	-2.28150
H	4.39290	1.04610	-3.38440
H	4.62640	2.38330	0.11690
H	3.61950	1.13160	0.87060
H	5.27050	0.74610	0.33440
H	-1.04820	-4.36170	-1.66040
H	0.56240	-4.90520	-2.12610
H	0.26610	-4.33190	-0.47230
H	-1.06200	-2.78960	-3.61360
H	0.13550	-1.49440	-3.74390

	H 0.60890 -3.17060 -4.06820 H -3.35540 0.25190 -4.34040 H -4.33540 1.52580 -3.59420 H -2.64150 1.83790 -4.00260 H -3.86960 -1.35080 -2.45490 H -3.53020 -0.89380 -0.77450 H -4.89340 -0.15660 -1.64780 H 0.31680 2.50850 1.93350 H 0.93490 4.13210 2.35820 H -0.78340 3.74050 2.60070 H 1.79010 4.66140 0.03690 H 1.48830 2.94650 -0.28500 H 0.85990 4.18750 -1.39260 Pd -1.01610 -0.76820 0.29280 O 2.38090 0.55020 3.05420 C 1.49550 0.59800 4.18120 C 0.82370 -0.77390 4.22190 C 1.83420 -1.69360 3.50150 C 2.98010 -0.75120 3.13840 H 0.81150 1.43520 4.03280 H 2.09490 0.77740 5.08580 H -0.11960 -0.74610 3.66840 H 0.61960 -1.08680 5.24960 H 1.38630 -2.10330 2.59120 H 2.18030 -2.52050 4.12760 H 3.45470 -0.96340 2.17860 H 3.74740 -0.72970 3.92620
IIa E = -1481.604449, E+ZPE = -1481.154873, H = -1481.125516, G = -1481.222120	
	Pd 0.03380 -0.02540 -0.88970 O 2.06470 0.55380 -1.87060 C 2.16340 -0.01270 -3.18280 C 2.51230 -1.48550 -2.96210 C 3.15770 -1.49720 -1.55780 C 3.16350 -0.02470 -1.15640 H 2.96310 0.50960 -3.72770 H 1.21300 0.15630 -3.69160 H 3.18740 -1.85340 -3.73930 H 1.60710 -2.09820 -2.97590 H 4.16590 -1.92010 -1.55480 H 2.54110 -2.07400 -0.86200 H 4.09100 0.47430 -1.47320 H 2.98550 0.16320 -0.09100 O 1.13180 -1.20630 2.03610 C 2.36880 -1.86990 2.33150 C 1.97900 -3.31380 2.67870 C 0.44280 -3.27550 2.79930 C 0.13810 -1.79070 2.88570 H 2.85480 -1.36570 3.17590 H 3.00220 -1.77550 1.44780 H 2.44930 -3.61900 3.61690 H 2.29770 -4.01180 1.90110 H 0.07090 -3.82260 3.66880 H -0.02250 -3.69400 1.90230 H 0.25660 -1.40540 3.90800 H -0.83710 -1.49140 2.49890 Pd 1.04260 0.81320 1.51690 O 0.95690 2.87100 1.06510 C -0.32770 3.47080 0.82150 C -0.47010 3.44630 -0.68750 C 0.97140 3.66790 -1.18110 C 1.83460 3.42380 0.06290 H -1.07460 2.88900 1.36240 H -0.30260 4.49840 1.21160 H -1.17190 4.20200 -1.04970 H -0.82530 2.45430 -0.99440 H 1.12110 4.68400 -1.55600

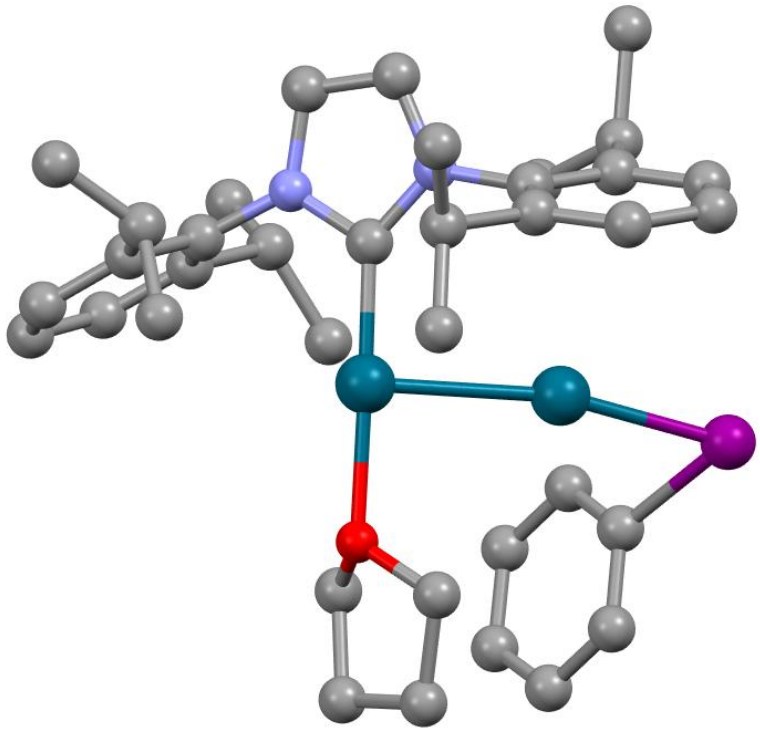
	H 1.22830 2.96250 -1.97370 H 2.24450 4.36050 0.46180 H 2.64540 2.71180 -0.08900 C -1.34450 -2.91460 -2.63430 C -1.46470 -3.21790 -1.25820 C -1.69090 -2.22910 -0.32570 C -1.77150 -0.85560 -0.73300 C -1.64410 -0.54240 -2.13800 C -1.44010 -1.60710 -3.06060 I -3.07680 0.38220 0.48890 H -1.19760 -3.71600 -3.35280 H -1.39130 -4.25050 -0.92550 H -1.83050 -2.48160 0.72050 H -2.01230 0.40670 -2.52140 H -1.39920 -1.37290 -4.12220
IIb E = -2176.065001, E+ZPE = -2175.278770, H = -2175.230271, G = -2175.364687	
	Pd 0.04410 -0.48700 -0.49210 Pd -2.07380 1.19620 -0.05250 C -1.60120 -0.21020 -3.32370 C -1.15770 -1.21200 -2.43450 C -1.76610 -1.39010 -1.17170 C -2.83630 -0.48530 -0.78850 C -3.31140 0.49450 -1.73240 C -2.66960 0.60490 -2.98930 I -4.24150 -1.25220 0.64710 H -1.12550 -0.11440 -4.29570 H -0.44850 -1.95770 -2.78370 H -1.65780 -2.33580 -0.64360 H -4.28430 0.96000 -1.59650 H -3.04690 1.33180 -3.70430 C 1.84740 -0.38840 0.46000 N 2.70410 0.48140 1.06890 C 3.83550 -0.15630 1.55890 C 3.68440 -1.47330 1.29070 N 2.47530 -1.59130 0.63250 C 2.58300 1.90570 1.10960 C 3.15290 2.62970 0.04860 C 3.14630 4.02450 0.12790 C 2.59830 4.67010 1.22820 C 2.01680 3.92930 2.25020 C 1.98730 2.53130 2.21890 C 1.92680 -2.80890 0.12270 C 2.28440 -3.21130 -1.17320 C 1.68250 -4.36570 -1.67910 C 0.76970 -5.08790 -0.91770 C 0.45620 -4.68040 0.37460 C 1.03310 -3.53420 0.92590 H 4.62350 0.38500 2.05860 H 4.31120 -2.32510 1.50500 C 3.70790 1.93920 -1.18180 H 3.57850 4.60810 -0.67980 H 2.61140 5.75520 1.28510 H 1.56800 4.43970 3.09860 C 1.25070 1.82330 3.34570 C 3.27430 -2.43200 -2.01580 H 1.93000 -4.69870 -2.68350 H 0.30650 -5.97980 -1.33090 H -0.25120 -5.25750 0.96390 C 0.67380 -3.09280 2.33020 C 0.93630 -4.19980 3.35140 C -0.77360 -2.60370 2.39800 C 2.60640 -1.84290 -3.25860 C 4.47930 -3.29680 -2.38840 C 5.08080 2.47220 -1.58710 C 2.70420 2.05110 -2.33310 C -0.14710 1.39230 2.88900

	C 1.98280 0.66520 4.02350 H 3.82410 0.87570 -0.95240 H 1.11320 2.59410 4.11460 H 3.64050 -1.59340 -1.41560 H 1.31710 -2.24600 2.58820 H 0.73820 -3.83340 4.36440 H 0.28900 -5.06720 3.18180 H 1.97570 -4.54260 3.31170 H -1.01430 -2.25460 3.40840 H -0.93310 -1.77310 1.69980 H -1.47610 -3.40450 2.14050 H 3.33250 -1.26790 -3.84410 H 2.20370 -2.63030 -3.90620 H 1.78580 -1.17580 -2.97600 H 5.21360 -2.70600 -2.94690 H 4.97340 -3.69760 -1.49700 H 4.18500 -4.14340 -3.01860 H 5.47790 1.88430 -2.42140 H 5.03450 3.51570 -1.91650 H 5.79480 2.41040 -0.75910 H 3.08370 1.53770 -3.22360 H 1.74530 1.59700 -2.05940 H 2.52750 3.10040 -2.59730 H -0.08850 0.65610 2.07740 H -0.69720 0.94070 3.72280 H -0.72170 2.24610 2.51680 H 1.46820 0.41720 4.95820 H 1.99170 -0.23690 3.40780 H 3.01760 0.92330 4.27090 O -1.49920 3.35040 0.32780 C -2.49900 4.24400 -0.18280 C -2.24710 4.32890 -1.69150 C -0.78440 3.85780 -1.84580 C -0.31340 3.69130 -0.40690 H -2.36200 5.22240 0.29850 H -3.47620 3.84410 0.09490 H -2.40030 5.34850 -2.05480 H -2.92580 3.66930 -2.23800 H -0.16260 4.57170 -2.39240 H -0.74260 2.89570 -2.36430 H 0.08220 4.63180 -0.00320 H 0.41180 2.89280 -0.25140
TS-IIIa E = -1481.586926, E+ZPE = -1481.139172, H = -1481.109166, G = -1481.211643	

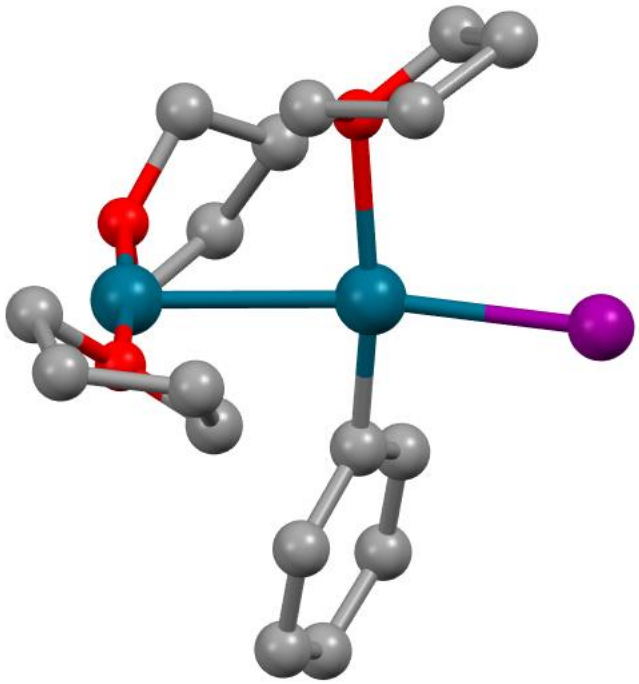


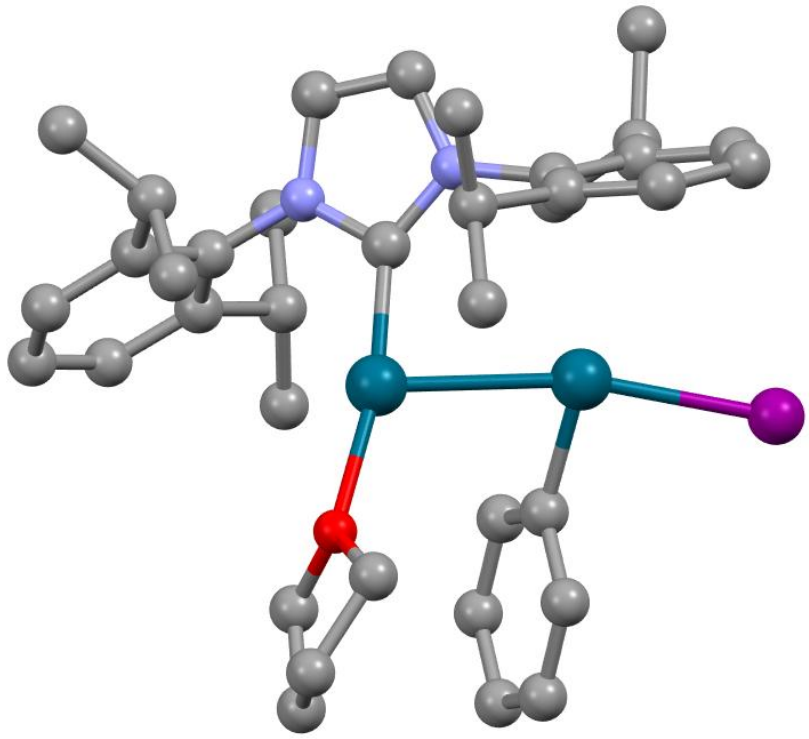
Pd	-0.05020	0.65920	0.20950
C	4.45370	-0.99660	1.02530
C	3.87130	-0.23570	2.03840
C	2.97980	0.78960	1.73150
C	2.66810	1.03770	0.39230
C	3.25400	0.29390	-0.63480
C	4.14260	-0.72780	-0.30710
I	1.41660	2.68910	-0.09910
H	5.15190	-1.79080	1.27260
H	4.10990	-0.43650	3.07920
H	2.52780	1.38260	2.51960
H	3.01640	0.50580	-1.67210
H	4.59620	-1.31190	-1.10340
O	-0.50870	-1.73100	-3.12280
C	0.59020	-0.86990	-2.87100
C	0.18620	0.44610	-3.51140
C	-1.28440	0.52450	-3.09390
C	-1.69420	-0.95240	-2.95520
H	1.48840	-1.33220	-3.29250
H	0.72920	-0.72450	-1.78040
H	0.28790	0.37980	-4.60020
H	0.77430	1.29600	-3.15250
H	-1.90710	1.07160	-3.80700
H	-1.35260	1.02050	-2.11520
H	-2.41120	-1.27630	-3.71790
H	-2.12330	-1.14700	-1.95930
O	-3.26170	0.01790	1.02140
C	-4.04110	0.40370	-0.12850
C	-4.82230	1.61340	0.34100
C	-3.78960	2.31560	1.22020
C	-3.08720	1.15580	1.90820
H	-4.65320	-0.45600	-0.41170
H	-3.36590	0.65750	-0.95340
H	-5.69190	1.30420	0.93110
H	-5.16690	2.22850	-0.49400
H	-4.23020	3.01080	1.93880
H	-3.07720	2.86590	0.59570
H	-3.54760	0.88940	2.86590
H	-2.01440	1.32000	2.04440
Pd	-1.74940	-1.39780	0.83750
O	-0.21930	-2.79270	0.73380
C	1.05340	-2.53330	1.36340
C	1.89850	-3.72530	0.96870
C	1.46550	-3.92860	-0.48140
C	-0.02710	-3.62210	-0.44170
H	1.46230	-1.59360	0.97320
H	0.86930	-2.42940	2.43490
H	1.64100	-4.59700	1.58050
H	2.96660	-3.52320	1.07490
H	1.66490	-4.93470	-0.85850
H	1.98270	-3.21010	-1.12650
H	-0.63410	-4.52240	-0.29680
H	-0.37520	-3.07990	-1.32430

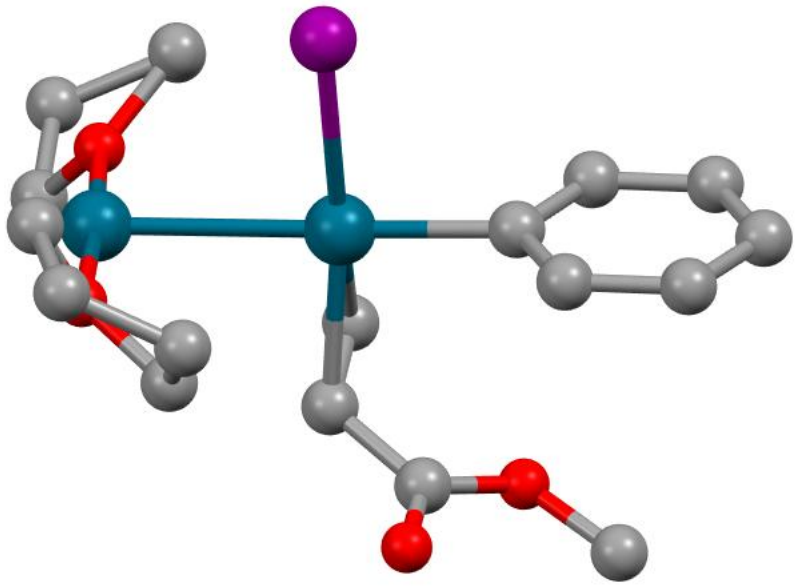
TS-IIIb E = -2176.047443, E+ZPE = -2175.261241, H = -2175.212755, G = -2175.348282

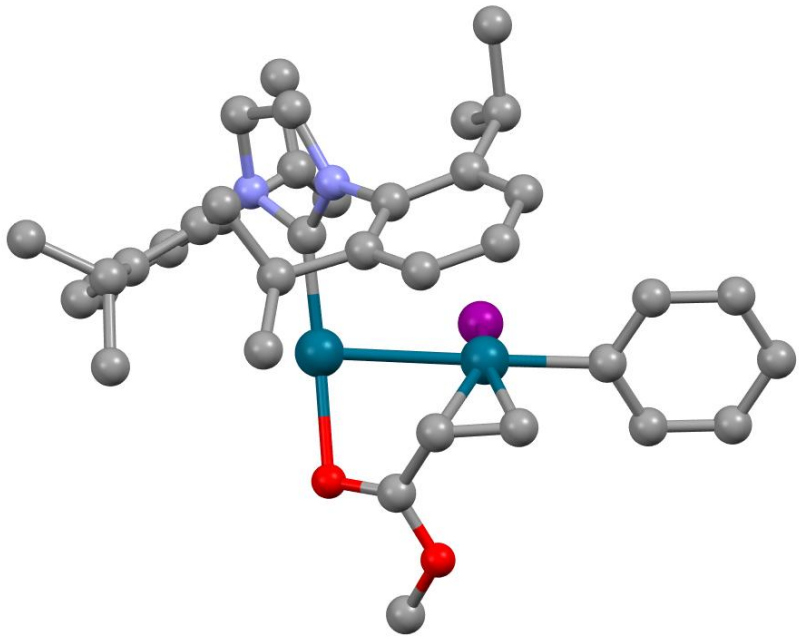


O	-0.06970	1.98520	-2.20850
C	0.32800	3.20740	-1.56800
C	0.95420	4.00710	-2.69640
C	1.64830	2.92570	-3.54500
C	1.02530	1.60670	-3.06560
H	1.05180	2.98250	-0.77510
H	-0.56690	3.65270	-1.12790
H	1.64810	4.76350	-2.32170
H	0.17410	4.51200	-3.27390
H	2.72740	2.91540	-3.37160
H	1.48210	3.08830	-4.61280
H	1.73100	1.00310	-2.47700
H	0.60610	0.98980	-3.86330
C	3.59040	1.44170	0.41880
C	3.00410	1.97400	1.57120
C	2.82490	3.35190	1.66410
C	3.24710	4.19570	0.63640
C	3.85170	3.65220	-0.49570
C	4.02680	2.27480	-0.61430
I	4.04440	-0.63950	0.31880
H	2.67980	1.31960	2.37330
H	2.35200	3.76500	2.55100
H	3.11000	5.26970	0.72060
H	4.19530	4.30100	-1.29710
H	4.49850	1.85370	-1.49640
Pd	1.59090	-0.36400	-0.21900
C	-1.68880	-0.71290	0.38920
N	-1.46440	-2.02060	0.71710
C	-2.43000	-2.50380	1.58610
C	-3.27330	-1.47700	1.84420
N	-2.80350	-0.39860	1.11480
C	-0.40500	-2.82550	0.19660
C	-0.52520	-3.30030	-1.12290
C	0.48210	-4.13070	-1.61630
C	1.56590	-4.48680	-0.82330
C	1.66070	-4.00280	0.47360
C	0.68840	-3.15490	1.01850
C	-3.44500	0.87590	1.01740
C	-4.41330	1.05800	0.01780
C	-4.99650	2.32230	-0.09450
C	-4.62840	3.35640	0.75860
C	-3.67640	3.14320	1.74950
C	-3.06670	1.89610	1.90370
H	-2.42800	-3.52550	1.93040
H	-4.15440	-1.41310	2.46370
C	-1.71230	-2.96750	-2.00530
H	0.40900	-4.50890	-2.63220
H	2.34090	-5.13750	-1.21890
H	2.51720	-4.27000	1.08810
C	0.90740	-2.72090	2.46280
C	-4.79710	-0.05190	-0.94010
H	-5.74220	2.49960	-0.86450
H	-5.08930	4.33480	0.65290
H	-3.39780	3.95890	2.41060
C	-2.00280	1.67930	2.95920
C	-2.42560	2.20590	4.32950
C	-0.67280	2.29170	2.51320
C	-4.25370	0.23600	-2.34090
C	-6.30720	-0.28700	-0.96640
C	-2.54080	-4.21870	-2.30160
C	-1.26800	-2.27100	-3.29100
C	0.46100	-1.31110	2.84350
C	0.34730	-3.75790	3.44220
H	-2.35150	-2.26320	-1.46650
H	1.99860	-2.73660	2.57970
H	-4.32680	-0.97640	-0.59050

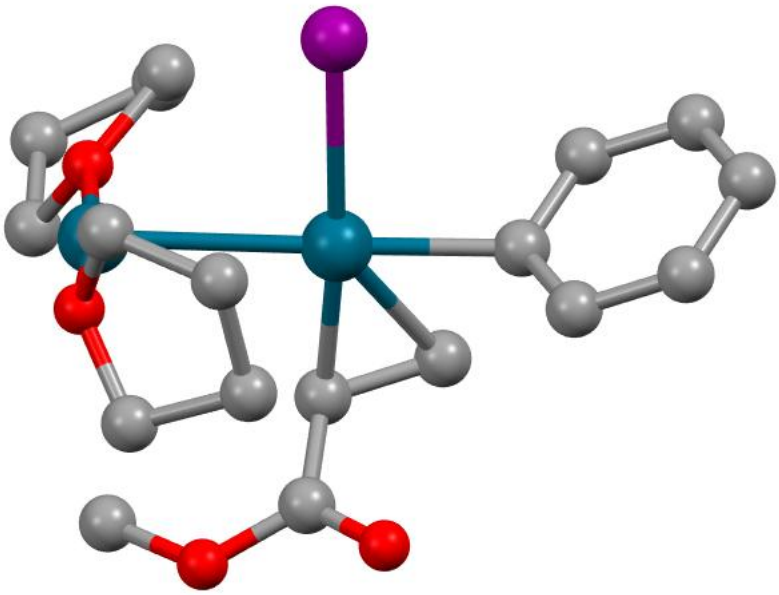
	H -1.84780 0.60050 3.05360 H -1.67100 1.94510 5.07920 H -2.52710 3.29660 4.33450 H -3.38170 1.77690 4.64770 H 0.10640 2.09060 3.25690 H -0.35250 1.86910 1.55290 H -0.76150 3.37880 2.39850 H -4.49220 -0.58800 -3.02280 H -4.68880 1.15400 -2.75250 H -3.16190 0.35630 -2.31190 H -6.54480 -1.13980 -1.61140 H -6.69550 -0.50080 0.03500 H -6.84650 0.58220 -1.35830 H -3.42110 -3.95970 -2.90050 H -1.96030 -4.95940 -2.86320 H -2.88750 -4.69450 -1.37800 H -2.13900 -1.98740 -3.89200 H -0.70450 -1.36200 -3.04960 H -0.63420 -2.91960 -3.90610 H -0.61910 -1.24400 2.99870 H 0.94670 -1.02250 3.78270 H 0.74650 -0.58730 2.06600 H 0.64910 -3.51120 4.46630 H -0.74680 -3.78060 3.41680 H 0.71240 -4.76460 3.21390 Pd -0.91630 0.52510 -0.87970
IVa E = -1481.661161, E+ZPE = -1481.210271, H = -1481.181022, G = -1481.276700	
	Pd 0.34620 0.48540 -0.04490 C 3.36010 -2.03590 2.64090 C 2.02220 -1.93290 3.01760 C 1.13640 -1.14610 2.27900 C 1.56970 -0.46000 1.13600 C 2.92670 -0.54170 0.78750 C 3.80970 -1.33030 1.52700 I 1.34280 2.79380 0.69520 H 4.04740 -2.64850 3.21800 H 1.65930 -2.46800 3.89220 H 0.09990 -1.08390 2.59400 H 3.30180 0.01070 -0.07000 H 4.85510 -1.38410 1.23180 O -1.01190 1.25350 -1.67160 C -0.75840 2.49480 -2.35250 C -1.70420 3.52770 -1.72360 C -2.65500 2.68290 -0.85370 C -2.41060 1.27250 -1.35940 H -0.97380 2.34490 -3.41780 H 0.30010 2.72550 -2.22600 H -2.24560 4.07380 -2.50070 H -1.15310 4.25120 -1.11810 H -3.70190 2.98210 -0.94880 H -2.37000 2.75130 0.20090 H -2.97880 1.06730 -2.27800 H -2.59220 0.47320 -0.64060 O -2.46930 -1.43350 0.97710 C -3.82600 -1.79190 0.63160 C -4.67800 -1.19920 1.73790 C -3.90020 0.06670 2.09060 C -2.46220 -0.40550 2.00000 H -3.87690 -2.88130 0.55990 H -4.06550 -1.35470 -0.34540 H -4.71640 -1.87750 2.59680 H -5.69940 -1.00140 1.40430 H -4.13710 0.45830 3.08260 H -4.09370 0.85380 1.35340 H -2.12670 -0.86510 2.93620 H -1.74900 0.36770 1.69940

	Pd -0.94170 -1.91090 -0.37930 O 0.44320 -2.42430 -1.83680 C 1.72720 -2.98000 -1.44110 C 2.76230 -2.34150 -2.36140 C 2.05470 -1.08540 -2.86870 C 0.62560 -1.56260 -2.98560 H 1.88770 -2.71810 -0.39410 H 1.66700 -4.06740 -1.54310 H 3.00100 -3.00550 -3.19840 H 3.68720 -2.12150 -1.82280 H 2.45270 -0.72150 -3.81920 H 2.10870 -0.27950 -2.12670 H 0.46720 -2.16370 -3.89050 H -0.12340 -0.77210 -2.92600
IVb E = -2176.117129, E+ZPE = -2175.329197, H = -2175.280463, G = -2175.414463	
	O 1.43460 2.35180 1.55750 C 1.88350 3.50460 0.80810 C 1.71460 4.69590 1.74500 C 1.65920 4.04870 3.12900 C 0.92300 2.75730 2.83580 H 1.28250 3.58560 -0.10100 H 2.92880 3.32340 0.53750 H 0.77280 5.20970 1.53130 H 2.52990 5.41590 1.64050 H 1.14040 4.66340 3.86870 H 2.66710 3.83200 3.49940 H -0.16010 2.91260 2.76120 H 1.12580 1.94970 3.54260 C -1.33130 2.14240 -0.46760 C -0.80210 2.41580 -1.73590 C -0.60500 3.73420 -2.14960 C -0.94100 4.79610 -1.31020 C -1.47640 4.52730 -0.05180 C -1.67130 3.21070 0.37010 I -4.27170 0.64740 -0.31510 H -0.54010 1.60110 -2.40490 H -0.18960 3.92680 -3.13610 H -0.79460 5.82190 -1.63690 H -1.75870 5.34560 0.60670 H -2.11120 3.02050 1.34480 Pd -1.67470 0.30030 0.04680 C 0.99890 -1.25140 -0.22680 N 0.19650 -2.34760 -0.16430 C 0.82490 -3.46590 -0.69240 C 2.03830 -3.05910 -1.13350 N 2.12090 -1.70660 -0.85040 C -1.11500 -2.38390 0.40600 C -1.23040 -2.36760 1.81670 C -2.49030 -2.59060 2.37140 C -3.59050 -2.85910 1.56520 C -3.45560 -2.85970 0.18640 C -2.22610 -2.60620 -0.43670 C 3.28010 -0.88220 -1.01540 C 4.27990 -0.94350 -0.03380 C 5.39520 -0.11680 -0.19820 C 5.49630 0.73230 -1.29260 C 4.48090 0.78160 -2.24360 C 3.34630 -0.02190 -2.12530 H 0.35120 -4.43410 -0.69990 H 2.84560 -3.59770 -1.60470 C -0.03310 -2.19980 2.73040 H -2.60260 -2.58270 3.45160 H -4.56090 -3.04850 2.01470 H -4.32490 -3.03410 -0.44120 C -2.23330 -2.62480 -1.96110 C 4.14290 -1.81340 1.20020

	H 6.18650 -0.13270 0.54580 H 6.37020 1.36840 -1.40420 H 4.57040 1.46100 -3.08490 C 2.22800 0.01790 -3.14740 C 2.39710 -1.10130 -4.17900 C 2.09360 1.37070 -3.83950 C 3.81520 -0.95020 2.42130 C 5.38320 -2.67150 1.44510 C 0.26420 -3.50250 3.47510 C -0.22500 -1.03170 3.69610 C -1.21750 -1.74190 -2.68260 C -2.19630 -4.05810 -2.50170 H 0.83660 -1.96030 2.11330 H -3.22060 -2.21820 -2.21470 H 3.29970 -2.49400 1.04600 H 1.29320 -0.16290 -2.60550 H 1.55890 -1.10010 -4.88420 H 3.32230 -0.96340 -4.75040 H 2.43760 -2.08740 -3.70640 H 1.19130 1.37830 -4.45990 H 2.01280 2.18630 -3.11420 H 2.94180 1.58060 -4.50040 H 3.67190 -1.57670 3.30890 H 4.62440 -0.24170 2.63190 H 2.89410 -0.37580 2.25500 H 5.21580 -3.33910 2.29680 H 5.62070 -3.28820 0.57210 H 6.26200 -2.05970 1.67530 H 1.15910 -3.38850 4.09680 H -0.56640 -3.78580 4.13120 H 0.43920 -4.32890 2.77800 H 0.68500 -0.87730 4.28650 H -0.43840 -0.11060 3.14230 H -1.04870 -1.21100 4.39580 H -0.21000 -2.16600 -2.67940 H -1.52350 -1.63400 -3.72880 H -1.17780 -0.74050 -2.23670 H -2.38300 -4.05490 -3.58100 H -1.22030 -4.52540 -2.33690 H -2.95790 -4.68610 -2.02870 Pd 1.00990 0.50590 0.56070
Va E = -1555.605409, E+ZPE = -1555.176239, H = -1555.144674, G = -1555.245376	
	Pd 0.42040 -0.26330 -0.08160 C 5.02010 -0.62020 -1.39860 C 4.15090 -1.68330 -1.63320 C 2.80510 -1.58730 -1.27380 C 2.32470 -0.42570 -0.66800 C 3.19070 0.64780 -0.45000 C 4.53560 0.54690 -0.81170 I -0.16470 0.99260 -2.29650 H 6.06690 -0.69730 -1.67980 H 4.51690 -2.59410 -2.10140 H 2.14000 -2.42530 -1.46830 H 2.82670 1.56620 0.00370 H 5.20240 1.38760 -0.63510 C 0.55960 -1.99900 1.18710 C 0.77740 -0.88510 1.97870 C 2.11560 -0.43270 2.43990 O 2.30490 0.63800 2.98130 O 3.06900 -1.33950 2.22350 C 4.39350 -0.93060 2.56730 H -0.43580 -2.42990 1.12730 H 1.39230 -2.61260 0.85770 H -0.05280 -0.41290 2.50050 H 5.04550 -1.74330 2.24790 H 4.65780 -0.00900 2.04490

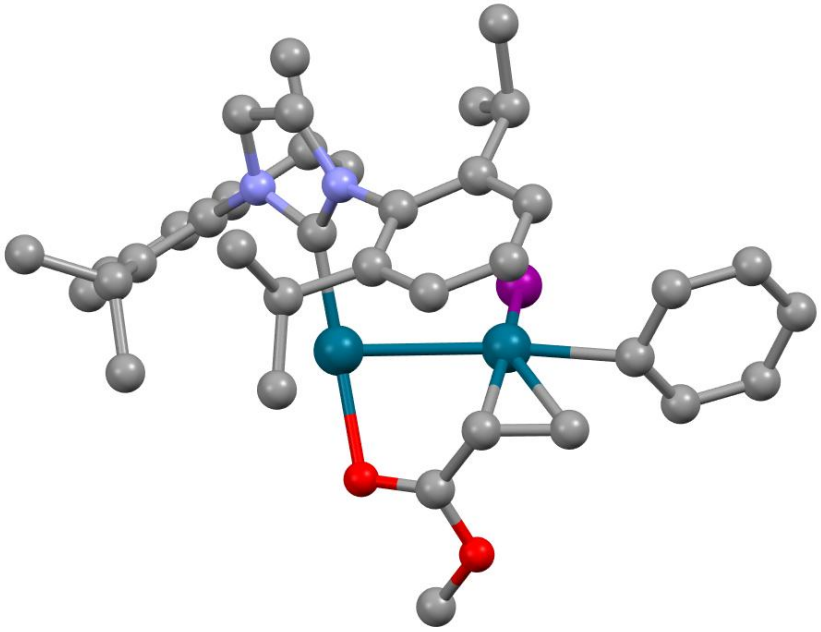
	H 4.48040 -0.77740 3.64640 O -2.70550 -1.78340 0.13100 C -2.27790 -2.45770 -1.07530 C -2.49420 -3.93380 -0.79440 C -3.66950 -3.91550 0.18120 C -3.35030 -2.70320 1.03490 H -1.23540 -2.18640 -1.26520 H -2.89580 -2.09200 -1.90240 H -1.60860 -4.36570 -0.31480 H -2.69940 -4.49650 -1.70800 H -3.75080 -4.82740 0.77750 H -4.61170 -3.76430 -0.35600 H -2.65540 -2.94510 1.84900 H -4.22820 -2.20400 1.45170 Pd -2.18530 0.16870 0.65020 O -1.78530 2.15680 1.18590 C -2.36770 3.18420 0.35140 C -1.66240 4.45770 0.77060 C -0.24850 3.94730 1.03850 C -0.49930 2.59940 1.69120 H -2.17040 2.94110 -0.69910 H -3.44520 3.17920 0.53290 H -2.10960 4.86320 1.68470 H -1.70360 5.22230 -0.00880 H 0.33930 4.60790 1.68040 H 0.28720 3.81160 0.09270 H -0.58360 2.66630 2.78130 H 0.25550 1.85190 1.43510
Vb E = -2250.044941, E+ZPE = -2249.278201, H = -2249.229308, G = -2249.362634	
	C 1.50030 0.45770 0.62430 N 1.22260 1.45390 1.51280 C 2.20270 1.55400 2.48580 C 3.11040 0.58620 2.22310 N 2.65790 -0.08050 1.09600 C 0.10040 2.33730 1.41320 C 0.17220 3.37680 0.46170 C -0.92620 4.22690 0.34300 C -2.04490 4.06500 1.15580 C -2.07070 3.05750 2.10700 C -0.99830 2.16810 2.26840 C 3.42620 -1.05710 0.38200 C 4.29310 -0.59930 -0.62170 C 5.05170 -1.55280 -1.30620 C 4.94880 -2.90120 -0.99210 C 4.08210 -3.32540 0.01030 C 3.29810 -2.41440 0.72070 H 2.16210 2.29990 3.26320 H 4.03350 0.32070 2.71380 C 1.42760 3.58480 -0.36670 H -0.90770 5.02890 -0.38720 H -2.89390 4.73470 1.05040 H -2.93910 2.94530 2.75160 C -1.11750 1.17190 3.41400 C 4.42160 0.86830 -0.97590 H 5.72850 -1.23040 -2.09270 H 5.54530 -3.63060 -1.53320 H 4.00800 -4.38390 0.23720 C 2.36220 -2.86910 1.82250 C 3.04220 -2.78090 3.19280 C 1.82510 -4.28060 1.60280 C 3.93990 1.13300 -2.40230 C 5.85080 1.37090 -0.76990 C 2.55960 4.21260 0.48390 C 1.19450 4.39680 -1.63670 C -0.49620 -0.20950 3.22770 C -0.64200 1.81390 4.72260

	H 1.75240 2.58840 -0.69090 H -2.19730 1.00970 3.52230 H 3.77390 1.43910 -0.30420 H 1.50440 -2.18650 1.82080 H 2.34780 -3.09500 3.97960 H 3.91810 -3.43890 3.23150 H 3.37350 -1.76570 3.42650 H 1.03120 -4.48790 2.32710 H 1.40450 -4.40140 0.60040 H 2.60340 -5.03890 1.74590 H 3.98560 2.20350 -2.63110 H 4.55440 0.60300 -3.13820 H 2.90070 0.80170 -2.53150 H 5.90850 2.44500 -0.97730 H 6.18580 1.20530 0.25930 H 6.55540 0.86490 -1.43890 H 2.90820 5.14790 0.03330 H 2.22830 4.44990 1.49890 H 3.42300 3.54660 0.56800 H 2.11340 4.41040 -2.23170 H 0.40060 3.97030 -2.25910 H 0.93450 5.43820 -1.41710 H 0.58920 -0.20660 3.35980 H -0.91160 -0.88810 3.98050 H -0.72590 -0.62750 2.24520 H -0.86030 1.15060 5.56670 H 0.43850 1.99000 4.70980 H -1.13900 2.77220 4.90510 Pd 0.78680 0.13040 -1.17360 C -2.90520 1.51220 -1.54020 C -1.59630 1.46700 -1.99720 C -1.15080 0.58050 -3.08230 O 0.03100 0.19960 -3.17890 O -2.08020 0.21000 -3.93870 C -1.70130 -0.79240 -4.89510 H -3.70240 1.03320 -2.09690 H -3.19230 2.27960 -0.82830 H -0.84010 2.15390 -1.62810 H -0.89900 -0.42470 -5.53780 H -1.37860 -1.69930 -4.37830 H -2.59890 -0.98690 -5.48060 C -3.78210 -0.46780 0.00240 C -4.24990 0.05780 1.20890 C -5.55410 -0.20120 1.63720 C -6.40910 -0.97740 0.85890 C -5.94990 -1.49510 -0.35130 C -4.64580 -1.24250 -0.77790 I -1.32810 -2.61000 0.18430 H -3.60090 0.67530 1.82390 H -5.89930 0.21060 2.58310 H -7.42440 -1.17710 1.19090 H -6.60720 -2.10400 -0.96810 H -4.30020 -1.66430 -1.71870 Pd -1.85400 -0.12690 -0.52490
TS-VIa E = -1555.581628, E+ZPE = -1555.152104, H = -1555.121894, G = -1555.217196	

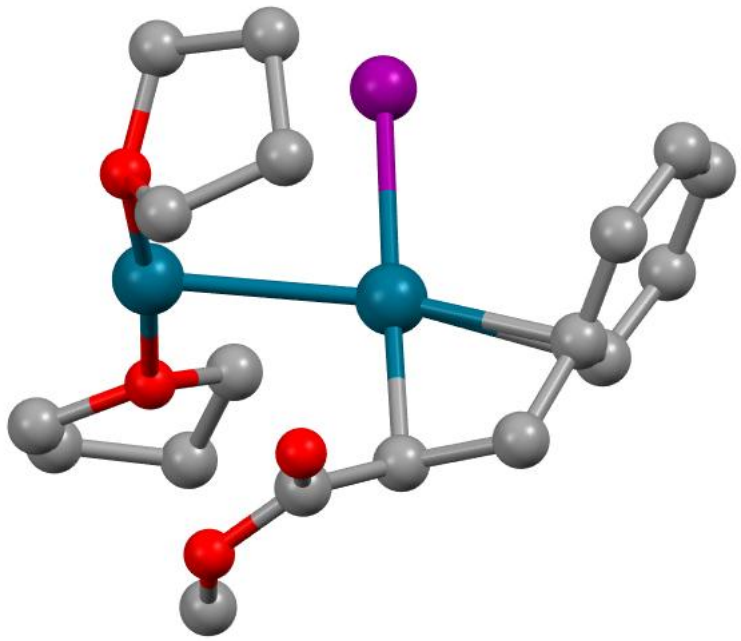


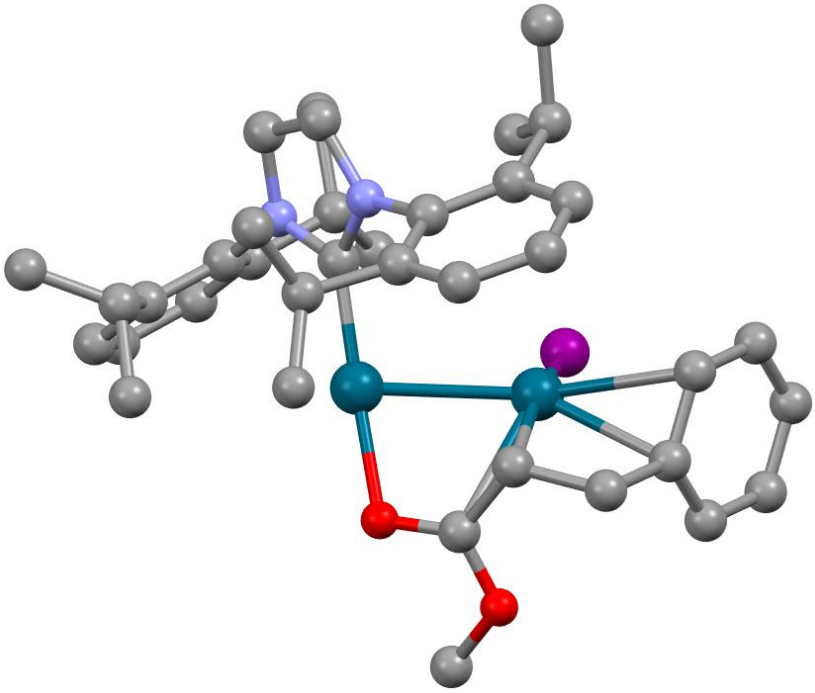
Pd	0.50680	-0.22640	0.40250
C	5.17230	-0.83820	0.95500
C	4.57400	0.39170	1.22950
C	3.19040	0.48820	1.34980
C	2.39350	-0.64770	1.16200
C	2.99350	-1.88560	0.91290
C	4.37980	-1.97500	0.80580
I	1.33700	-0.53340	-2.12180
H	6.25260	-0.91170	0.86760
H	5.18690	1.27970	1.36110
H	2.72370	1.43610	1.60360
H	2.38090	-2.77410	0.78530
H	4.83990	-2.93760	0.59810
C	0.89320	-0.82150	2.53880
C	-0.34610	-0.15040	2.30700
C	-0.44040	1.24650	2.78350
O	0.53430	1.92000	3.06330
O	-1.65450	1.81020	2.93770
C	-2.84410	1.08630	2.63860
H	0.87260	-1.90530	2.60620
H	1.58150	-0.33430	3.21970
H	-1.25100	-0.74260	2.21320
H	-2.96710	0.22610	3.30400
H	-3.66490	1.78510	2.80690
H	-2.85060	0.76600	1.58520
O	-2.50810	-1.57230	-0.37910
C	-3.57660	-1.90760	0.52740
C	-3.74040	-3.40410	0.36580
C	-2.29020	-3.85190	0.19550
C	-1.68830	-2.74040	-0.64880
H	-4.45080	-1.31880	0.24040
H	-3.28250	-1.64410	1.55110
H	-4.32410	-3.62740	-0.53340
H	-4.23490	-3.85960	1.22700
H	-2.19160	-4.82660	-0.28760
H	-1.79430	-3.90010	1.17130
H	-1.75060	-2.93810	-1.72320
H	-0.65340	-2.50070	-0.39140
Pd	-1.92400	0.39700	-0.69970
O	-1.54510	2.40800	-1.12180
C	-0.73600	2.73180	-2.28130
C	0.57240	3.32620	-1.74410
C	0.37540	3.36070	-0.22160
C	-1.13030	3.31960	-0.08380
H	-0.59990	1.80940	-2.84710
H	-1.30180	3.45230	-2.88240
H	0.72630	4.33090	-2.14680
H	1.42960	2.70820	-2.02220
H	0.81260	4.24420	0.25000
H	0.80580	2.46610	0.24310
H	-1.58350	4.29760	-0.29660
H	-1.50600	2.94470	0.86710

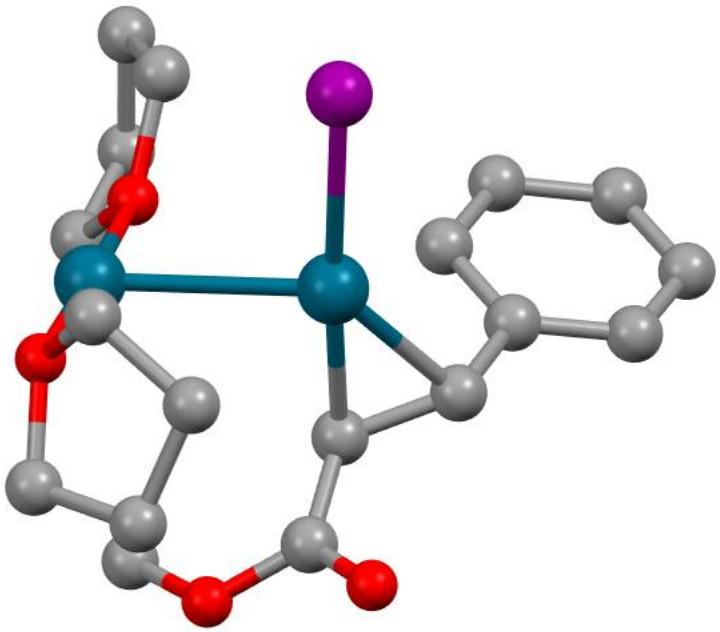
TS-VIb E = -2250.037927, E+ZPE = -2249.270884, H = -2249.222267, G = -2249.354237

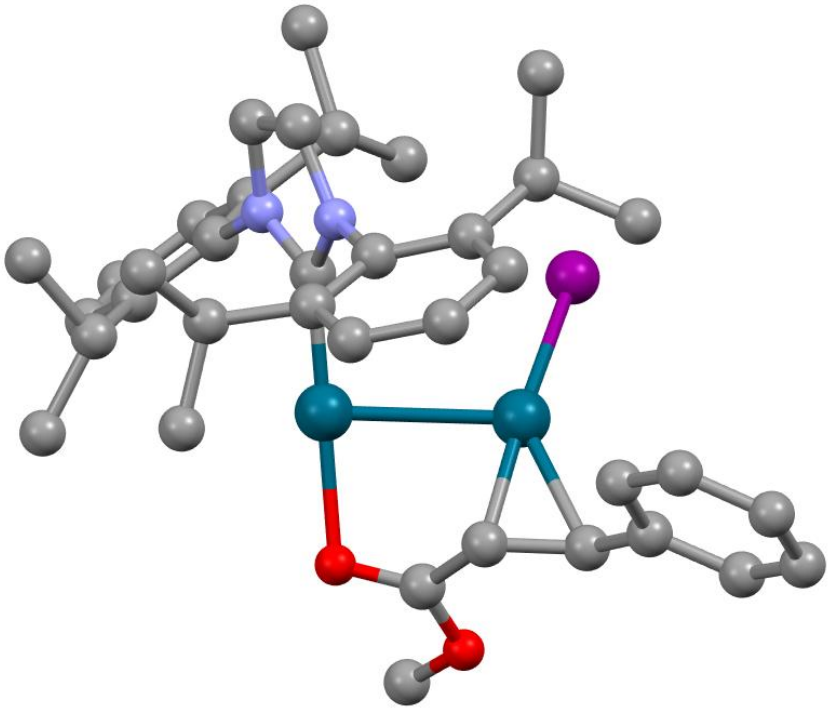


C	1.57250	0.33810	0.66100
N	1.32300	1.26540	1.63020
C	2.29210	1.24500	2.61730
C	3.16130	0.26250	2.28420
N	2.69930	-0.28750	1.09910
C	0.26400	2.22390	1.56370
C	0.43350	3.32230	0.69850
C	-0.60770	4.24700	0.60390
C	-1.76910	4.09230	1.35230
C	-1.89190	3.01880	2.22280
C	-0.88170	2.05670	2.35660
C	3.43710	-1.23790	0.32030
C	4.38790	-0.74250	-0.58410
C	5.10780	-1.67130	-1.34050
C	4.88980	-3.03360	-1.18690
C	3.94550	-3.49600	-0.27580
C	3.19420	-2.61010	0.49890
H	2.26970	1.92280	3.45590
H	4.06260	-0.08600	2.76340
C	1.72700	3.56410	-0.05620
H	-0.50390	5.10240	-0.05680
H	-2.57340	4.81780	1.26680
H	-2.79040	2.91460	2.82630
C	-1.11160	0.98030	3.40800
C	4.63360	0.74140	-0.77150
H	5.84420	-1.31910	-2.05740
H	5.45740	-3.74370	-1.78220
H	3.78410	-4.56390	-0.17330
C	2.17150	-3.10720	1.50100
C	2.76490	-3.15950	2.91300
C	1.59230	-4.47050	1.13530
C	4.10680	1.20950	-2.12840
C	6.11020	1.09830	-0.59930
C	2.57130	4.60700	0.68090
C	1.49960	3.96770	-1.51100
C	-0.53800	-0.40910	3.14540
C	-0.67880	1.49560	4.78550
H	2.29120	2.62760	-0.06950
H	-2.20210	0.86150	3.44210
H	4.07790	1.28130	0.00130
H	1.34420	-2.38780	1.50530
H	2.00720	-3.49950	3.62730
H	3.60650	-3.86110	2.95210
H	3.12470	-2.18330	3.24850
H	0.75620	-4.70380	1.80150
H	1.21580	-4.48890	0.10860
H	2.33340	-5.27020	1.24840
H	4.26660	2.28570	-2.25480
H	4.61250	0.69140	-2.95080
H	3.02920	1.01340	-2.22180
H	6.24630	2.18290	-0.66890
H	6.48720	0.77080	0.37510
H	6.73190	0.63680	-1.37390
H	2.05800	5.57480	0.71590
H	2.77670	4.29840	1.71120
H	3.53100	4.75090	0.17220
H	2.46190	4.08480	-2.02010
H	0.92770	3.20340	-2.04750
H	0.96820	4.92130	-1.59720
H	0.53650	-0.46630	3.34010
H	-1.02730	-1.12520	3.81440
H	-0.72510	-0.73770	2.12090
H	-0.96090	0.77650	5.56240
H	0.40730	1.62770	4.83290
H	-1.14710	2.45610	5.02370
Pd	0.83610	0.30210	-1.14960

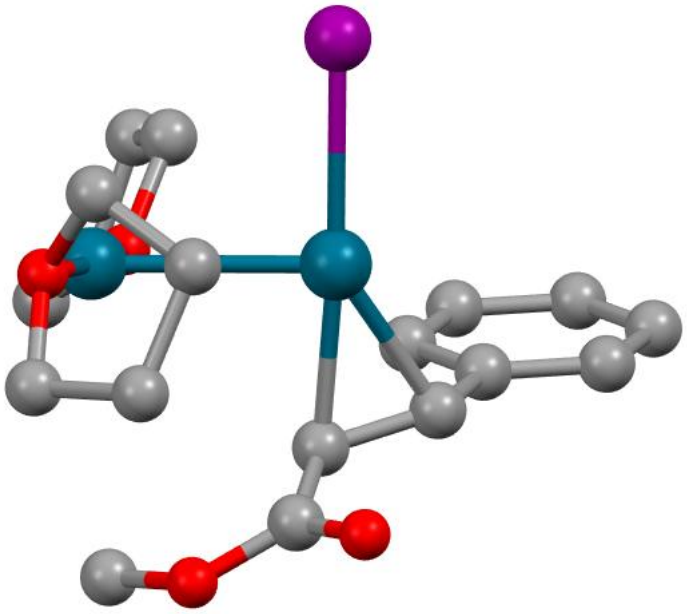
	C -3.15750 1.50280 -1.45540 C -1.76740 1.59420 -1.76190 C -1.19410 0.95050 -2.94680 O 0.02660 0.72020 -3.07170 O -2.05670 0.61460 -3.89040 C -1.54320 -0.17700 -4.97130 H -3.82690 1.19650 -2.25130 H -3.55250 2.26800 -0.79570 H -1.13610 2.33670 -1.27890 H -0.78240 0.37680 -5.52530 H -1.11850 -1.10800 -4.58810 H -2.40050 -0.38550 -5.61020 C -3.87850 -0.01330 -0.26770 C -4.25810 0.43020 1.00260 C -5.43370 -0.03910 1.58640 C -6.25350 -0.92870 0.89510 C -5.89450 -1.34360 -0.38760 C -4.71870 -0.88270 -0.97240 I -1.66220 -2.68780 0.12630 H -3.63200 1.13910 1.53680 H -5.71100 0.29940 2.58160 H -7.17260 -1.28970 1.34810 H -6.53160 -2.03260 -0.93620 H -4.44330 -1.21350 -1.97040 Pd -1.80360 -0.10160 -0.57530
VIIa E = -1555.626966, E+ZPE = -1555.194737, H = -1555.164534, G = -1555.259782	
	Pd -0.60910 -0.03060 -0.58880 C -4.10440 -1.68020 -1.01020 C -4.32340 -0.34550 -0.64390 C -3.48650 0.65420 -1.10910 C -2.40660 0.34900 -1.96890 C -2.18130 -1.00810 -2.30660 C -3.03780 -2.01030 -1.83180 I -1.23630 -1.66020 1.48710 H -4.76920 -2.45690 -0.64400 H -5.15430 -0.09350 0.00850 H -3.66310 1.69230 -0.84020 H -1.40740 -1.25800 -3.02830 H -2.86190 -3.04390 -2.11440 C -1.56620 1.43570 -2.61300 C -0.12880 1.12890 -2.22930 C 0.68850 2.31800 -1.91960 O 0.22480 3.37920 -1.53020 O 2.02880 2.27240 -2.09380 C 2.64910 1.12210 -2.65470 H -1.72100 1.46070 -3.70020 H -1.85170 2.40910 -2.20780 H 0.35500 0.42950 -2.91290 H 2.34500 0.97450 -3.69700 H 3.72160 1.32510 -2.63070 H 2.43900 0.22610 -2.06550 O 2.61240 -1.04490 -0.20730 C 4.04720 -1.16870 -0.03770 C 4.36850 -2.62090 -0.36690 C 3.18800 -3.04580 -1.23930 C 2.03890 -2.32010 -0.57510 H 4.30690 -0.89120 0.98790 H 4.51210 -0.46090 -0.73120 H 4.39400 -3.22090 0.54800 H 5.33380 -2.71750 -0.86910 H 3.03540 -4.12740 -1.25510 H 3.31670 -2.69420 -2.26880 H 1.68700 -2.83240 0.32660 H 1.18150 -2.10750 -1.21900 Pd 1.64990 0.42010 0.89650 O 0.88940 1.91850 2.11570

	C -0.03210 1.57000 3.17870 C -1.40570 2.08880 2.73940 C -1.10950 2.92420 1.48240 C 0.38420 3.15140 1.56160 H 0.01530 0.48880 3.30980 H 0.32420 2.06840 4.08770 H -1.85400 2.69340 3.53210 H -2.08200 1.26060 2.51320 H -1.66850 3.86250 1.44530 H -1.32960 2.34860 0.57640 H 0.64030 3.95570 2.26460 H 0.86740 3.32430 0.60120
VIIb E = -2250.092909, E+ZPE = -2249.323124, H = -2249.274464, G = -2249.407308	
	C -1.62520 0.35260 -0.59690 N -1.43440 1.24310 -1.61060 C -2.47670 1.20520 -2.51910 C -3.33160 0.24800 -2.08830 N -2.78790 -0.26980 -0.92400 C -0.34540 2.16970 -1.66630 C -0.39610 3.28730 -0.81050 C 0.67690 4.17900 -0.83750 C 1.75500 3.97220 -1.69070 C 1.76260 2.87690 -2.54220 C 0.71490 1.94670 -2.55780 C -3.46580 -1.18770 -0.05710 C -4.32360 -0.65310 0.91540 C -4.98200 -1.54990 1.76090 C -4.79290 -2.91900 1.62810 C -3.94000 -3.42010 0.64980 C -3.25310 -2.56710 -0.21610 H -2.50680 1.85070 -3.38250 H -4.27090 -0.10230 -2.48630 C -1.60160 3.57940 0.06320 H 0.66500 5.04940 -0.18860 H 2.58620 4.67200 -1.69780 H 2.59890 2.72540 -3.22060 C 0.81730 0.83870 -3.59670 C -4.52690 0.83950 1.08160 H -5.64600 -1.16850 2.53150 H -5.31120 -3.60410 2.29340 H -3.79910 -4.49260 0.56560 C -2.33350 -3.10660 -1.29370 C -3.06820 -3.21760 -2.63390 C -1.71430 -4.45270 -0.93040 C -3.86620 1.33200 2.36940 C -6.00660 1.22100 1.04100 C -2.51490 4.59220 -0.63230 C -1.22360 4.04900 1.46580 C 0.21300 -0.52140 -3.25870 C 0.29770 1.34420 -4.94780 H -2.16600 2.65010 0.18220 H 1.89630 0.67540 -3.71400 H -4.03810 1.34780 0.24460 H -1.51370 -2.38890 -1.41350 H -2.38510 -3.58210 -3.40880 H -3.90320 -3.92400 -2.55840 H -3.46980 -2.25720 -2.96790 H -0.95110 -4.71580 -1.66900 H -1.23220 -4.42420 0.05090 H -2.46000 -5.25610 -0.92930 H -3.97880 2.41640 2.47360 H -4.31040 0.85620 3.25060 H -2.79080 1.10150 2.37730 H -6.11660 2.30940 1.09490 H -6.47980 0.87740 0.11550 H -6.55950 0.79070 1.88260

	H -3.41380 4.77230 -0.03210 H -2.00260 5.55110 -0.77180 H -2.83120 4.23350 -1.61730 H -2.12740 4.18080 2.06970 H -0.58670 3.31510 1.97040 H -0.69900 5.01020 1.45370 H -0.87430 -0.54050 -3.37240 H 0.62270 -1.26950 -3.94590 H 0.46540 -0.83690 -2.24400 H 0.47640 0.59380 -5.72580 H -0.78010 1.53500 -4.90990 H 0.79360 2.27250 -5.24920 Pd -0.74490 0.36370 1.14640 C 3.52800 1.82100 1.43640 C 2.03740 1.55270 1.53430 C 1.50060 0.92020 2.72590 O 0.27090 0.74780 2.93990 O 2.39230 0.50720 3.62110 C 1.89390 -0.29080 4.69920 H 3.98800 1.94470 2.42150 H 3.69310 2.74250 0.87040 H 1.37360 2.32470 1.14490 H 2.76890 -0.55880 5.29120 H 1.18540 0.27520 5.30800 H 1.40950 -1.19130 4.31320 C 4.16920 0.65600 0.69910 C 4.09360 0.59710 -0.70910 C 4.70650 -0.44510 -1.41170 C 5.38910 -1.44040 -0.72450 C 5.46110 -1.39920 0.67080 C 4.85570 -0.36800 1.37670 I 1.72290 -2.73420 -0.37660 H 3.60970 1.40880 -1.24690 H 4.64380 -0.47050 -2.49570 H 5.86430 -2.25110 -1.26870 H 5.99260 -2.17940 1.20830 H 4.91660 -0.33390 2.46070 Pd 1.83370 -0.14900 0.37050
TS-VIIIa E = -1555.607125, E+ZPE = -1555.179536, H = -1555.149457, G = -1555.244591	
	Pd -0.07700 0.59680 -0.63720 C -5.59600 0.10960 -0.79290 C -5.24190 0.44410 -2.09720 C -3.91290 0.35900 -2.50500 C -2.92450 -0.06930 -1.61420 C -3.28820 -0.39730 -0.30140 C -4.61320 -0.30990 0.10490 I 0.39470 2.88240 0.55860 H -6.63140 0.18260 -0.47270 H -6.00040 0.77640 -2.80020 H -3.63610 0.62260 -3.52270 H -2.51900 -0.69900 0.40430 H -4.88090 -0.55920 1.12820 C -1.52550 -0.18340 -2.08680 C -0.65010 -1.18940 -1.59150 C 0.46520 -1.63110 -2.45610 O 0.82030 -1.03490 -3.45610 O 1.11760 -2.76480 -2.13550 C 0.74140 -3.53490 -0.99720 H -1.35180 0.13320 -3.11390 H -0.90750 1.37690 -1.68370 H -1.02270 -1.87010 -0.83390 H -0.27600 -3.92570 -1.09660 H 1.43940 -4.37300 -0.96410 H 0.83960 -2.94160 -0.07470 O -0.53770 -1.14670 2.02710 C -0.98170 -2.46580 2.39860

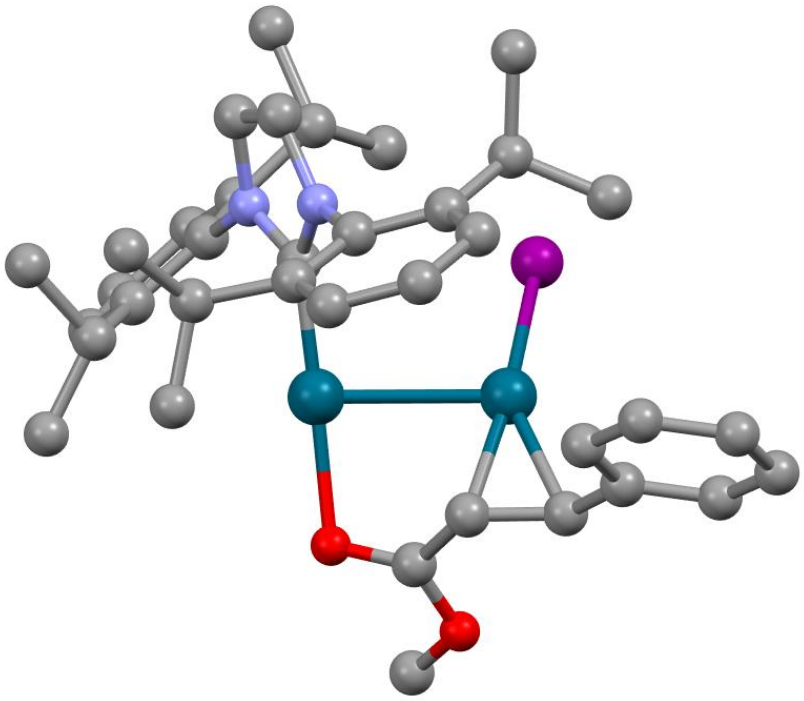
	C -2.33150 -2.22520 3.04080 C -2.08550 -0.92360 3.80410 C -1.15030 -0.14720 2.88520 H -0.26750 -2.90790 3.10450 H -1.01000 -3.06870 1.48760 H -2.63210 -3.05130 3.68950 H -3.09790 -2.09060 2.26990 H -1.59270 -1.13590 4.75810 H -3.00300 -0.36720 4.00950 H -0.36180 0.38900 3.41790 H -1.67260 0.55450 2.22860 Pd 1.35160 -0.83720 1.21090 O 3.28090 -0.54120 0.46680 C 3.72680 0.79110 0.13730 C 3.52400 0.88080 -1.35970 C 3.87960 -0.53490 -1.84500 C 3.80460 -1.39580 -0.57720 H 3.13810 1.49560 0.72580 H 4.78740 0.86650 0.41330 H 4.14180 1.65870 -1.81490 H 2.47130 1.10720 -1.56620 H 4.88870 -0.57080 -2.26390 H 3.17940 -0.88120 -2.60780 H 4.79580 -1.73470 -0.25360 H 3.14280 -2.25620 -0.66180
TS-VIIIb E = -2250.068960, E+ZPE = -2249.304994, H = -2249.256040, G = -2249.390380	
	C -1.36060 0.73620 -0.51970 N -0.83160 1.49130 -1.52460 C -1.75420 1.70330 -2.53770 C -2.88700 1.06390 -2.17120 N -2.63190 0.47440 -0.94230 C 0.41320 2.19930 -1.45570 C 0.45490 3.38550 -0.70310 C 1.66070 4.08970 -0.66330 C 2.76690 3.65310 -1.38090 C 2.68780 2.49510 -2.14500 C 1.51510 1.73620 -2.19240 C -3.63390 -0.19810 -0.16520 C -4.16620 0.45890 0.96360 C -5.17220 -0.19380 1.67680 C -5.64450 -1.43910 1.27820 C -5.11080 -2.05890 0.15850 C -4.08960 -1.45800 -0.58470 H -1.52100 2.29660 -3.40760 H -3.84590 0.98180 -2.65700 C -0.75780 3.94600 0.01180 H 1.72230 5.00430 -0.07980 H 3.69230 4.22210 -1.35170 H 3.55480 2.16640 -2.70920 C 1.45020 0.48890 -3.04800 C -3.72450 1.85350 1.36650 H -5.59930 0.28170 2.55350 H -6.43290 -1.92660 1.84520 H -5.48580 -3.03160 -0.14430 C -3.53980 -2.16430 -1.80790 C -4.48680 -2.00450 -3.00130 C -3.28290 -3.64910 -1.54900 C -3.84150 2.12560 2.86270 C -4.48450 2.90930 0.55920 C -1.13550 5.31850 -0.54870 C -0.54030 4.00520 1.52300 C 1.19140 0.85400 -4.51260 C 2.71300 -0.36240 -2.92890 H -1.60210 3.27770 -0.17500 H 0.61000 -0.11720 -2.69270 H -2.66010 1.94540 1.11730

	H -2.57880 -1.70360 -2.06050 H -4.06820 -2.49490 -3.88680 H -5.45750 -2.46670 -2.78730 H -4.66740 -0.95520 -3.25170 H -2.74360 -4.08490 -2.39620 H -2.67760 -3.80200 -0.65150 H -4.21810 -4.20860 -1.43550 H -3.37160 3.08610 3.09740 H -4.88350 2.18680 3.19480 H -3.33850 1.35110 3.45150 H -4.14180 3.91570 0.82460 H -4.34150 2.77680 -0.51750 H -5.55950 2.85280 0.76680 H -2.04870 5.68590 -0.06790 H -0.34560 6.05650 -0.37140 H -1.31620 5.27110 -1.62760 H -1.43340 4.39350 2.02480 H -0.32790 3.00570 1.92250 H 0.29920 4.66040 1.78080 H 2.01040 1.46370 -4.91170 H 1.11650 -0.05290 -5.12220 H 0.26260 1.41940 -4.63460 H 2.57640 -1.30570 -3.46670 H 3.58690 0.13970 -3.35840 H 2.93360 -0.60400 -1.88430 Pd -0.68010 0.38840 1.27170 C 3.26530 -0.95470 1.70910 C 2.19480 -0.10160 2.09200 C 1.21230 -0.48580 3.10490 O 0.11550 0.09450 3.22520 O 1.55880 -1.48750 3.89400 C 0.53770 -1.98860 4.76880 H 3.42490 -1.83810 2.32320 H 2.71440 -2.05790 0.47480 H 2.18920 0.95540 1.83700 H 0.98930 -2.83400 5.28610 H 0.23630 -1.22160 5.48520 H -0.32900 -2.31490 4.18880 C 4.47930 -0.44740 1.03290 C 5.66980 -1.17300 1.15330 C 6.84020 -0.71690 0.55490 C 6.83440 0.46920 -0.17560 C 5.64980 1.19360 -0.30570 C 4.47990 0.73970 0.29090 I 0.40790 -2.90990 -1.22980 H 5.67350 -2.09950 1.72240 H 7.75730 -1.28970 0.65910 H 7.74650 0.82520 -0.64610 H 5.63440 2.11530 -0.88060 H 3.56090 1.30200 0.15940 Pd 1.40870 -1.20990 0.50420
IXa E = -1555.609627, E+ZPE = -1555.180992, H = -1555.150426, G = -1555.247656	

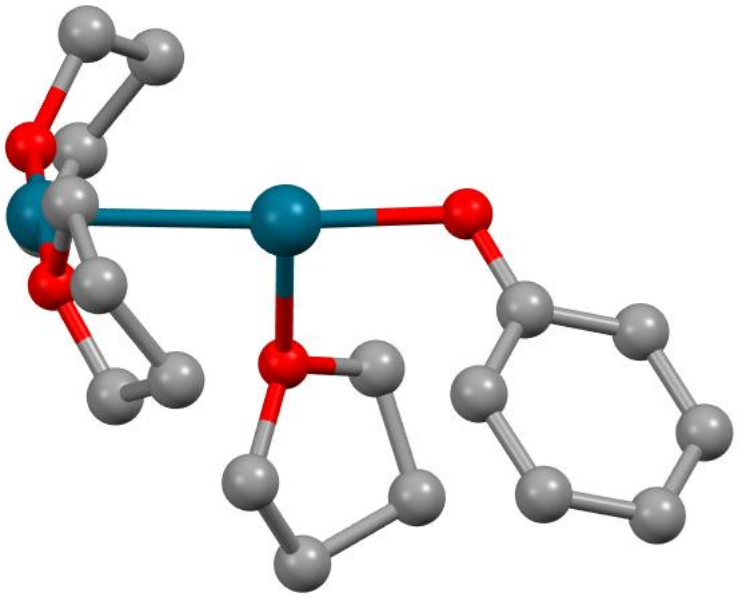


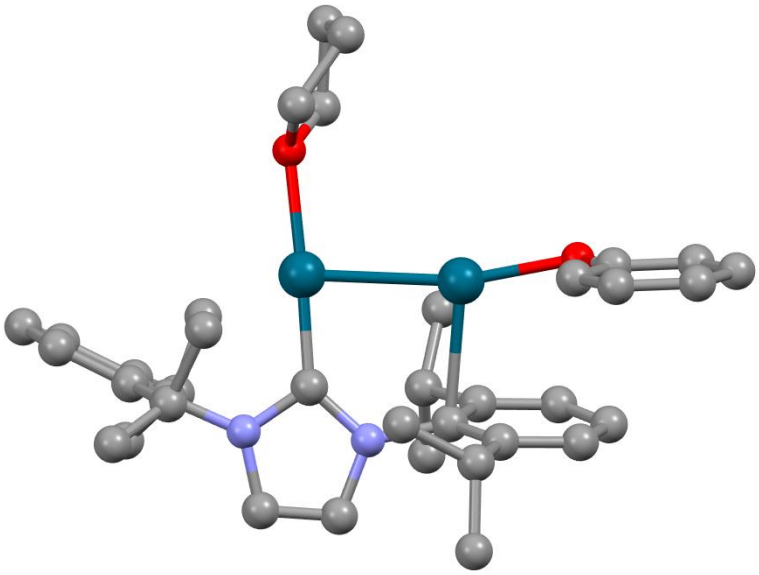
Pd	-0.04820	-0.73120	0.65820
C	-5.43780	-0.30220	0.90070
C	-4.97720	-0.96960	2.03360
C	-3.65250	-0.83170	2.43470
C	-2.76670	-0.02380	1.71070
C	-3.24110	0.64490	0.57240
C	-4.56390	0.50590	0.17270
I	0.40080	-2.78080	-0.87090
H	-6.47120	-0.41200	0.58460
H	-5.65080	-1.60050	2.60660
H	-3.29170	-1.35470	3.31700
H	-2.56440	1.25880	-0.01370
H	-4.91600	1.02770	-0.71320
C	-1.37590	0.09810	2.17810
C	-0.47740	1.08260	1.74630
C	0.69160	1.40790	2.59430
O	1.08200	0.70730	3.50810
O	1.34820	2.55930	2.35830
C	0.91770	3.46390	1.34340
H	-1.15290	-0.38580	3.12590
H	-0.48900	-1.86440	1.57820
H	-0.80140	1.81020	1.01220
H	-0.08660	3.84710	1.54840
H	1.62540	4.29400	1.36910
H	0.95240	2.98520	0.35160
O	-0.77740	1.39290	-1.76950
C	-1.07290	2.70020	-2.29310
C	-2.52100	2.58520	-2.71990
C	-2.56730	1.17620	-3.31970
C	-1.50790	0.39880	-2.53500
H	-0.41270	2.91790	-3.14270
H	-0.88420	3.41940	-1.49270
H	-2.80360	3.36050	-3.43590
H	-3.17670	2.66530	-1.84660
H	-2.30400	1.20850	-4.38070
H	-3.55360	0.71520	-3.23020
H	-0.80780	-0.13550	-3.18250
H	-1.92180	-0.30410	-1.80840
Pd	1.16970	0.96930	-1.13980
O	3.17990	0.62140	-0.64390
C	3.68830	-0.72480	-0.55630
C	3.67260	-1.02390	0.92860
C	4.02450	0.33310	1.56560
C	3.83250	1.34080	0.42570
H	3.04640	-1.36520	-1.16160
H	4.70830	-0.72470	-0.96420
H	4.37310	-1.81880	1.19580
H	2.66400	-1.33740	1.22120
H	5.05890	0.35670	1.91850
H	3.37120	0.55550	2.41160
H	4.79240	1.70220	0.03720
H	3.20810	2.19410	0.68270

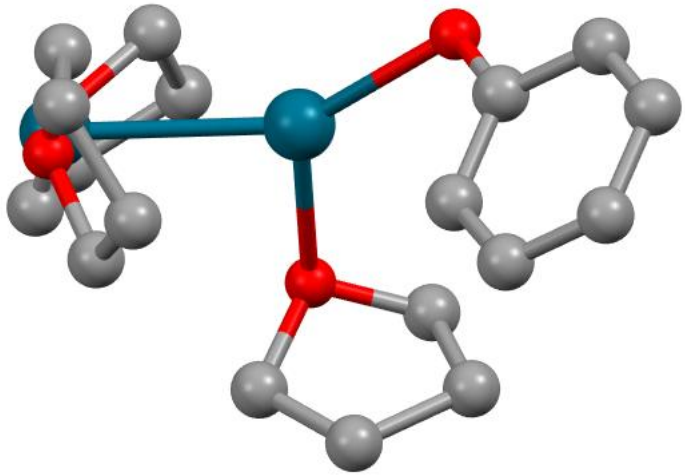
IXb E = -2250.071753, E+ZPE = -2249.306439, H = -2249.257329, G = -2249.391234

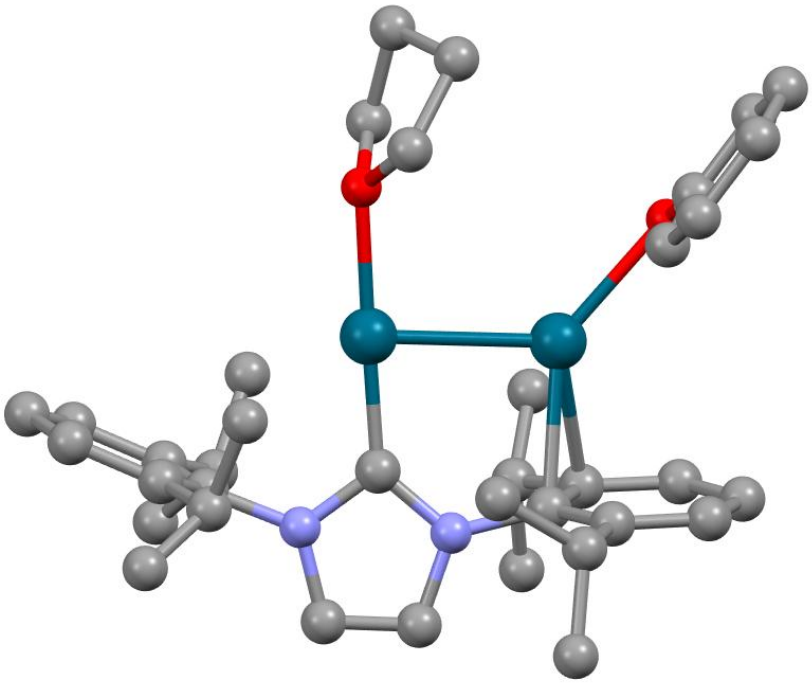


C	1.27370	-0.75770	-0.52170
N	0.68980	-1.48470	-1.51600
C	1.57870	-1.73630	-2.55000
C	2.74900	-1.15670	-2.20500
N	2.55060	-0.56160	-0.96750
C	-0.58060	-2.14250	-1.42810
C	-0.65700	-3.33260	-0.68420
C	-1.88360	-4.00050	-0.64940
C	-2.97650	-3.52530	-1.36320
C	-2.86550	-2.36040	-2.11240
C	-1.67050	-1.63790	-2.15440
C	3.60020	0.06080	-0.21070
C	4.07490	-0.58720	0.95020
C	5.11340	0.02390	1.65350
C	5.67800	1.21620	1.21480
C	5.21080	1.81940	0.05780
C	4.16070	1.26060	-0.67830
H	1.29600	-2.31000	-3.41840
H	3.69720	-1.11830	-2.71610
C	0.54020	-3.93590	0.02150
H	-1.97160	-4.91880	-0.07510
H	-3.91710	-4.06900	-1.34070
H	-3.72340	-1.99780	-2.66960
C	-1.56920	-0.38340	-2.99460
C	3.54650	-1.93950	1.39390
H	5.49510	-0.44460	2.55430
H	6.48880	1.67140	1.77670
H	5.66170	2.74620	-0.28330
C	3.70750	1.94400	-1.95310
C	4.70630	1.68260	-3.08540
C	3.52270	3.45100	-1.76940
C	3.70540	-2.20560	2.88680
C	4.19300	-3.05840	0.57240
C	0.87120	-5.31680	-0.54750
C	0.32980	-3.99500	1.53370
C	-1.39220	-0.73950	-4.47300
C	-2.77340	0.53640	-2.80240
H	1.40390	-3.29360	-0.16630
H	-0.68080	0.16670	-2.66730
H	2.46710	-1.95580	1.19200
H	2.73680	1.52400	-2.23660
H	4.34880	2.12650	-4.02080
H	5.67850	2.13080	-2.84990
H	4.87130	0.61490	-3.25780
H	3.04320	3.87700	-2.65700
H	2.89300	3.67700	-0.90510
H	4.48250	3.96340	-1.64040
H	3.17220	-3.12450	3.15130
H	4.75280	-2.34590	3.17560
H	3.28910	-1.38990	3.48720
H	3.78910	-4.03330	0.86710
H	4.01780	-2.93000	-0.50010
H	5.27670	-3.07790	0.73740
H	1.77620	-5.71430	-0.07520
H	0.06030	-6.03120	-0.36760
H	1.04540	-5.27010	-1.62760
H	1.20990	-4.42220	2.02710
H	0.16250	-2.98970	1.93970
H	-0.53360	-4.61770	1.79360
H	-2.26310	-1.28940	-4.84860
H	-1.28250	0.17030	-5.07310
H	-0.50670	-1.36150	-4.63770
H	-2.61320	1.47650	-3.33990
H	-3.69670	0.08810	-3.18550
H	-2.92200	0.77810	-1.74480
Pd	0.64280	-0.35170	1.27940

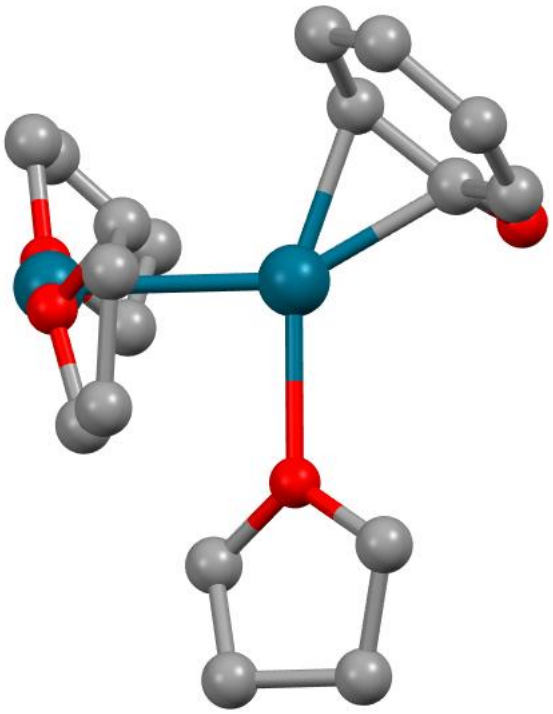
	C -3.21560 0.96120 1.75370 C -2.15940 0.13160 2.14730 C -1.18590 0.52510 3.16750 O -0.06760 -0.01430 3.25940 O -1.56830 1.48280 3.99070 C -0.56720 1.98480 4.88860 H -3.35100 1.88950 2.30220 H -2.41290 2.44210 0.26880 H -2.09510 -0.91150 1.84800 H -1.05000 2.79210 5.43760 H -0.24110 1.20040 5.57470 H 0.28880 2.36410 4.32560 C -4.38820 0.51610 0.98380 C -5.44820 1.41540 0.80230 C -6.58640 1.04160 0.09850 C -6.68660 -0.24260 -0.43480 C -5.63910 -1.14470 -0.25750 C -4.49780 -0.77120 0.44270 I -0.11790 2.83280 -1.14590 H -5.36780 2.41840 1.21440 H -7.39660 1.75310 -0.03400 H -7.57500 -0.53800 -0.98570 H -5.70850 -2.14720 -0.66990 H -3.68880 -1.48520 0.55730 Pd -1.39650 1.32450 0.54060
Xa E = -1259.619098, E+ZPE = -1259.157082, H = -1259.127940, G = -1259.222143	
	C 1.58830 -2.50670 0.60320 C 2.64630 -2.41010 1.68700 C 1.86130 -1.78640 2.83910 C 0.99700 -0.77700 2.10620 O 0.70400 -1.38750 0.83450 H 1.97640 -2.41970 -0.41320 H 0.99650 -3.42630 0.69370 H 3.45250 -1.74130 1.36810 H 3.07700 -3.38460 1.93070 H 2.49660 -1.31230 3.59140 H 1.23840 -2.54020 3.33370 H 1.54340 0.15670 1.93040 H 0.04440 -0.55260 2.59570 O -2.92530 -1.42860 -0.05310 C -2.47280 -2.43470 0.89180 C -2.57750 -3.74640 0.13790 C -2.23900 -3.31500 -1.28690 C -2.96010 -1.98710 -1.39620 H -1.43770 -2.20690 1.16190 H -3.11510 -2.36700 1.77330 H -3.59680 -4.14460 0.18750 H -1.89140 -4.49750 0.53710 H -2.57220 -4.02490 -2.04770 H -1.15880 -3.16460 -1.39550 H -4.01400 -2.11000 -1.67110 H -2.48180 -1.27570 -2.07040 C -0.56070 2.80520 1.30750 C 0.04800 4.01620 0.61950 C -1.15890 4.66340 -0.05690 C -1.92910 3.44700 -0.52450 O -1.75890 2.49020 0.54830 H -0.87890 3.01710 2.33360 H 0.09250 1.93020 1.29990 H 0.77320 3.69560 -0.13590 H 0.55380 4.67540 1.32890 H -0.88520 5.31710 -0.88830 H -1.74920 5.23920 0.66410 H -1.50660 3.02780 -1.44350 H -3.00280 3.60330 -0.65120 C 2.98330 1.06460 -0.28790

	C 4.16260 1.46580 0.33040 C 5.36720 0.81040 0.07360 C 5.36500 -0.25720 -0.82720 C 4.19290 -0.66980 -1.44910 C 2.95960 -0.02330 -1.19280 O 1.87070 -0.45240 -1.79190 H 2.04350 1.57610 -0.08290 H 4.13840 2.30520 1.02260 H 6.28580 1.12440 0.56040 H 6.29280 -0.78200 -1.04600 H 4.19840 -1.50500 -2.14520 Pd 0.09550 -0.07210 -0.85620 H -0.38670 0.82130 -1.98630 Pd -2.34090 0.52950 0.24570
Xb E = -1954.073368, E+ZPE = -1953.275623, H = -1953.227482, G = -1953.359909	
	O 1.12020 3.16000 -0.00560 C 0.63710 3.90970 -1.14830 C -0.18440 5.04570 -0.56560 C 0.49080 5.27650 0.78450 C 0.79430 3.85640 1.21890 H 0.06200 3.23390 -1.78450 H 1.51250 4.27190 -1.69910 H -1.22150 4.72510 -0.41890 H -0.18000 5.92690 -1.21180 H -0.14800 5.79520 1.50330 H 1.41670 5.84930 0.66160 H -0.08030 3.37680 1.67160 H 1.65120 3.76060 1.89070 Pd -1.62390 0.69160 0.38810 C 1.10120 -0.90510 -0.01560 N 0.22310 -1.89450 0.29850 C 0.81670 -3.14550 0.21030 C 2.09340 -2.94390 -0.19200 N 2.24460 -1.57550 -0.32630 C -1.11890 -1.72120 0.77190 C -1.29840 -1.41210 2.14600 C -2.58370 -1.53490 2.68080 C -3.64720 -1.95540 1.89490 C -3.45580 -2.22950 0.54730 C -2.20040 -2.11550 -0.05460 C 3.46320 -0.89070 -0.63360 C 4.28920 -0.49980 0.43210 C 5.44650 0.21700 0.11860 C 5.76240 0.52040 -1.20090 C 4.93100 0.10780 -2.23660 C 3.76180 -0.60970 -1.97560 H 0.27740 -4.04840 0.44840 H 2.90060 -3.63260 -0.38690 C -0.13190 -1.05640 3.04730 H -2.74320 -1.30630 3.73050 H -4.63890 -2.04800 2.32790 H -4.30220 -2.51420 -0.07170 C -2.11710 -2.44880 -1.53730 C 3.94380 -0.80860 1.87540 H 6.10480 0.54400 0.91860 H 6.66600 1.08090 -1.42480 H 5.18980 0.35180 -3.26280 C 2.82810 -1.01360 -3.09750 C 3.56740 -1.63750 -4.27960 C 1.98720 0.18670 -3.54050 C 3.54460 0.46620 2.62140 C 5.08450 -1.53550 2.58760 C 0.15690 -2.19440 4.02780 C -0.36140 0.26850 3.77090 C -1.06400 -1.70060 -2.35240 C -2.01470 -3.96010 -1.76650

	H 0.75160 -0.92330 2.41790 H -3.09270 -2.13430 -1.92820 H 3.07640 -1.47670 1.88080 H 2.14080 -1.76860 -2.70250 H 2.84750 -1.99660 -5.02240 H 4.21990 -0.91440 -4.78060 H 4.18260 -2.48700 -3.96510 H 1.26530 -0.11020 -4.30930 H 1.43360 0.60910 -2.69180 H 2.62490 0.97490 -3.95770 H 3.27110 0.23510 3.65690 H 4.36980 1.18710 2.64240 H 2.68320 0.94400 2.13580 H 4.78060 -1.80770 3.60400 H 5.36370 -2.45320 2.05950 H 5.97820 -0.90730 2.66730 H 1.03570 -1.95630 4.63730 H -0.68760 -2.36040 4.70600 H 0.35540 -3.13370 3.50070 H 0.51520 0.52650 4.37510 H -0.53170 1.07290 3.04580 H -1.22730 0.22500 4.44040 H -0.06410 -2.12550 -2.22700 H -1.31760 -1.77130 -3.41560 H -1.01960 -0.64120 -2.07800 H -2.11490 -4.18470 -2.83410 H -1.04650 -4.34940 -1.43540 H -2.80130 -4.50140 -1.23140 Pd 1.06640 1.02180 -0.02040 H -1.55020 2.12110 -0.10940 O -3.62890 0.90520 0.72370 C -4.49390 0.72200 -0.24250 C -5.87590 0.66350 0.06820 C -4.14110 0.56240 -1.60450 C -6.82990 0.45460 -0.91910 H -6.17100 0.78180 1.10800 C -5.10720 0.35540 -2.58380 H -3.08410 0.59820 -1.86220 C -6.46240 0.29560 -2.25780 H -7.88050 0.41230 -0.63830 H -4.79230 0.23630 -3.61880 H -7.21320 0.13010 -3.02500
TS-XIa E = -1259.576287, E+ZPE = -1259.118309, H = -1259.087894, G = -1259.192401	
	C -0.43850 -3.28090 0.87510 C 0.79060 -3.10460 1.76710 C 0.40030 -1.92690 2.68700 C -0.99550 -1.53410 2.19760 O -1.07190 -2.00100 0.85000 H -0.21270 -3.56230 -0.15580 H -1.13640 -4.01650 1.30230 H 1.66750 -2.84850 1.16590 H 1.01690 -4.01860 2.32220 H 1.10100 -1.09580 2.56530 H 0.38760 -2.20260 3.74470 H -1.18620 -0.45710 2.18100 H -1.77550 -2.03170 2.79310 O -3.26090 0.23370 -0.56340 C -4.11310 -0.30790 0.46600 C -4.96500 -1.33220 -0.25530 C -3.95850 -1.92190 -1.24120 C -3.15690 -0.70470 -1.66950 H -3.49240 -0.77660 1.23640 H -4.67090 0.52500 0.90080 H -5.78920 -0.84200 -0.78450 H -5.38160 -2.07390 0.43060 H -4.42640 -2.42250 -2.09230

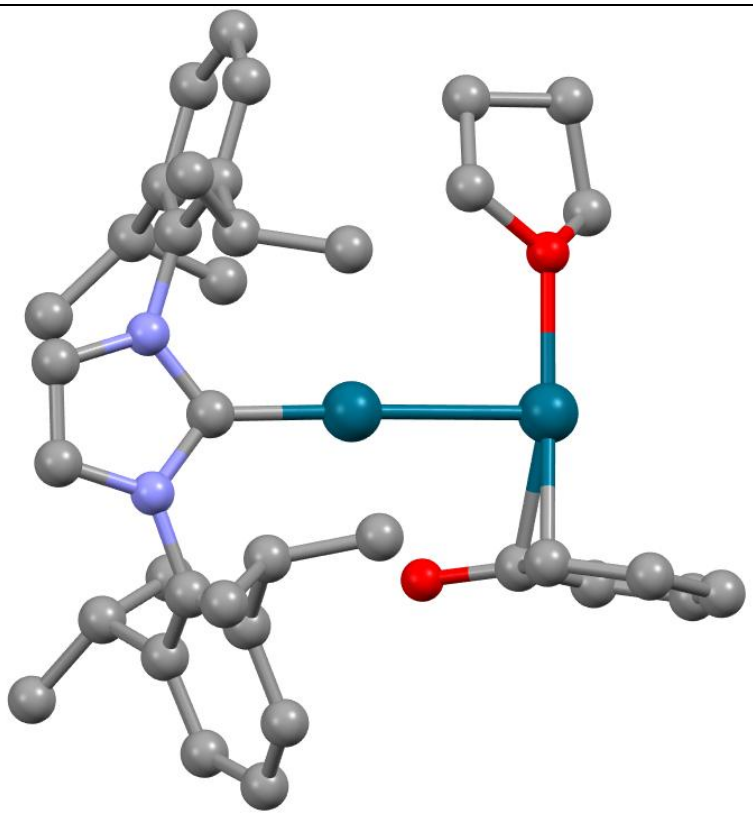
	H -3.30540 -2.63390 -0.72720 H -3.57790 -0.20850 -2.55070 H -2.09590 -0.91500 -1.84020 C 0.74060 2.42450 1.60210 C 2.08880 3.05680 1.27500 C 1.73880 4.10070 0.21480 C 0.64480 3.39300 -0.55500 O -0.11800 2.72650 0.47330 H 0.26650 2.86160 2.48670 H 0.79480 1.33900 1.71910 H 2.76390 2.30710 0.85060 H 2.56260 3.48500 2.16160 H 2.58730 4.36180 -0.42210 H 1.35020 5.01520 0.67580 H 1.04860 2.64300 -1.24470 H -0.04290 4.05060 -1.09120 C 3.17350 -0.51040 0.18150 C 4.39210 -0.46060 0.85240 C 5.57460 -0.80720 0.20050 C 5.51690 -1.19950 -1.13800 C 4.30580 -1.24250 -1.81990 C 3.10690 -0.90470 -1.16600 O 1.95660 -0.98530 -1.84120 H 2.23620 -0.25260 0.67900 H 4.41360 -0.15280 1.89530 H 6.52490 -0.77340 0.72520 H 6.42990 -1.47280 -1.66200 H 4.26340 -1.54370 -2.86300 Pd 0.11220 -0.49400 -0.63660 H 1.17160 0.08330 -1.61090 Pd -1.69080 1.48130 -0.03700
TS-XIb E = -1954.041374, E+ZPE = -1953.246442, H = -1953.197971, G = -1953.333433	
	O 0.33320 2.88580 -0.80930 C 1.39410 3.42540 0.01860 C 2.45430 3.92280 -0.94920 C 1.63530 4.25370 -2.19500 C 0.62390 3.12470 -2.20330 H 1.75280 2.63620 0.68250 H 0.96260 4.23670 0.61580 H 3.17400 3.12610 -1.16520 H 3.00230 4.77890 -0.54820 H 2.23180 4.27570 -3.11030 H 1.13160 5.22010 -2.08220 H 1.04180 2.21060 -2.63990 H -0.32040 3.36280 -2.69990 Pd 1.61840 -0.53360 -0.63070 C -1.37750 -0.62610 0.34680 N -0.88750 -1.86530 0.64300 C -1.89280 -2.72140 1.06990 C -3.04210 -2.00730 1.06320 N -2.70730 -0.73880 0.62250 C 0.44900 -2.32020 0.39580 C 0.74040 -2.81430 -0.90840 C 1.94270 -3.51990 -1.09180 C 2.81420 -3.73770 -0.03440 C 2.52300 -3.22030 1.22510 C 1.34940 -2.50440 1.47800 C -3.63040 0.33010 0.39600 C -4.21350 0.44420 -0.87570 C -5.08070 1.51750 -1.09190 C -5.35400 2.42970 -0.07880 C -4.76990 2.28440 1.17470 C -3.89560 1.22820 1.44070 H -1.69470 -3.74990 1.32730 H -4.05420 -2.27590 1.32310 C -0.28200 -2.75200 -2.03000

	H 2.17170 -3.92030 -2.07490 H 3.73170 -4.29690 -0.19260 H 3.22260 -3.36970 2.04370 C 1.11990 -2.03290 2.90580 C -3.89000 -0.52350 -1.99650 H -5.54210 1.64310 -2.06730 H -6.02960 3.25970 -0.26700 H -4.99130 3.00430 1.95720 C -3.22370 1.09890 2.79220 C -4.20980 1.23850 3.95080 C -2.08100 2.11010 2.91280 C -2.97270 0.14010 -3.02640 C -5.15030 -1.08420 -2.65430 C -0.91830 -4.12690 -2.24450 C 0.31310 -2.20400 -3.32470 C 0.47520 -0.65810 3.07230 C 0.37180 -3.08630 3.72980 H -1.07020 -2.05860 -1.72350 H 2.12910 -1.96020 3.33040 H -3.34250 -1.36820 -1.56600 H -2.78490 0.09760 2.85220 H -3.69960 1.04800 4.90090 H -4.63490 2.24640 4.00510 H -5.03720 0.52690 3.86130 H -1.55740 1.99000 3.86780 H -1.35320 1.97120 2.10090 H -2.46110 3.13690 2.85850 H -2.71060 -0.56810 -3.82040 H -3.46410 1.00270 -3.49130 H -2.04530 0.48640 -2.55230 H -4.87970 -1.83760 -3.40180 H -5.80880 -1.55760 -1.91850 H -5.72300 -0.30400 -3.16720 H -1.69890 -4.06960 -3.01120 H -0.17330 -4.85930 -2.57560 H -1.37600 -4.50380 -1.32400 H -0.46260 -2.12950 -4.09440 H 0.73330 -1.20480 -3.15750 H 1.10840 -2.84730 -3.71720 H -0.60510 -0.68810 2.91030 H 0.64500 -0.30110 4.09410 H 0.89340 0.07350 2.37360 H 0.35990 -2.79760 4.78660 H -0.66780 -3.18190 3.40130 H 0.84780 -4.06910 3.65170 Pd -0.58940 1.03980 -0.22650 H 2.39830 0.66490 -1.18960 O 3.73920 0.09610 -1.29840 C 4.47830 0.64930 -0.34290 C 5.74470 1.18010 -0.66500 C 4.05240 0.73830 0.99800 C 6.54240 1.76050 0.31480 H 6.08350 1.12180 -1.69610 C 4.85330 1.33250 1.96770 H 3.07180 0.32870 1.24680 C 6.10680 1.84780 1.63830 H 7.51690 2.15710 0.03830 H 4.49320 1.38930 2.99270 H 6.73300 2.30790 2.39720
XIIa E = -1259.619943, E+ZPE = -1259.155909, H = -1259.125955, G = -1259.222687	

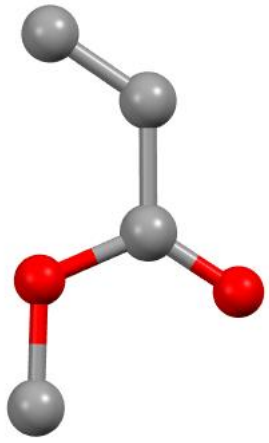


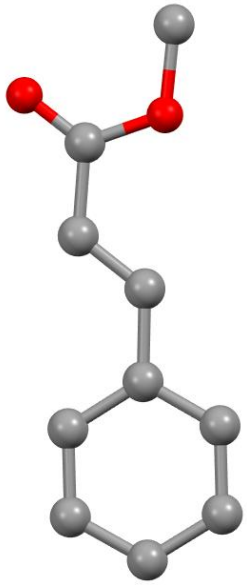
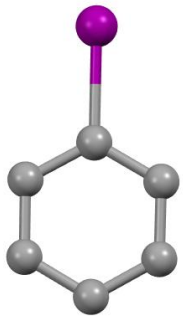
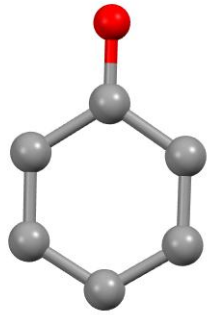
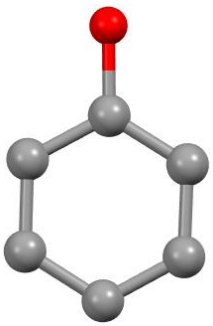
Pd	0.00500	0.79490	-0.45970
Pd	-0.74120	-1.30830	1.13160
O	1.21960	-1.43780	1.87080
C	2.21040	-2.02790	1.00820
C	3.55950	-1.72900	1.67490
C	3.22930	-0.65720	2.73300
C	1.81880	-0.22760	2.36790
H	2.13080	-1.55680	0.02350
H	1.97120	-3.09010	0.92600
H	4.27360	-1.36010	0.93410
H	3.98720	-2.62190	2.13670
H	3.92350	0.18650	2.71420
H	3.24390	-1.08900	3.73780
H	1.80430	0.52840	1.57100
H	1.20860	0.12040	3.20300
C	-3.65530	-0.38900	1.18460
C	-4.88280	-0.34810	0.29870
C	-4.25210	-0.16660	-1.08200
C	-2.95560	-0.96830	-0.98830
O	-2.71300	-1.16620	0.42600
H	-3.24830	0.61490	1.35960
H	-3.79390	-0.89390	2.14300
H	-5.56410	0.46250	0.56860
H	-5.42460	-1.29780	0.36050
H	-4.02840	0.89180	-1.25330
H	-4.89130	-0.51500	-1.89670
H	-2.09880	-0.43330	-1.41540
H	-3.02910	-1.96310	-1.43870
O	0.99660	-0.69150	-1.87460
C	2.19950	-0.39540	-2.60090
C	2.38600	-1.54960	-3.57620
C	1.68630	-2.70040	-2.85380
C	0.50180	-1.98980	-2.22650
H	2.08250	0.57680	-3.08940
H	3.02610	-0.32710	-1.88230
H	3.44000	-1.74520	-3.78860
H	1.87850	-1.33470	-4.52290
H	2.33560	-3.11720	-2.07550
H	1.38250	-3.51090	-3.52130
H	0.11870	-2.45220	-1.30950
H	-0.32530	-1.88060	-2.94160
H	-1.35190	2.58570	-2.13050
C	-0.68370	2.60560	0.32870
C	-0.04970	2.87130	1.58140
C	1.25680	3.30770	1.64780
C	1.99270	3.51200	0.45800
C	1.41330	3.30060	-0.77670
C	0.06240	2.85680	-0.88490
O	-0.56560	3.14250	-2.08390
H	-1.77450	2.61160	0.29420
H	-0.63410	2.75070	2.49080
H	1.72050	3.50080	2.61130
H	3.02420	3.85050	0.51210
H	1.95350	3.51590	-1.69550

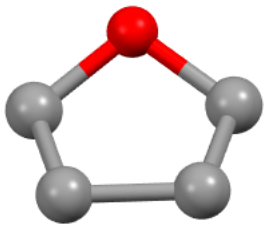
XIIb E = -1954.073431, E+ZPE = -1953.272692, H = -1953.224590, G = -1953.357763

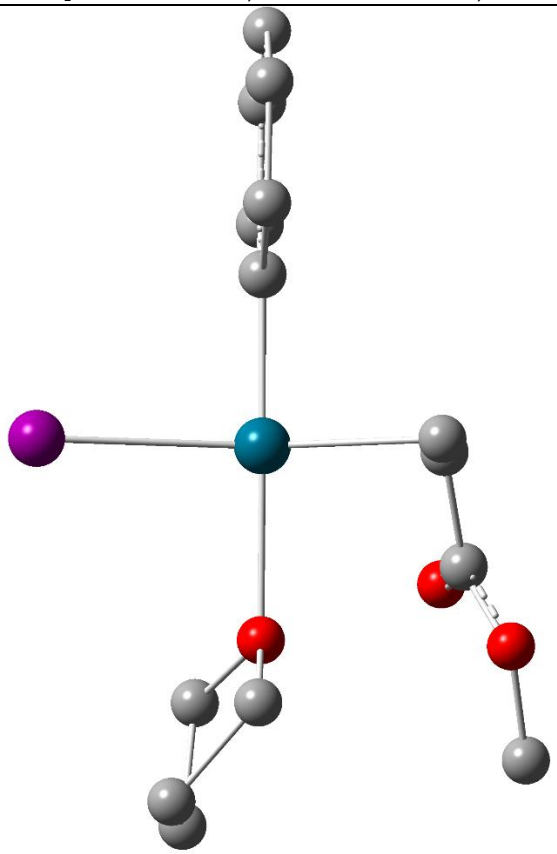


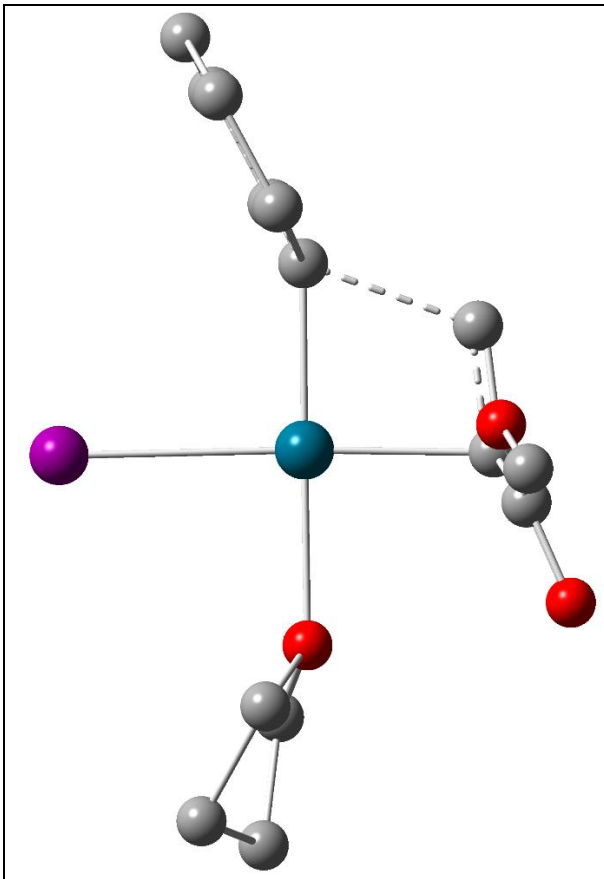
Pd	0.15530	-0.09400	0.08690
C	-1.50360	0.91500	-0.09300
N	-1.64870	2.27240	-0.16130
C	-2.98000	2.65550	-0.11930
C	-3.70630	1.51550	-0.05500
N	-2.79530	0.47040	-0.04970
C	-0.55220	3.18930	-0.13940
C	-0.11070	3.63510	1.11910
C	0.94350	4.54970	1.16210
C	1.52940	5.01320	-0.00870
C	1.08120	4.54800	-1.23840
C	0.03890	3.61990	-1.33970
C	-3.13400	-0.91320	0.05230
C	-3.08660	-1.52470	1.31350
C	-3.36420	-2.89270	1.37840
C	-3.68580	-3.61120	0.23370
C	-3.75470	-2.97210	-0.99990
C	-3.48450	-1.60730	-1.11710
H	-3.28060	3.69110	-0.15200
H	-4.77170	1.34850	-0.01560
C	-0.70450	3.10810	2.41050
H	1.30720	4.90180	2.12350
H	2.34070	5.73480	0.03600
H	1.55180	4.90190	-2.15270
C	-0.27370	3.10080	-2.73540
C	-2.77080	-0.75240	2.57880
H	-3.32840	-3.39800	2.33980
H	-3.89330	-4.67560	0.30280
H	-4.01720	-3.54420	-1.88450
C	-3.51480	-0.91410	-2.46560
C	-4.64620	-1.40830	-3.36410
C	-2.16030	-1.05220	-3.16540
C	-1.48690	-1.25730	3.23640
C	-3.95080	-0.79360	3.55130
C	-1.15820	4.23290	3.34010
C	0.29150	2.17500	3.10250
C	0.61530	1.88890	-3.04070
C	-1.73350	2.80020	-3.06940
H	-1.58750	2.51260	2.16120
H	0.03870	3.90830	-3.41040
H	-2.60300	0.29290	2.30180
H	-3.68350	0.15340	-2.28570
H	-4.69810	-0.79210	-4.26790
H	-4.48960	-2.44300	-3.68700
H	-5.61680	-1.35320	-2.86000
H	-2.16420	-0.51460	-4.12050
H	-1.35440	-0.64600	-2.54540
H	-1.93410	-2.10510	-3.36590
H	-1.28000	-0.69500	4.15370
H	-1.56060	-2.31790	3.50280
H	-0.63850	-1.12480	2.55320
H	-3.73740	-0.18030	4.43370
H	-4.86520	-0.41130	3.08520
H	-4.15080	-1.81430	3.89590
H	-1.64520	3.81410	4.22730
H	-0.31570	4.84200	3.68510
H	-1.87300	4.89740	2.84340
H	-0.14330	1.76090	4.01900
H	0.55740	1.34110	2.43950
H	1.20920	2.70880	3.37550
H	0.42380	1.07630	-2.32630
H	0.42290	1.51740	-4.05380
H	1.67650	2.15020	-2.96870
H	-1.82780	2.66870	-4.15300
H	-2.08640	1.88110	-2.59770
H	-2.39830	3.61790	-2.77440

	H -0.11270 -1.93340 -1.03020 Pd 2.46210 -1.56710 0.23060 C 1.17020 -3.15980 0.79110 C 2.04540 -3.97220 1.56710 C 2.98100 -4.79190 0.96470 C 3.08370 -4.81440 -0.44120 C 2.25630 -4.03750 -1.22890 C 1.26820 -3.20170 -0.63540 O 0.29220 -2.73420 -1.45670 H 0.27890 -2.73580 1.24930 H 1.92700 -3.97270 2.64750 H 3.62920 -5.42040 1.56800 H 3.81830 -5.45860 -0.91690 H 2.30030 -4.08310 -2.31310 O 3.67110 0.20610 0.11130 C 3.14780 1.54770 0.29880 C 4.03690 2.45390 -0.54430 C 5.31640 1.63530 -0.70740 C 4.75890 0.23260 -0.82850 H 3.21290 1.76770 1.36900 H 2.09310 1.55750 -0.00450 H 4.19980 3.42170 -0.06480 H 3.57630 2.63240 -1.52130 H 5.94870 1.71530 0.18360 H 5.90480 1.92500 -1.58160 H 5.45460 -0.56260 -0.54900 H 4.37460 0.03760 -1.83830
CH2CHCOOMe E = -306.137805, E+ZPE = -306.041619, H = -306.034055, G = -306.072107	
	C -2.17530 0.72330 0.00000 C -1.47580 -0.41120 0.00000 C 0.00000 -0.48060 0.00000 O 0.61920 -1.52550 0.00000 O 0.58490 0.72470 0.00000 C 2.01210 0.70710 0.00000 H -3.26150 0.70990 0.00000 H -1.68640 1.69290 0.00000 H -1.96290 -1.38210 0.00000 H 2.32230 1.75200 0.00000 H 2.39490 0.20130 0.89030 H 2.39490 0.20130 -0.89030
I- E = -297.892567, E+ZPE = -297.892567, H = -297.890206, G = -297.909415	
	I 0.00000 0.00000 0.00000
PhCHCHCOOMe E = -536.955220, E+ZPE = -536.776659, H = -536.764671, G = -536.814832	

	C -0.16600 -0.26060 -0.00020 C -1.06600 0.73720 -0.00020 C -2.51930 0.52630 -0.00040 O -3.32810 1.43470 0.00030 O -2.87250 -0.76970 0.00020 C -4.27760 -1.01440 0.00020 C 1.28750 -0.12850 -0.00010 H -0.53910 -1.28290 -0.00040 H -0.77680 1.78350 -0.00010 H -4.39110 -2.09870 0.00070 H -4.74780 -0.58720 0.89000 H -4.74760 -0.58810 -0.89020 C 2.06110 -1.29850 -0.00020 C 3.45000 -1.23710 -0.00000 C 4.09010 -0.00080 0.00010 C 3.33310 1.17200 0.00020 C 1.94690 1.11170 0.00000 H 1.55860 -2.26250 -0.00030 H 4.03230 -2.15390 -0.00010 H 5.17500 0.05220 0.00020 H 3.82950 2.13820 0.00030 H 1.37290 2.03340 0.00010
PhI E = -529.113161, E+ZPE = -529.022277, H = -529.015494, G = -529.053963	
	C 0.00010 3.32600 0.00000 C 1.20520 2.62790 0.00000 C 1.21420 1.23490 0.00000 C 0.00000 0.55080 0.00000 C -1.21420 1.23490 0.00000 C -1.20510 2.62790 0.00000 I -0.00000 -1.54230 0.00000 H -0.00000 4.41240 0.00000 H 2.14930 3.16590 0.00000 H 2.15350 0.69090 0.00000 H -2.15350 0.69100 0.00000 H -2.14910 3.16600 0.00000
PhO- E = -306.628058, E+ZPE = -306.536335, H = -306.530150, G = -306.565199	
	C 1.20840 -0.28720 -0.00000 C 1.19810 1.09930 0.00000 C -0.00000 -1.07980 -0.00000 C -0.00000 1.82510 0.00000 C -1.19810 1.09930 0.00000 C -1.20840 -0.28720 -0.00000 O 0.00000 -2.34300 -0.00000 H 2.15480 -0.82770 -0.00000 H 2.14780 1.63600 0.00000 H 0.00000 2.91180 0.00000 H -2.14780 1.63600 0.00000 H -2.15480 -0.82770 -0.00000
PhOH E = -307.143253, E+ZPE = -307.037512, H = -307.031116, G = -307.066447	
	C 1.21550 0.25350 -0.00000 C 1.21880 -1.13640 0.00000 C -0.00000 0.94250 -0.00000 C 0.02200 -1.85240 0.00000 C -1.18520 -1.15840 0.00000 C -1.20360 0.23370 -0.00000 O 0.04790 2.29690 -0.00000 H -0.85400 2.64220 -0.00000 H 2.14220 0.81940 -0.00000 H 2.16830 -1.66470 0.00000 H 0.03130 -2.93800 0.00000 H -2.12660 -1.70100 0.00000 H -2.14950 0.77170 -0.00000
THF E = -232.201383, E+ZPE = -232.083745, H = -232.078769, G = -232.110652	

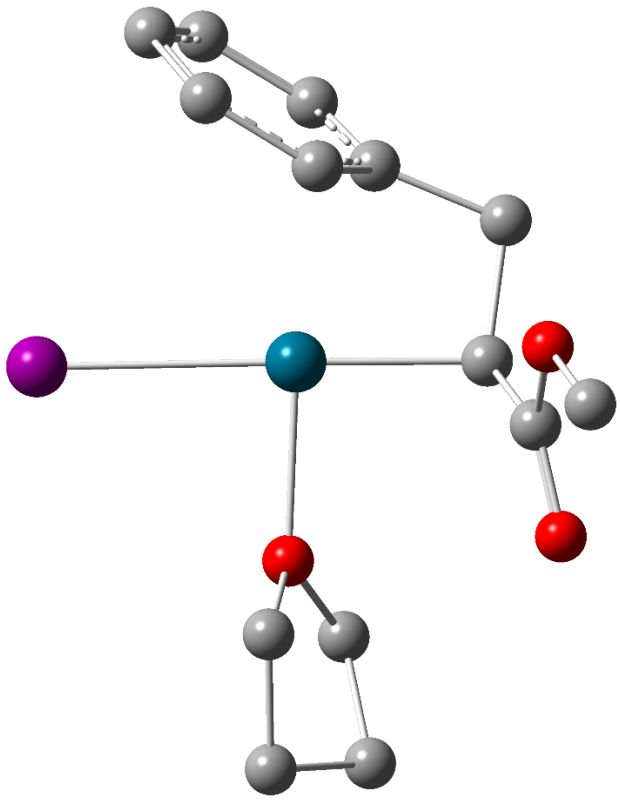


	O -0.00150 -1.19750 -0.30260 C -1.12280 -0.46580 0.15900 C -0.76990 1.01210 -0.04930 C 0.77390 1.00840 -0.05420 C 1.12040 -0.46910 0.16270 H -1.29780 -0.67260 1.22810 H -2.00090 -0.79710 -0.40260 H -1.18980 1.64120 0.74010 H -1.15990 1.37250 -1.00520 H 1.20250 1.64220 0.72680 H 1.15910 1.35820 -1.01600 H 1.28830 -0.67200 1.23380 H 2.00040 -0.80630 -0.39240
IVa-Pd$_1$ E = -1195.469187, E+ZPE = -1195.159353, H = -1195.136761, G = -1195.213649	
	O -1.93290 -0.33670 -0.11270 C -2.53590 -0.93800 -1.27990 C -3.40920 -2.06020 -0.74650 C -3.79990 -1.53820 0.63450 C -2.51100 -0.88570 1.09260 H -1.73750 -1.28350 -1.94200 H -3.12030 -0.16180 -1.78700 H -2.82300 -2.98010 -0.65030 H -4.26530 -2.25840 -1.39590 H -4.12380 -2.32630 1.31840 H -4.60150 -0.79550 0.55360 H -1.81410 -1.61920 1.51310 H -2.64150 -0.06120 1.79730 Pd 0.21170 0.22810 -0.15200 C 4.76460 1.57620 0.13570 C 4.28100 1.05810 -1.06370 C 2.95230 0.64460 -1.17000 C 2.10260 0.75320 -0.06840 C 2.58310 1.26960 1.13600 C 3.91420 1.67920 1.23400 I 0.94300 -2.27030 0.20320 H 5.80000 1.89560 0.21470 H 4.93920 0.96750 -1.92420 H 2.59010 0.22940 -2.10660 H 1.93030 1.35000 2.00190 H 4.28260 2.07840 2.17560 C -0.15750 1.91110 -1.46930 C -0.39710 2.33130 -0.17470 C -1.76080 2.42200 0.41560 O -1.96820 2.50870 1.60870 O -2.71810 2.43460 -0.51370 C -4.05580 2.44670 -0.01460 H 0.79350 2.11940 -1.94950 H -0.98190 1.61640 -2.11360 H 0.37250 2.83920 0.40050 H -4.70020 2.44070 -0.89360 H -4.24820 1.56360 0.59970 H -4.23840 3.34520 0.58030
TS-Va-Pd$_1$ E = -1195.444861, E+ZPE = -1195.135766, H = -1195.113450, G = -1195.192238	



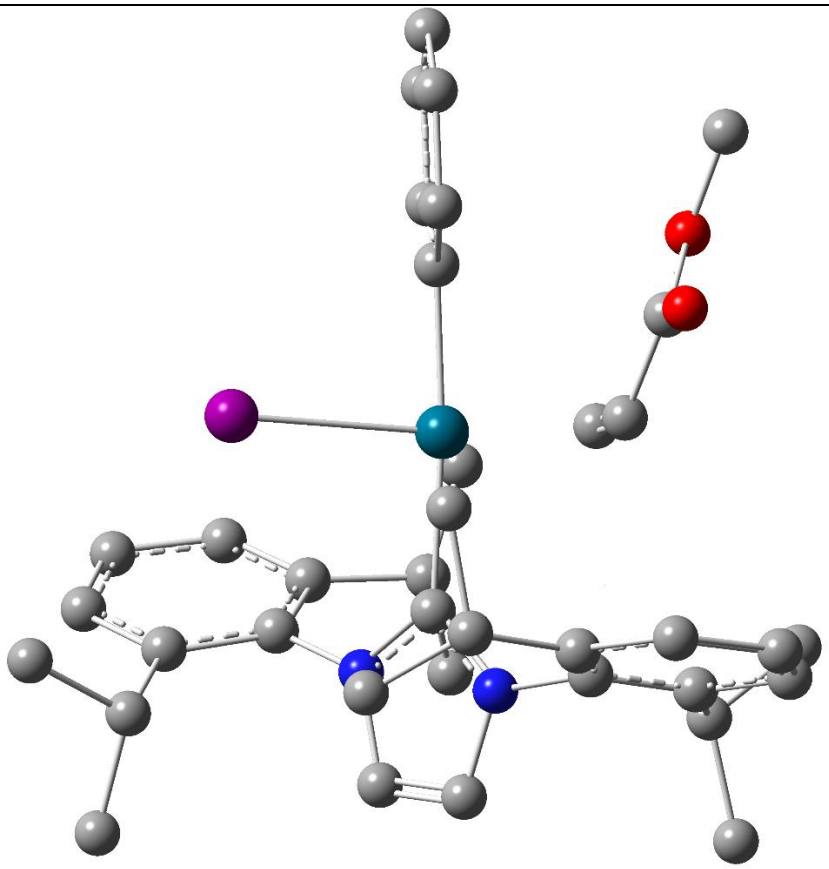
O	-2.11310	0.33560	-0.39230
C	-2.79730	0.44370	0.88170
C	-3.76920	1.60060	0.71560
C	-4.01950	1.61610	-0.79160
C	-2.64170	1.29410	-1.33170
H	-2.05130	0.61370	1.66220
H	-3.30140	-0.51190	1.05400
H	-3.29580	2.53720	1.02770
H	-4.67850	1.45650	1.30370
H	-4.38770	2.57810	-1.15610
H	-4.73320	0.83540	-1.07540
H	-1.99280	2.17750	-1.34470
H	-2.63690	0.82140	-2.31710
Pd	-0.03520	-0.18970	-0.43850
C	4.62250	-0.31610	0.20980
C	3.77260	-0.92730	1.13190
C	2.43740	-1.14940	0.81210
C	1.93720	-0.73210	-0.42890
C	2.79740	-0.14190	-1.36270
C	4.13400	0.07060	-1.03730
I	0.58810	2.23800	0.55550
H	5.66650	-0.15020	0.45970
H	4.15180	-1.23770	2.10170
H	1.77920	-1.64250	1.52210
H	2.41960	0.16120	-2.33530
H	4.79430	0.54140	-1.76040
C	0.81850	-2.18470	-1.32060
C	-0.58580	-2.03760	-1.21450
C	-1.37090	-2.73070	-0.16760
O	-2.56820	-2.91990	-0.23210
O	-0.61300	-3.12470	0.86830
C	-1.31720	-3.77600	1.92640
H	1.25920	-2.05000	-2.30260
H	1.30540	-2.92280	-0.69470
H	-1.16270	-1.78180	-2.10080
H	-0.56220	-4.04000	2.66680
H	-2.05720	-3.10330	2.36790
H	-1.82020	-4.67510	1.56180

VIa-Pd_1 E = -1195.484739, E+ZPE = -1195.172860, H = -1195.150671, G = -1195.227714

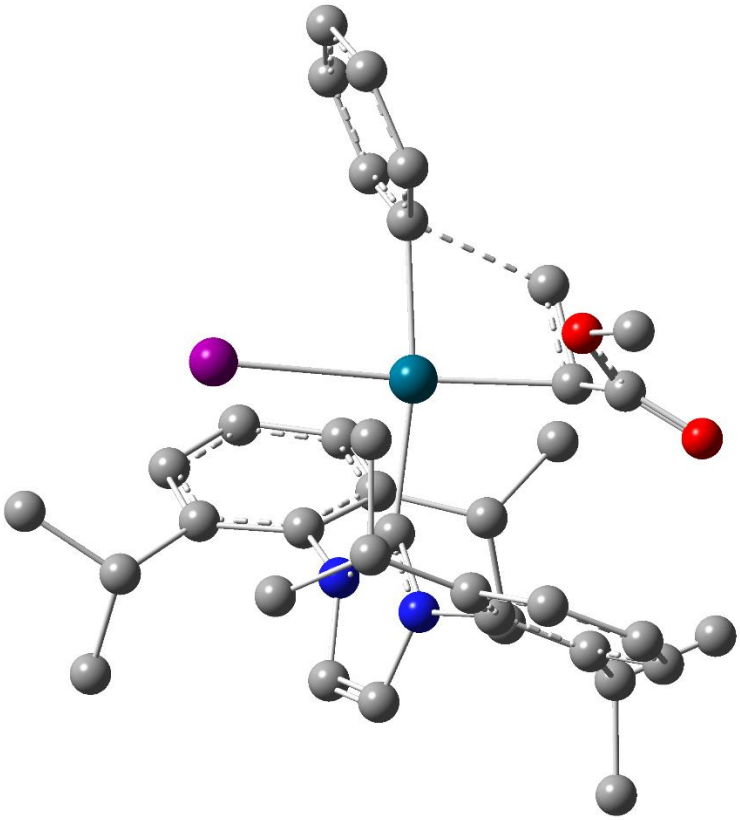


O	1.46560	-1.34500	-0.36190
C	2.13220	-1.71860	0.86340
C	3.13710	-2.76460	0.42720
C	3.56360	-2.23570	-0.94110
C	2.26010	-1.70710	-1.51390
H	1.36270	-2.08250	1.54820
H	2.62320	-0.83360	1.28160
H	2.65160	-3.74160	0.33210
H	3.96770	-2.85210	1.13160
H	4.00870	-3.00090	-1.58160
H	4.27630	-1.41450	-0.82150
H	1.70060	-2.46950	-2.06630
H	2.39280	-0.82790	-2.14690
Pd	-0.04000	0.14540	-0.28590
C	-3.59030	1.42630	0.40850
C	-2.50840	1.64120	1.24030
C	-1.25180	1.95610	0.69230
C	-1.09800	2.08100	-0.71160
C	-2.21140	1.79740	-1.54210
C	-3.43640	1.48730	-0.98660
I	-1.77320	-1.87830	0.42410
H	-4.56290	1.19420	0.83190
H	-2.62020	1.58000	2.31810
H	-0.43810	2.26530	1.34340
H	-2.09550	1.87670	-2.61950
H	-4.28900	1.29620	-1.63130
C	0.19540	2.65530	-1.27040
C	1.22150	1.57390	-1.00200
C	2.27410	1.78320	0.01460
O	3.34780	1.20750	0.02490
O	1.92270	2.67580	0.95910
C	2.88460	2.88490	1.99270
H	0.08710	2.83050	-2.34330
H	0.43580	3.60630	-0.78690
H	1.64900	1.11740	-1.89580
H	2.45260	3.63740	2.65270
H	3.06710	1.95990	2.54620
H	3.82890	3.24510	1.57660

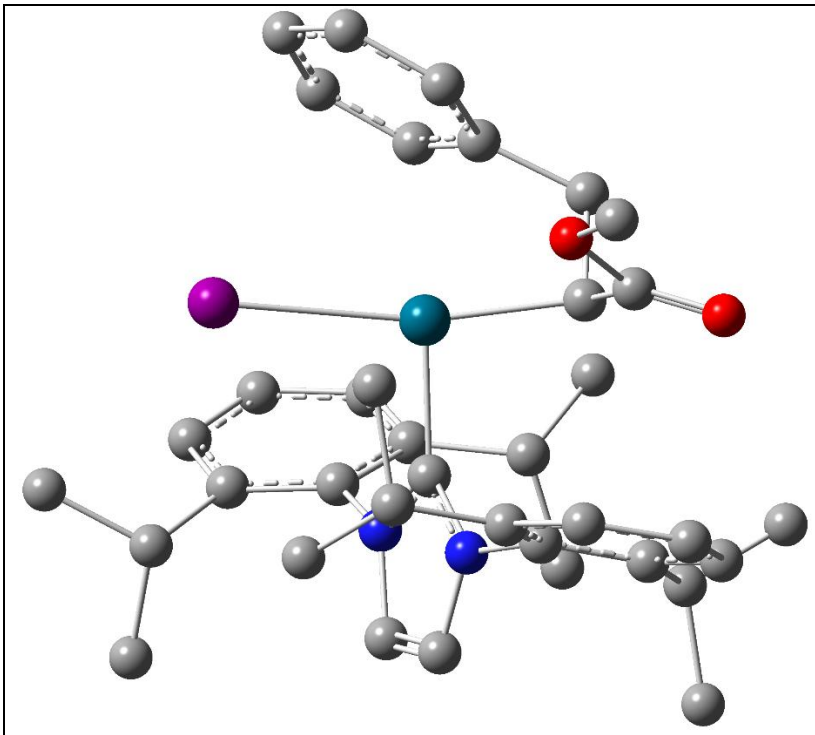
IVb-Pd_1 E = -2122.100255, E+ZPE = -2121.333223, H = -2121.285876, G = -2121.413946



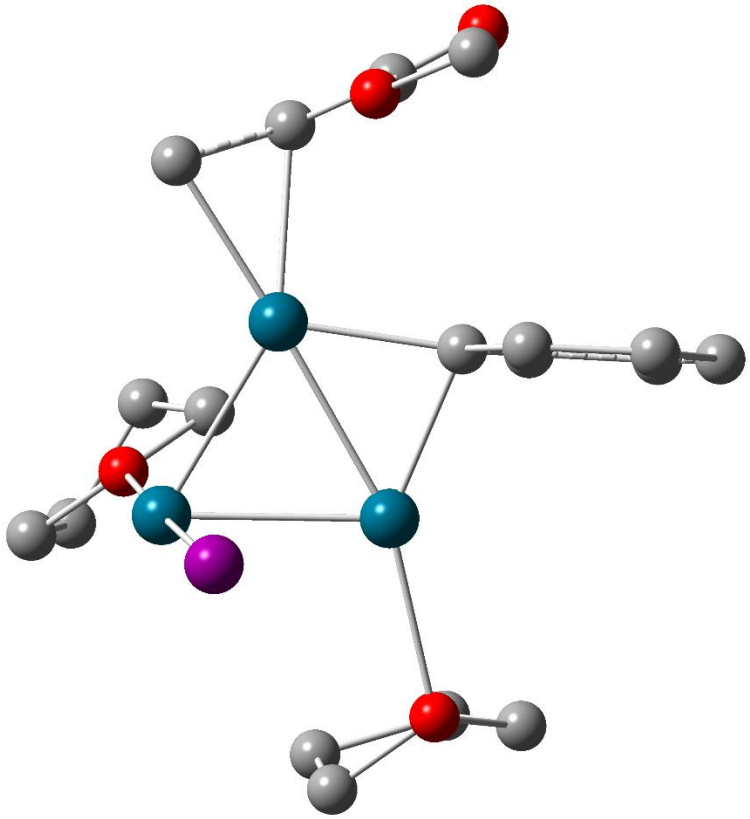
Pd	0.54840	-0.69980	0.07770
C	2.88690	-4.91780	0.40530
C	3.01570	-4.14680	-0.74890
C	2.34770	-2.92670	-0.85940
C	1.54500	-2.45320	0.18370
C	1.41410	-3.23880	1.33270
C	2.08130	-4.45990	1.44520
I	-1.10230	-2.08540	-1.45080
H	3.40480	-5.86960	0.49020
H	3.63340	-4.49710	-1.57280
H	2.45480	-2.34430	-1.77110
H	0.78250	-2.90680	2.15400
H	1.96430	-5.05570	2.34770
C	-0.68310	1.07740	-0.02920
N	-0.35750	2.33390	-0.44370
C	-1.43000	3.20370	-0.36230
C	-2.46470	2.48870	0.12390
N	-2.00260	1.19750	0.30770
C	0.93870	2.82460	-0.81340
C	1.63750	3.56470	0.16520
C	2.88640	4.08380	-0.17340
C	3.42500	3.87520	-1.43730
C	2.70900	3.15860	-2.38300
C	1.44330	2.62420	-2.10750
C	-2.86830	0.17410	0.82330
C	-2.68160	-0.26330	2.14420
C	-3.53340	-1.25970	2.62710
C	-4.55390	-1.77120	1.83700
C	-4.75690	-1.27510	0.55550
C	-3.92510	-0.29130	0.01750
H	-1.35200	4.23500	-0.66590
H	-3.47520	2.77240	0.36670
C	1.08120	3.80550	1.55760
H	3.44580	4.65250	0.56300
H	4.40180	4.27980	-1.68710
H	3.12670	3.00860	-3.37540
C	0.79270	1.85540	-3.24870
C	-1.68160	0.38990	3.07510
H	-3.40640	-1.62300	3.64230
H	-5.20660	-2.54680	2.22790
H	-5.57360	-1.66390	-0.04480
C	-4.22510	0.26570	-1.36310
C	-5.37600	1.27760	-1.29110
C	-4.58320	-0.81250	-2.38630
C	-0.91890	-0.61590	3.93260
C	-2.39020	1.43110	3.94660
C	0.52140	5.22580	1.68350
C	2.12130	3.56260	2.65340
C	1.40600	0.45470	-3.33890
C	-0.73200	1.78820	-3.29370
H	0.25780	3.10160	1.72140
H	1.10450	2.39870	-4.15070
H	-0.95430	0.92480	2.46100
H	-3.32860	0.78130	-1.72370
H	-5.56130	1.71180	-2.27960
H	-6.29700	0.78230	-0.96350
H	-5.17940	2.09780	-0.59560
H	-4.66370	-0.36080	-3.38070
H	-3.82380	-1.59650	-2.42910
H	-5.54910	-1.27800	-2.16230
H	-0.12770	-0.10930	4.49540
H	-1.57240	-1.10660	4.66130
H	-0.45840	-1.39400	3.31660
H	-1.67030	1.94030	4.59720
H	-2.88970	2.18940	3.33450
H	-3.14750	0.95900	4.58260

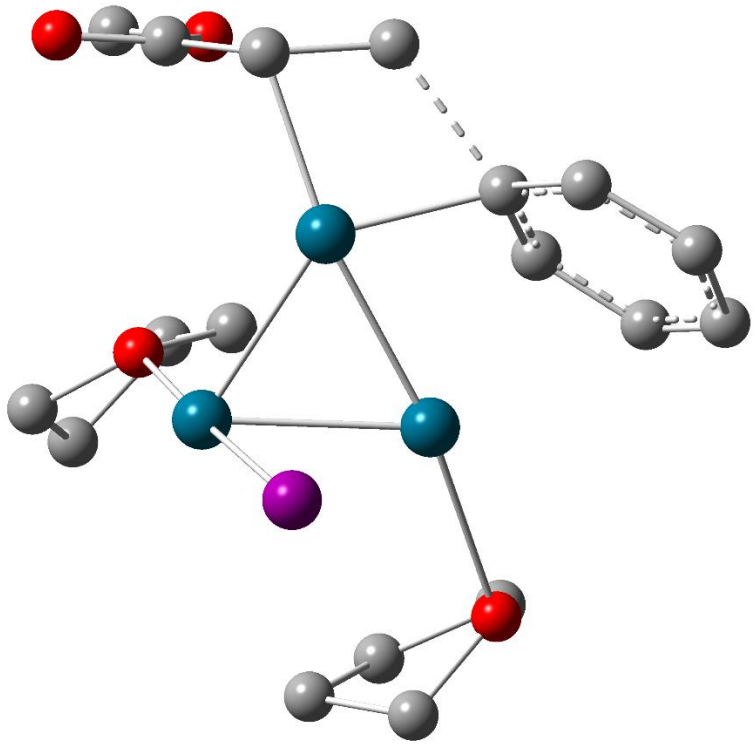
	H 0.09780 5.38080 2.68180 H 1.31650 5.96510 1.53590 H -0.26300 5.42740 0.94890 H 1.63750 3.59010 3.63560 H 2.61440 2.59290 2.54350 H 2.89640 4.33600 2.65240 H 1.18680 -0.12070 -2.43340 H 0.98780 -0.09300 -4.19040 H 2.49290 0.50110 -3.45720 H -1.03630 1.42820 -4.28210 H -1.13940 1.08880 -2.56000 H -1.19300 2.76870 -3.14080 C 1.64700 0.07490 1.79840 C 2.43650 0.28570 0.68640 C 3.68350 -0.46660 0.38330 O 4.31650 -0.30980 -0.64020 O 4.07200 -1.25110 1.38910 C 5.25020 -2.01840 1.14450 H 1.01200 0.86830 2.17310 H 1.85930 -0.75000 2.47120 H 2.37840 1.21630 0.13430 H 5.35520 -2.68180 2.00280 H 5.14370 -2.60160 0.22790 H 6.12330 -1.36490 1.06250
TS-Vb-Pd$_1$ E = -2122.086258, E+ZPE = -2121.318628, H = -2121.272453, G = -2121.395881	
	Pd 0.23000 0.89510 0.44300 C 2.85960 4.87360 1.17850 C 1.61880 4.97090 0.54760 C 0.74980 3.88310 0.53280 C 1.13040 2.67290 1.12230 C 2.36360 2.58410 1.77400 C 3.22600 3.67930 1.79560 I 2.03850 1.10990 -1.55410 H 3.53310 5.72600 1.19380 H 1.32350 5.90080 0.06760 H -0.22260 3.96680 0.05590 H 2.66330 1.65120 2.24570 H 4.18900 3.59420 2.29280 C -0.30650 -0.95480 -0.30840 N -1.39410 -1.40960 -0.98580 C -1.20910 -2.71260 -1.42190 C 0.00650 -3.10100 -0.98680 N 0.54830 -2.02290 -0.30770 C -2.71210 -0.83430 -1.04270 C -3.64310 -1.33580 -0.10870 C -4.96410 -0.89960 -0.19970 C -5.35050 0.00430 -1.17880 C -4.41620 0.47520 -2.09040 C -3.07890 0.06090 -2.06060 C 1.79300 -2.09190 0.40700 C 1.74650 -2.04890 1.81480 C 2.95920 -2.04430 2.50590 C 4.16950 -2.13010 1.82800 C 4.18270 -2.26750 0.44780 C 2.99920 -2.26020 -0.29680 H -1.96320 -3.23040 -1.99220 H 0.52760 -4.03810 -1.08610 C -3.27120 -2.35580 0.95410 H -5.69610 -1.27200 0.51030 H -6.38360 0.33530 -1.23920 H -4.72350 1.16900 -2.86920 C -2.17210 0.64760 -3.12950 C 0.43600 -2.15460 2.57140 H 2.95600 -1.99480 3.58980 H 5.10390 -2.12040 2.38210 H 5.13040 -2.37950 -0.06910

	C 3.06440 -2.53150 -1.78840 C 3.20260 -4.04110 -2.03090 C 4.21770 -1.81530 -2.49170 C 0.47050 -1.53060 3.96240 C 0.01590 -3.62650 2.65690 C -3.78400 -3.74830 0.57430 C -3.78850 -1.97650 2.34280 C -1.60670 1.98850 -2.65300 C -1.08250 -0.26500 -3.68810 H -2.18000 -2.40650 1.01400 H -2.84540 0.86790 -3.96830 H -0.32870 -1.63130 1.99430 H 2.12930 -2.18350 -2.23980 H 3.16440 -4.26020 -3.10340 H 4.16550 -4.39830 -1.64840 H 2.42250 -4.62700 -1.53630 H 4.11910 -1.93890 -3.57530 H 4.22470 -0.74560 -2.27070 H 5.18800 -2.23480 -2.20520 H -0.54180 -1.49620 4.37790 H 1.08440 -2.11420 4.65710 H 0.86550 -0.51030 3.94120 H -0.94140 -3.72170 3.18140 H -0.09670 -4.07330 1.66420 H 0.76310 -4.20970 3.20720 H -3.47990 -4.48370 1.32740 H -4.87870 -3.75330 0.52200 H -3.40100 -4.07990 -0.39460 H -3.35580 -2.64540 3.09500 H -3.54450 -0.94270 2.59600 H -4.87740 -2.08160 2.40540 H -1.01190 1.86430 -1.74320 H -0.96050 2.42800 -3.42060 H -2.41370 2.69590 -2.43610 H -0.67130 0.19050 -4.59520 H -0.25130 -0.40210 -2.99450 H -1.47940 -1.24870 -3.95970 C -0.34650 1.84880 2.39300 C -1.33870 0.98620 1.85860 C -2.59820 1.62220 1.40050 O -3.70560 1.26070 1.73920 O -2.38140 2.70550 0.64100 C -3.55210 3.42060 0.24740 H 0.32770 1.45390 3.14670 H -0.59580 2.89530 2.51450 H -1.47530 0.00580 2.30060 H -3.20140 4.25300 -0.36240 H -4.21810 2.77760 -0.33240 H -4.08710 3.79740 1.12350
VIb-Pd_1 E = -2122.136719, E+ZPE = -2121.365996, H = -2121.319846, G = -2121.443610	

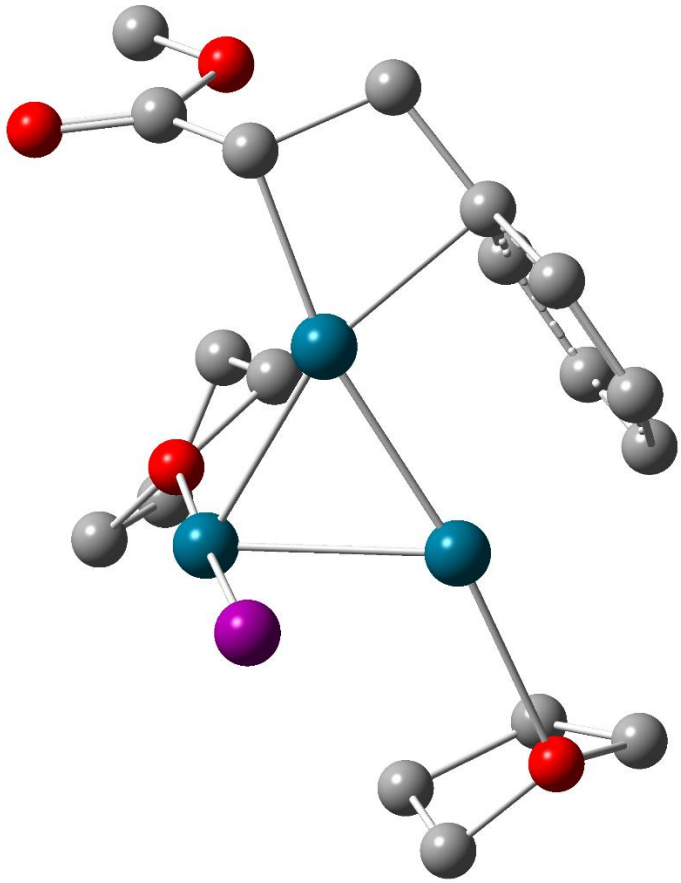


Pd	0.13370	-0.86920	-0.33600
C	2.90200	-3.75830	-1.40050
C	1.62130	-4.25020	-1.17490
C	0.50790	-3.54120	-1.62500
C	0.66290	-2.32920	-2.31970
C	1.96710	-1.83650	-2.51750
C	3.07340	-2.54480	-2.06790
I	1.94350	-1.59440	1.55990
H	3.76770	-4.31230	-1.04930
H	1.48180	-5.18830	-0.64580
H	-0.48990	-3.93650	-1.46540
H	2.10230	-0.89600	-3.04450
H	4.07070	-2.14810	-2.23380
C	-0.27150	0.91850	0.38660
N	-1.35570	1.40950	1.04070
C	-1.11250	2.68950	1.51350
C	0.13660	3.01970	1.12830
N	0.64300	1.93190	0.43580
C	-2.68900	0.87270	1.08250
C	-3.59350	1.38840	0.13040
C	-4.92400	0.97950	0.20330
C	-5.34360	0.09130	1.18400
C	-4.43430	-0.39130	2.11380
C	-3.08740	-0.00670	2.10140
C	1.91140	1.95390	-0.24160
C	1.90660	2.06110	-1.64710
C	3.13970	2.04500	-2.30000
C	4.32890	1.96130	-1.58480
C	4.30610	1.93160	-0.19850
C	3.10000	1.93800	0.50910
H	-1.85380	3.23220	2.07720
H	0.70300	3.92540	1.26430
C	-3.17760	2.39130	-0.93170
H	-5.63750	1.35970	-0.52090
H	-6.38410	-0.21820	1.23050
H	-4.76840	-1.07290	2.89230
C	-2.21510	-0.61330	3.18960
C	0.62380	2.28650	-2.42620
H	3.17180	2.11130	-3.38230
H	5.27840	1.94350	-2.11270
H	5.24130	1.90280	0.35140
C	3.12440	2.02660	2.02320
C	3.31660	3.48700	2.45550
C	4.22550	1.18300	2.66600
C	0.71800	1.89940	-3.89870
C	0.18180	3.75020	-2.30800
C	-3.59190	3.81180	-0.53430
C	-3.74550	2.05800	-2.31280
C	-1.77170	-2.01770	2.76910
C	-1.03810	0.21570	3.69740
H	-2.08610	2.36950	-1.01040
H	-2.89340	-0.73650	4.04430
H	-0.15160	1.66360	-1.97350
H	2.16000	1.66780	2.39940
H	3.26620	3.56990	3.54660
H	4.30090	3.84770	2.13560
H	2.57040	4.16290	2.03050
H	4.08450	1.16360	3.75170
H	4.21130	0.15270	2.30430
H	5.21820	1.60590	2.47670
H	-0.27970	1.92740	-4.34900
H	1.34750	2.59580	-4.46370
H	1.12300	0.89260	-4.03630
H	-0.74900	3.91150	-2.86320
H	0.00860	4.04780	-1.27030
H	0.94430	4.41580	-2.72840

	H -3.26280 4.52990 -1.29360 H -4.68250 3.88350 -0.45350 H -3.16430 4.11650 0.42450 H -3.26080 2.68110 -3.07260 H -3.59970 1.00490 -2.56470 H -4.82000 2.26680 -2.36320 H -1.17030 -1.97960 1.85600 H -1.16500 -2.47930 3.55560 H -2.63710 -2.66120 2.58070 H -0.65730 -0.24350 4.61580 H -0.20780 0.24550 2.98910 H -1.33460 1.24170 3.93710 C -0.53030 -1.58440 -2.89960 C -1.28010 -0.80040 -1.80370 C -2.53180 -1.51170 -1.39760 O -3.64570 -1.22580 -1.78820 O -2.30340 -2.57980 -0.61350 C -3.45600 -3.34390 -0.26190 H -0.16580 -0.87940 -3.64960 H -1.19370 -2.28970 -3.41670 H -1.56540 0.19110 -2.15110 H -3.09420 -4.15220 0.37360 H -4.17640 -2.72720 0.28040 H -3.93550 -3.75450 -1.15490
IVa-Pd_3 E = -1683.553783, E+ZPE = -1683.125048, H = -1683.093156, G = -1683.195697	
	O 2.11980 1.88070 0.94020 C 1.72020 1.53000 2.28050 C 2.61790 2.36340 3.17240 C 3.92400 2.36550 2.38030 C 3.43580 2.47720 0.94450 H 1.88070 0.45530 2.43120 H 0.65240 1.74610 2.37130 H 2.72030 1.93300 4.17140 H 2.22250 3.38030 3.26870 H 4.45810 1.42100 2.52970 H 4.59350 3.18610 2.64870 H 4.06380 1.94300 0.22560 H 3.33150 3.51920 0.62200 C -2.12060 2.76830 0.15820 C -2.62230 1.97520 1.19700 C -3.86430 1.18350 1.11290 O -4.40450 0.67250 2.07490 O -4.35140 1.08720 -0.13620 C -5.53310 0.30060 -0.26300 H -1.42480 3.57330 0.39100 H -2.65440 2.84690 -0.78570 H -2.29730 2.14050 2.22110 H -5.76740 0.28540 -1.32780 H -5.36320 -0.71610 0.10050 H -6.36050 0.74650 0.29630 Pd 0.32630 -1.11680 0.04180 Pd -1.02980 0.96690 0.14980 Pd 1.24770 1.01580 -0.84890 C -1.56500 -0.89120 0.76730 C -1.17710 -1.37370 2.04740 C -1.66890 -2.60690 2.50580 C -2.56170 -3.34040 1.73590 C -2.97220 -2.85280 0.48820 C -2.49210 -1.64300 0.00310 H -0.58420 -0.75110 2.71240 H -1.37440 -2.96240 3.49040 H -2.95300 -4.28420 2.10510 H -3.67090 -3.42820 -0.11450 H -2.81770 -1.26940 -0.96330 I 0.20120 -0.05180 -2.86190 O 2.02740 -2.58340 -0.25580

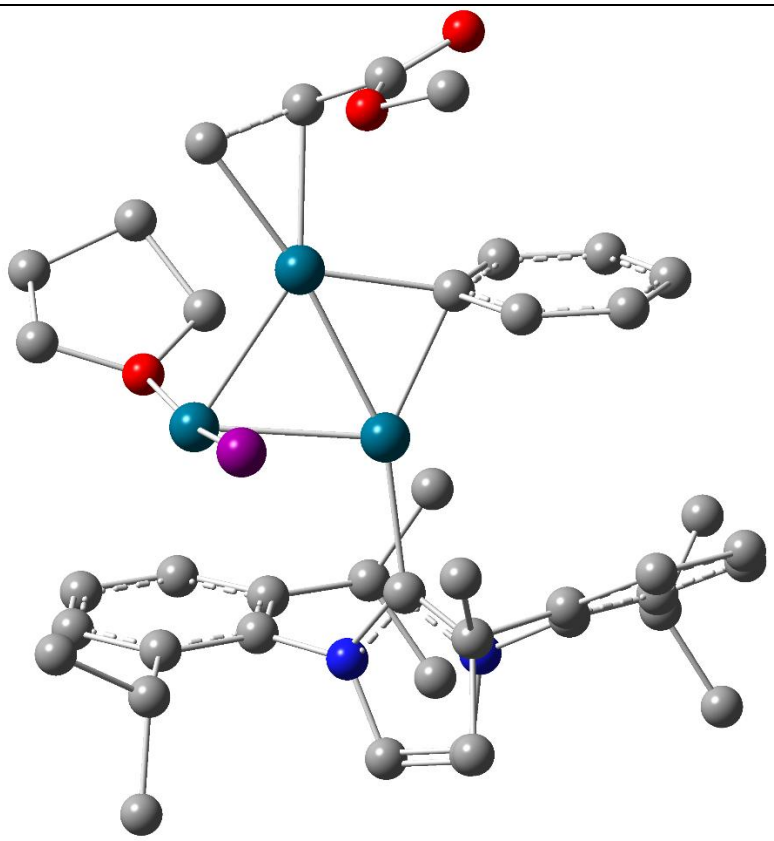
	C 2.30070 -3.29670 0.96140 C 3.19600 -2.36660 1.78100 C 3.82720 -1.43930 0.71820 C 3.28470 -1.98160 -0.60000 H 2.82190 -4.22790 0.70250 H 1.34310 -3.53960 1.42580 H 3.94300 -2.93310 2.34250 H 2.60260 -1.79070 2.49700 H 4.91980 -1.44750 0.73900 H 3.48820 -0.40930 0.85870 H 3.93630 -2.76120 -1.01700 H 3.09030 -1.22290 -1.36080
TS-Va-Pd_3 E = -1683.519290, E+ZPE = -1683.090651, H = -1683.058872, G = -1683.159087	
	O 1.51200 2.14120 0.18940 C 1.43620 2.15920 -1.25260 C 1.98400 3.51410 -1.66110 C 1.53490 4.39710 -0.49870 C 1.73530 3.47770 0.69250 H 0.38810 2.03870 -1.55000 H 2.01010 1.30560 -1.62010 H 1.59290 3.83950 -2.62840 H 3.07730 3.48740 -1.72090 H 0.47590 4.65690 -0.60470 H 2.11030 5.32130 -0.40620 H 1.03670 3.66040 1.51300 H 2.75960 3.52510 1.08060 C 2.34230 -2.54720 -0.94460 C 2.91950 -1.99270 0.26480 C 3.79950 -0.81910 0.27870 O 4.39510 -0.42270 1.26460 O 3.89400 -0.20530 -0.92100 C 4.69600 0.97210 -0.92540 H 2.28320 -3.63150 -0.96250 H 2.66960 -2.10820 -1.88440 H 3.07150 -2.65150 1.11710 H 4.68010 1.34140 -1.95140 H 4.28710 1.72190 -0.24350 H 5.72340 0.74470 -0.62830 Pd -1.20080 -0.32720 -0.53700 Pd 0.95720 -1.29630 0.23940 Pd 0.11130 0.82320 1.23340 C 0.40400 -2.38930 -1.35410 C -0.09100 -1.39440 -2.25180 C -1.32010 -1.61850 -2.89730 C -1.99570 -2.83470 -2.72790 C -1.44090 -3.83630 -1.93810 C -0.25110 -3.61520 -1.23840 H 0.53970 -0.55580 -2.54050 H -1.70180 -0.87520 -3.59200 H -2.93900 -3.00130 -3.23960 H -1.95490 -4.78700 -1.82570 H 0.13380 -4.37600 -0.56520 I -1.60510 -0.71780 2.25980 O -3.02480 1.09440 -1.29850 C -2.61720 1.98630 -2.34590 C -2.29600 3.33790 -1.68260 C -2.53820 3.07500 -0.19120 C -3.51120 1.91300 -0.23200 H -3.43270 2.08130 -3.07450 H -1.75790 1.53070 -2.84470 H -2.97160 4.11370 -2.05440 H -1.27260 3.66320 -1.88650 H -2.93000 3.94460 0.34270 H -1.61410 2.74380 0.30250 H -4.53240 2.25240 -0.46270 H -3.52840 1.30130 0.67300

VIa E = -1683.585869, E+ZPE = -1683.154264, H = -1683.122987, G = -1683.220794

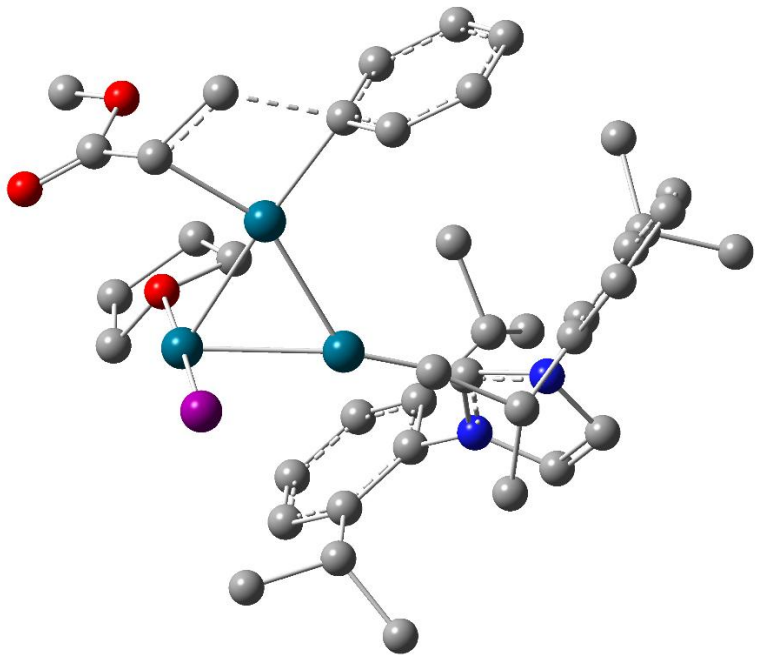


O	-0.36830	2.54150	-0.68320
C	-0.83220	2.77060	0.65970
C	-1.08430	4.26320	0.72680
C	0.04120	4.80350	-0.15330
C	0.10350	3.77320	-1.27030
H	-0.05220	2.46000	1.36590
H	-1.71590	2.14780	0.81130
H	-1.05170	4.64250	1.75120
H	-2.06200	4.50570	0.29610
H	0.98360	4.81780	0.40530
H	-0.14830	5.80970	-0.53460
H	1.11280	3.61320	-1.66000
H	-0.56390	4.02320	-2.10250
C	-3.35990	-1.78960	1.30240
C	-3.24780	-1.21130	-0.10790
C	-3.80530	0.09590	-0.43230
O	-4.08350	0.49090	-1.55490
O	-3.97580	0.89380	0.65960
C	-4.47520	2.19460	0.37520
H	-3.74850	-2.81190	1.28460
H	-4.00090	-1.18710	1.95170
H	-3.39400	-1.92080	-0.92190
H	-4.45720	2.73870	1.32120
H	-3.85440	2.70440	-0.36670
H	-5.50070	2.14750	-0.00390
Pd	1.19780	-0.58420	0.69770
Pd	-1.17660	-0.87150	0.03320
Pd	0.31670	0.57610	-1.32560
C	-1.91710	-1.78060	1.79800
C	-1.33430	-0.54520	2.21570
C	0.03350	-0.47880	2.61640
C	0.82960	-1.65500	2.57110
C	0.22240	-2.89630	2.19850
C	-1.09820	-2.95890	1.82090
H	-1.97720	0.31860	2.35730
H	0.38970	0.41050	3.12940
H	1.79560	-1.67700	3.06970
H	0.82410	-3.80010	2.21650
H	-1.54180	-3.90550	1.52470
I	1.10600	-1.71800	-1.99270
O	3.50450	-0.04790	1.09440
C	3.64190	0.77870	2.25360
C	3.20850	2.18240	1.81600
C	3.34020	2.13820	0.27830
C	3.96870	0.77370	0.01770
H	4.69470	0.77100	2.56860
H	3.03610	0.34360	3.05140
H	3.84410	2.94770	2.26900
H	2.17580	2.38520	2.11370
H	3.94680	2.95320	-0.12490
H	2.35020	2.17600	-0.18990
H	5.06660	0.82180	0.05540
H	3.65880	0.30300	-0.91770

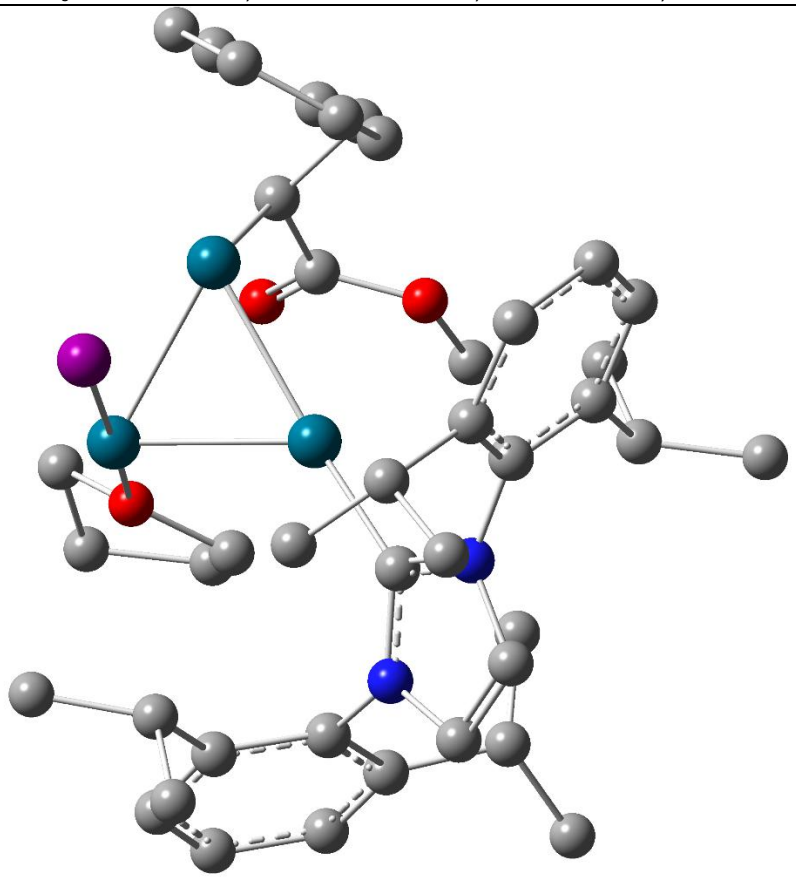
IVb-Pd_3 E =, E+ZPE =, H =, G =



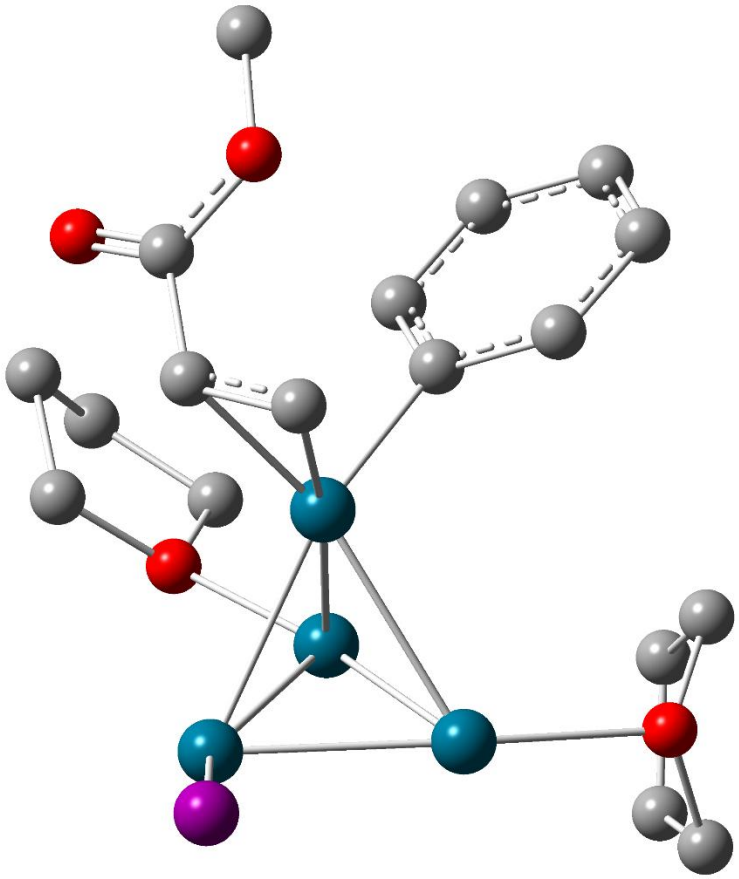
O	-2.88460	-1.73020	-0.93420
C	-2.89320	-1.21520	-2.28170
C	-4.35820	-1.05620	-2.63820
C	-4.99430	-2.20290	-1.85600
C	-4.20640	-2.16300	-0.55920
H	-2.39740	-1.95210	-2.92410
H	-2.32800	-0.27920	-2.28520
H	-4.53020	-1.11480	-3.71580
H	-4.73460	-0.09220	-2.27700
H	-4.83070	-3.15480	-2.37330
H	-6.06680	-2.07680	-1.68910
H	-4.11270	-3.13120	-0.06050
H	-4.63060	-1.43520	0.14430
C	-3.89440	2.24320	0.14610
C	-3.28900	3.03280	-0.84860
C	-2.60270	4.30770	-0.59350
O	-2.24410	5.07890	-1.46520
O	-2.40060	4.55670	0.71720
C	-1.66120	5.74020	0.99420
H	-4.66040	1.52530	-0.14440
H	-3.93320	2.59250	1.17560
H	-3.54660	2.89300	-1.89550
H	-1.55030	5.77570	2.07860
H	-0.67720	5.70520	0.51820
H	-2.19280	6.62970	0.64340
Pd	0.21660	0.28340	-0.31050
Pd	-1.96910	1.46980	-0.20360
Pd	-1.75210	-0.83640	0.71330
C	-0.30530	2.10600	-1.22430
C	-0.24010	2.04390	-2.64000
C	0.75460	2.71780	-3.34120
C	1.70380	3.48920	-2.66430
C	1.65900	3.57450	-1.27650
C	0.66570	2.90270	-0.55920
H	-0.98800	1.47540	-3.18760
H	0.78810	2.64710	-4.42610
H	2.47170	4.01990	-3.22050
H	2.38820	4.17760	-0.74200
H	0.60490	3.03150	0.51920
I	-0.83990	0.51120	2.63220
C	1.66310	-1.13730	0.01850
N	1.57320	-2.49590	-0.02200
C	2.78760	-3.09570	0.27370
C	3.66990	-2.09600	0.49350
N	2.96810	-0.91200	0.33390
C	0.38980	-3.25280	-0.32010
C	-0.36650	-3.74260	0.76350
C	-1.48530	-4.52910	0.47630
C	-1.83880	-4.81750	-0.83380
C	-1.06790	-4.33300	-1.88080
C	0.06820	-3.54770	-1.65880
C	3.61090	0.36980	0.29500
C	3.65200	1.15840	1.45570
C	4.32020	2.38200	1.37580
C	4.93390	2.78960	0.19610
C	4.89010	1.98120	-0.93210
C	4.22520	0.75280	-0.90770
H	2.91320	-4.16620	0.26560
H	4.72280	-2.11110	0.72720
C	0.03790	-3.50400	2.20720
H	-2.08210	-4.92350	1.29260
H	-2.71090	-5.43200	-1.04060
H	-1.33760	-4.57790	-2.90500
C	0.86170	-3.12760	-2.89010
C	3.04760	0.67390	2.75660
H	4.36620	3.02310	2.25020

	H 5.45210 3.74400 0.15890 H 5.37820 2.30540 -1.84660 C 4.23690 -0.14670 -2.12710 C 5.61570 -0.78810 -2.30190 C 3.80510 0.57710 -3.39930 C 2.55960 1.80870 3.65160 C 4.04630 -0.20580 3.51580 C 0.92980 -4.64090 2.71910 C -1.16280 -3.35120 3.14020 C 0.78150 -1.63370 -3.20480 C 2.31010 -3.62100 -2.90340 H 0.60850 -2.56950 2.24380 H 0.36170 -3.64240 -3.72000 H 2.17750 0.05860 2.50350 H 3.51660 -0.95110 -1.95710 H 5.60800 -1.48490 -3.14730 H 6.37980 -0.02740 -2.49840 H 5.91760 -1.34310 -1.40790 H 3.78450 -0.12660 -4.23870 H 2.80740 1.00870 -3.28800 H 4.49610 1.38440 -3.66530 H 1.89220 2.48900 3.11390 H 2.00510 1.39610 4.50040 H 3.39170 2.39320 4.06020 H 3.59590 -0.57780 4.44260 H 4.36010 -1.07140 2.92540 H 4.94340 0.36610 3.78010 H 1.21910 -4.45400 3.75910 H 0.39070 -5.59460 2.68460 H 1.84520 -4.75110 2.13290 H -0.82930 -2.98320 4.11560 H -1.89150 -2.63430 2.74650 H -1.67170 -4.30720 3.30630 H 1.25430 -1.02490 -2.42970 H 1.28490 -1.42590 -4.15570 H -0.25580 -1.30160 -3.29290 H 2.73310 -3.48050 -3.90420 H 2.94470 -3.07580 -2.20120 H 2.37210 -4.68700 -2.66000
TS-Vb-Pd$_3$ E = -2610.183255, E+ZPE = -2609.296378, H = -2609.239868, G = -2609.392446	
	O 2.98720 0.87720 -1.19870 C 1.96440 1.31100 -2.11240 C 2.71030 2.13420 -3.15960 C 3.99910 2.58820 -2.44080 C 3.87500 1.99390 -1.03990 H 1.23230 1.90980 -1.56210 H 1.47570 0.41200 -2.49160 H 2.10210 2.97950 -3.49050 H 2.94880 1.52750 -4.03680 H 4.09020 3.67620 -2.39400 H 4.88540 2.19890 -2.94840 H 3.42890 2.70980 -0.33860 H 4.80960 1.60910 -0.62610 C 1.49950 -3.75070 -1.46240 C 2.56980 -3.09050 -0.77030 C 3.64580 -2.36980 -1.47880 O 4.73150 -2.11680 -0.99070 O 3.31690 -2.03710 -2.74050 C 4.31290 -1.30600 -3.45030 H 1.16440 -4.68520 -1.02290 H 1.56440 -3.77090 -2.54530 H 2.88340 -3.47000 0.19930 H 3.88270 -1.09050 -4.42880 H 4.55170 -0.37920 -2.92470 H 5.22380 -1.90000 -3.56670 Pd -0.00900 0.23350 0.59140

	Pd 1.00830 -1.78670 -0.44490 Pd 2.45860 -0.08990 0.65300 C -0.32230 -3.00250 -1.46330 C -0.71990 -2.63910 -2.75850 C -1.99270 -2.96430 -3.21830 C -2.88190 -3.65510 -2.39620 C -2.49100 -4.02370 -1.10950 C -1.21620 -3.71480 -0.64870 H -0.02240 -2.12150 -3.41210 H -2.28840 -2.68180 -4.22540 H -3.87290 -3.91200 -2.75910 H -3.17990 -4.55920 -0.46270 H -0.90490 -4.03050 0.34360 I 1.90790 -1.26030 2.79040 C -1.79950 1.12030 0.46160 N -3.10610 0.84180 0.75170 C -3.83630 1.99400 1.00550 C -2.98780 3.03490 0.86680 N -1.76140 2.49070 0.52700 C -3.79590 -0.40700 0.61200 C -4.52890 -0.57870 -0.57970 C -5.33010 -1.71350 -0.70310 C -5.40610 -2.64560 0.32380 C -4.67300 -2.45240 1.48520 C -3.85520 -1.32990 1.66710 C -0.64140 3.29880 0.14430 C -0.64050 3.82950 -1.15670 C 0.42760 4.65560 -1.51860 C 1.44650 4.93730 -0.61790 C 1.42140 4.39530 0.66360 C 0.37650 3.56580 1.07650 H -4.88520 1.95640 1.25410 H -3.13720 4.09920 0.96180 C -4.52350 0.45230 -1.69460 H -5.91100 -1.85940 -1.60930 H -6.04220 -3.52060 0.22120 H -4.73750 -3.17990 2.29090 C -3.09180 -1.27010 2.97980 C -1.71980 3.47450 -2.16190 H 0.46200 5.08010 -2.51720 H 2.26800 5.58410 -0.91400 H 2.22690 4.62350 1.35380 C 0.32890 2.99560 2.48100 C -0.57430 3.83890 3.38500 C 1.70740 2.82710 3.10970 C -1.28220 2.27300 -3.00470 C -2.11960 4.64950 -3.05130 C -5.87380 1.16940 -1.77100 C -4.15670 -0.15800 -3.04540 C -1.82370 -2.11730 2.85460 C -2.76390 0.10400 3.56010 H -3.75980 1.20070 -1.46670 H -3.74820 -1.76750 3.70630 H -2.61270 3.17340 -1.60450 H -0.11150 1.99030 2.40440 H -0.62700 3.39660 4.38560 H -0.18010 4.85720 3.48420 H -1.59380 3.90730 2.99490 H 1.61660 2.27300 4.04910 H 2.37760 2.25800 2.45580 H 2.17650 3.79050 3.33990 H -1.05870 1.40740 -2.37330 H -2.07310 1.99160 -3.70810 H -0.38570 2.51510 -3.58730 H -2.98260 4.37120 -3.66530 H -2.39450 5.52870 -2.45940

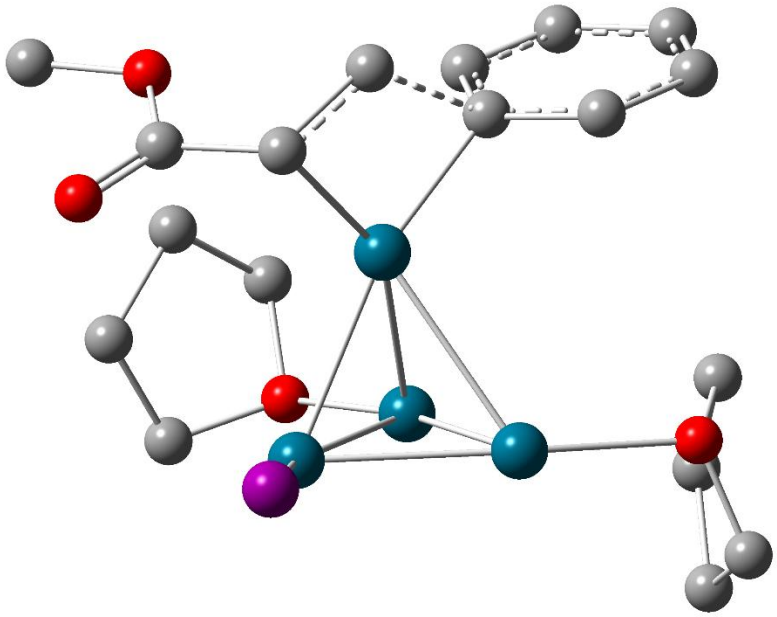
	H -1.31570 4.93950 -3.73630 H -5.84630 1.95430 -2.53500 H -6.67520 0.47050 -2.03630 H -6.13870 1.63520 -0.81670 H -4.15810 0.61820 -3.81850 H -3.16270 -0.60930 -3.01160 H -4.87130 -0.92910 -3.35350 H -1.15670 -1.68690 2.09690 H -1.28370 -2.14500 3.80720 H -2.05890 -3.14570 2.56180 H -2.43260 -0.02380 4.59640 H -1.95200 0.59510 3.01710 H -3.63250 0.76970 3.56760
VIb-Pd_3 E = -2610.216741, E+ZPE = -2609.327075, H = -2609.271786, G = -2609.416923	
	O -2.11680 -2.60390 -0.22920 C -2.84900 -1.86680 0.77560 C -3.79010 -2.87910 1.42250 C -3.79530 -4.04760 0.43390 C -2.37670 -4.01190 -0.09770 H -3.36880 -1.06550 0.25320 H -2.13220 -1.43210 1.47330 H -4.78560 -2.45850 1.58750 H -3.37740 -3.20700 2.37980 H -4.50570 -3.86840 -0.38050 H -4.03650 -5.00350 0.90560 H -2.25250 -4.45930 -1.08670 H -1.66280 -4.44390 0.61060 C 2.48500 -2.05500 2.71570 C 1.29800 -2.72930 2.03950 C -0.01100 -2.67400 2.71340 O -0.86670 -3.54300 2.64580 O -0.17030 -1.58220 3.48780 C -1.36040 -1.54410 4.26670 H 2.99790 -2.72050 3.42490 H 2.15560 -1.17020 3.26360 H 1.48770 -3.77620 1.77920 H -1.28810 -0.64570 4.88000 H -2.25070 -1.49100 3.63660 H -1.43260 -2.42850 4.90620 Pd 0.01400 0.08340 0.20710 Pd 1.57220 -1.85660 0.21940 Pd -0.43570 -1.88350 -1.24980 C 3.41230 -1.63130 1.59010 C 3.72550 -0.27280 1.36130 C 4.62110 0.08600 0.36210 C 5.22190 -0.89030 -0.43690 C 4.91920 -2.23290 -0.23620 C 4.02290 -2.60810 0.76790 H 3.26390 0.49060 1.98150 H 4.84520 1.13580 0.20180 H 5.92040 -0.60020 -1.21640 H 5.38190 -2.99730 -0.85390 H 3.83300 -3.66160 0.95890 I 1.64550 -1.15400 -2.50360 C -0.73320 1.94560 -0.07480 N -0.04480 3.12410 0.03120 C -0.82810 4.22260 -0.27720 C -2.04440 3.74020 -0.61530 N -1.96890 2.35980 -0.48940 C 1.30510 3.23770 0.48490 C 1.53500 3.16470 1.87000 C 2.84570 3.30860 2.32920 C 3.88880 3.53990 1.44160 C 3.63090 3.62320 0.07960 C 2.33850 3.47570 -0.43650 C -3.11320 1.52240 -0.68030

	C -4.08050 1.49080 0.33800 C -5.23180 0.73040 0.11520 C -5.40020 0.02370 -1.06990 C -4.41970 0.06220 -2.05560 C -3.25720 0.81940 -1.88810 H -0.45020 5.23140 -0.22380 H -2.95160 4.23840 -0.92060 C 0.41550 2.94110 2.86510 H 3.04640 3.24580 3.39530 H 4.90470 3.65210 1.81060 H 4.44820 3.80410 -0.61460 C 2.18640 3.64860 -1.94080 C -3.85260 2.18730 1.66580 H -5.99840 0.68180 0.88200 H -6.29940 -0.56640 -1.22520 H -4.56320 -0.49980 -2.97270 C -2.21440 0.92100 -2.98320 C -2.43720 2.18630 -3.81760 C -2.16460 -0.30410 -3.88940 C -3.15280 1.22970 2.63570 C -5.13130 2.75000 2.28070 C 0.35020 4.06200 3.90270 C 0.55620 1.57120 3.52400 C 1.11120 2.81740 -2.63640 C 2.03980 5.13250 -2.29580 H -0.53190 2.94190 2.31840 H 3.14960 3.31880 -2.35030 H -3.17550 3.03040 1.49370 H -1.23860 0.99760 -2.49100 H -1.65560 2.28200 -4.57900 H -3.40620 2.14600 -4.32920 H -2.41890 3.09050 -3.20230 H -1.30760 -0.22490 -4.56570 H -2.04390 -1.22730 -3.30880 H -3.06450 -0.39920 -4.50780 H -2.20810 0.86630 2.21710 H -2.94120 1.73270 3.58610 H -3.79190 0.36400 2.84610 H -4.88620 3.33960 3.17010 H -5.66440 3.40050 1.57950 H -5.81830 1.95780 2.59760 H -0.50690 3.90950 4.56790 H 1.25070 4.09180 4.52580 H 0.23840 5.04140 3.42570 H -0.26000 1.40100 4.23390 H 0.52170 0.77390 2.77160 H 1.50110 1.48890 4.07400 H 0.11140 3.23920 -2.50490 H 1.31690 2.79720 -3.71240 H 1.10180 1.78660 -2.27390 H 2.05930 5.26530 -3.38330 H 1.08860 5.53210 -1.92910 H 2.84810 5.73240 -1.86490
IVa-Pd_4 E = -1811.480902, E+ZPE = -1811.049928, H = -1811.014443, G = -1811.126030	



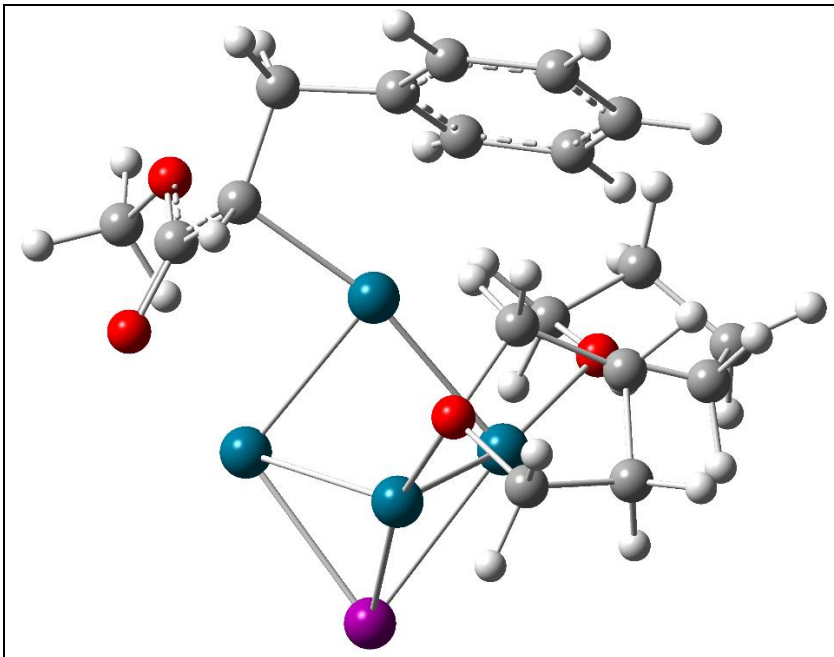
O	1.54030	0.44210	2.82520
C	2.74590	1.19450	3.07460
C	3.60180	0.27090	3.91830
C	3.27450	-1.09260	3.31320
C	1.78940	-0.97880	3.01230
H	2.45670	2.12440	3.57050
H	3.22940	1.43050	2.11810
H	3.28860	0.31490	4.96690
H	4.66250	0.52670	3.85980
H	3.48930	-1.92710	3.98480
H	3.83610	-1.24820	2.38630
H	1.16410	-1.30640	3.84930
H	1.48950	-1.50830	2.10620
O	-0.99950	3.13090	-1.59100
C	0.40190	3.45740	-1.71100
C	0.77580	4.11660	-0.38750
C	-0.56790	4.64690	0.15930
C	-1.57150	4.27860	-0.92750
H	0.50200	4.15430	-2.55300
H	0.93880	2.53630	-1.93210
H	1.51460	4.90790	-0.53730
H	1.20070	3.37180	0.29640
H	-0.55770	5.72470	0.33870
H	-0.82570	4.14370	1.09590
H	-1.67280	5.07550	-1.67550
H	-2.56190	3.99590	-0.56580
Pd	0.25320	1.08310	1.24640
Pd	-1.77390	-0.56320	1.08830
Pd	0.23030	-0.75250	-0.62640
Pd	-1.50470	1.32470	-0.55490
C	1.86590	-0.04210	-1.43720
C	1.87860	0.34170	-2.78020
C	3.02720	0.91890	-3.32700
C	4.16350	1.10920	-2.54400
C	4.15160	0.71360	-1.20710
C	3.00900	0.13400	-0.65330
H	0.99720	0.20510	-3.40140
H	3.02700	1.22120	-4.37140
H	5.05450	1.55860	-2.97330
H	5.03510	0.85080	-0.58800
H	3.01390	-0.18230	0.38560
C	0.12840	-2.40290	-2.01250
C	0.74090	-2.82960	-0.83750
C	2.20070	-3.02540	-0.66880
O	2.72610	-3.23780	0.40750
O	2.87380	-2.95930	-1.82040
C	4.29350	-3.04720	-1.70320
H	-0.93690	-2.56430	-2.15810
H	0.72440	-2.19030	-2.89470
H	0.15020	-3.28060	-0.04240
H	4.68290	-2.90580	-2.71130
H	4.67430	-2.26670	-1.04070
H	4.58860	-4.02690	-1.31800
I	-3.56930	-1.78430	-0.21720

TS-Va-Pd_4 E = -1811.459967, E+ZPE = -1811.028694, H = -1810.994167, G = -1811.102346



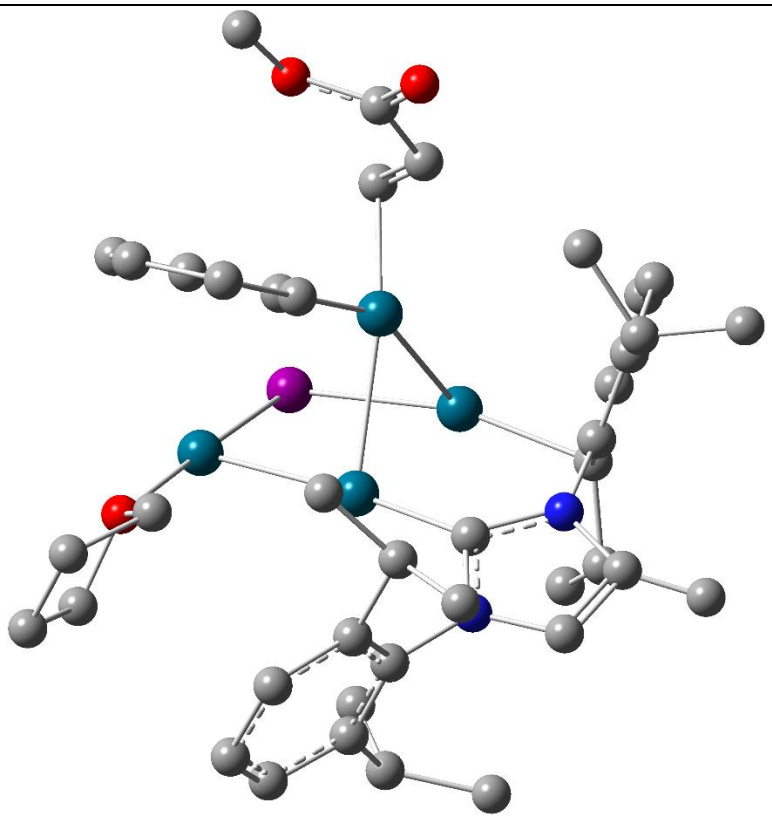
O	-0.56450	1.51630	3.09160
C	-0.52310	2.90080	2.69550
C	0.89540	3.13110	2.18030
C	1.71910	2.00160	2.83760
C	0.70900	1.29080	3.72780
H	-0.73650	3.50820	3.58480
H	-1.31120	3.05580	1.95620
H	1.25360	4.12700	2.45280
H	0.93110	3.03700	1.09260
H	2.56940	2.37190	3.41560
H	2.08920	1.31020	2.07270
H	0.66440	1.73740	4.73010
H	0.84970	0.21250	3.81300
O	-3.21730	-1.65700	-0.78150
C	-3.95900	-0.46940	-0.42700
C	-4.33900	-0.64710	1.04270
C	-4.20510	-2.16530	1.28740
C	-3.90450	-2.72380	-0.09610
H	-4.84500	-0.43340	-1.07370
H	-3.32050	0.38850	-0.63310
H	-5.35080	-0.27880	1.23030
H	-3.64600	-0.09300	1.68670
H	-5.10860	-2.61040	1.71100
H	-3.36880	-2.37030	1.96220
H	-4.82350	-2.94200	-0.65600
H	-3.25570	-3.60170	-0.11080
Pd	-0.99910	0.16640	1.46170
Pd	1.11710	-1.13420	0.78790
Pd	0.32230	0.63470	-0.89030
Pd	-1.12710	-1.62170	-0.30770
C	-0.88780	1.91950	-1.92410
C	-1.78730	1.34200	-2.83090
C	-3.05840	1.88880	-2.99050
C	-3.43570	3.02020	-2.26810
C	-2.52600	3.61830	-1.39490
C	-1.24830	3.08740	-1.23680
H	-1.49710	0.46040	-3.39590
H	-3.75580	1.42560	-3.68360
H	-4.42710	3.44460	-2.39710
H	-2.80620	4.51180	-0.84290
H	-0.53380	3.56990	-0.57570
C	0.98050	1.90740	-2.63980
C	1.99520	1.16040	-1.96400
C	2.98270	1.80570	-1.06830
O	3.99890	1.26860	-0.67740
O	2.65310	3.07060	-0.75090
C	3.59260	3.75020	0.08120
H	0.68390	1.53680	-3.61620
H	1.03040	2.98850	-2.56280
H	2.36110	0.23550	-2.40420
H	3.16900	4.73790	0.26300
H	3.73680	3.21880	1.02470
H	4.55680	3.84390	-0.42560
I	2.55700	-2.67870	-0.64380

VIa-Pd_4 E = -1811.525280, E+ZPE = -1811.093287, H = -1811.058979, G = -1811.169464



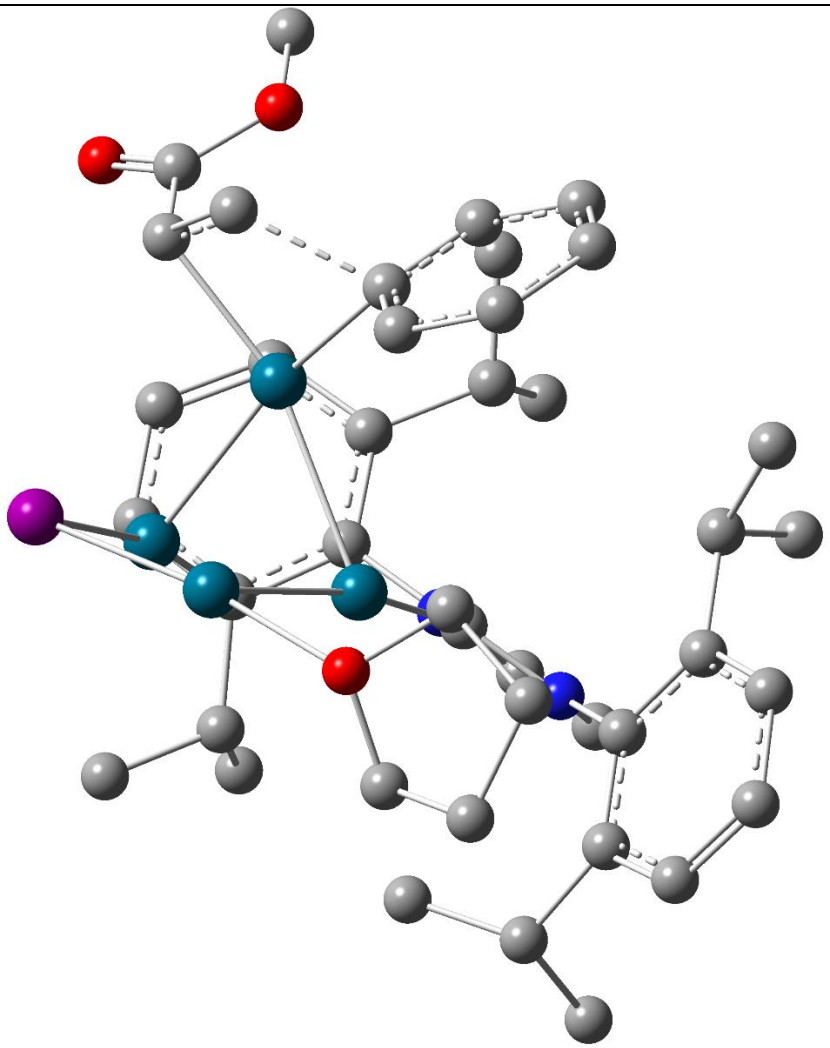
O	1.19250	0.97470	2.73410
C	1.20800	2.09500	3.64370
C	1.95880	1.61640	4.88620
C	2.71000	0.38030	4.38920
C	1.72540	-0.18710	3.38750
H	0.17810	2.39500	3.86060
H	1.71440	2.91860	3.12930
H	1.25010	1.33240	5.67060
H	2.61920	2.38860	5.28780
H	2.94760	-0.32580	5.18850
H	3.64100	0.66350	3.88550
H	0.91470	-0.73850	3.88200
H	2.16380	-0.82090	2.61300
O	-0.90470	2.10630	-2.61820
C	0.42330	2.53240	-2.27600
C	0.23590	3.54230	-1.14640
C	-1.19620	4.07870	-1.36830
C	-1.67150	3.32110	-2.60640
H	0.87600	2.99490	-3.16450
H	0.98840	1.64110	-1.99540
H	0.99460	4.32820	-1.18000
H	0.30640	3.02670	-0.18060
H	-1.22560	5.15980	-1.52820
H	-1.83080	3.84030	-0.50960
H	-1.44600	3.87870	-3.52700
H	-2.72880	3.04930	-2.60140
Pd	-0.42830	0.72440	1.29770
Pd	-1.16350	-1.95070	-0.31860
Pd	0.92960	-0.51670	-0.52050
Pd	-1.72730	0.71520	-1.06090
C	3.33400	-0.17700	-1.62180
C	3.62910	0.88880	-2.47700
C	3.74220	2.18260	-1.97890
C	3.51710	2.44640	-0.62510
C	3.21680	1.40250	0.23950
C	3.14440	0.08390	-0.24380
H	3.77380	0.69560	-3.53670
H	3.99170	2.99750	-2.65310
H	3.58410	3.46310	-0.24970
H	3.04440	1.58570	1.29460
H	3.11670	-0.74840	0.46380
C	3.12480	-1.58550	-2.11910
C	1.65150	-1.88580	-1.93460
C	1.21140	-3.04920	-1.20420
O	0.01740	-3.45090	-1.18920
O	2.14930	-3.70660	-0.51450
C	1.68130	-4.73120	0.36400
H	3.41860	-1.67140	-3.17020
H	3.73850	-2.28340	-1.54150
H	1.00810	-1.66410	-2.78750
H	2.57040	-5.12050	0.86030
H	0.98920	-4.31570	1.10270
H	1.18250	-5.52840	-0.19180
I	-2.89400	-0.39580	0.90810

IVb-Pd_4 E = -2738.178968, E+ZPE = -2737.292350, H = -2737.232195, G = -2737.390818



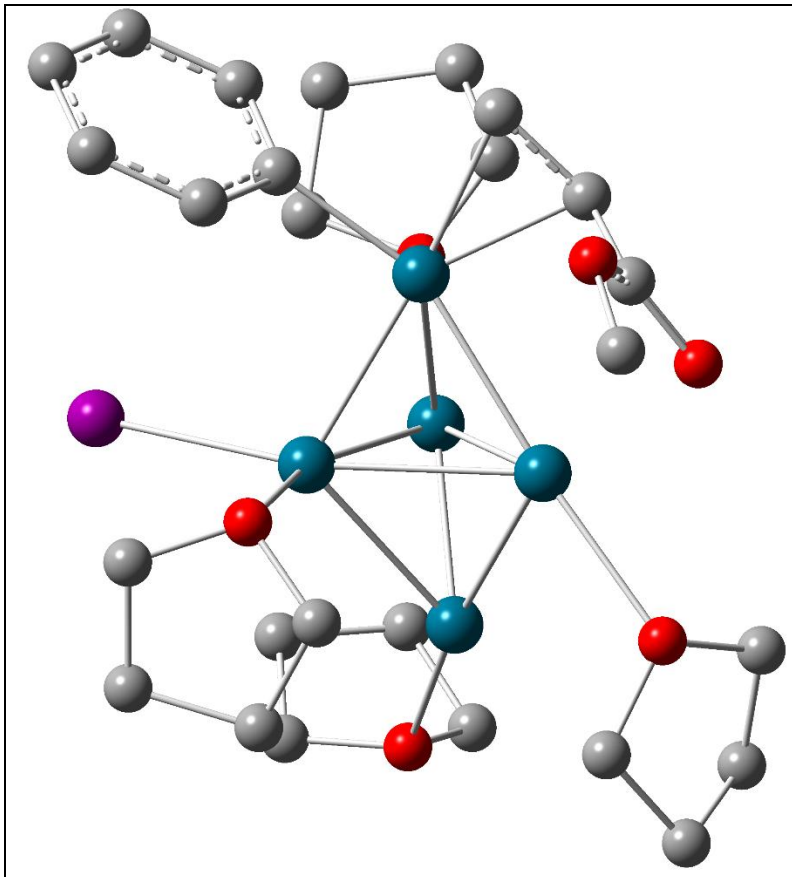
O	-2.23570	2.48810	-1.57700
C	-2.74300	2.37810	-0.23740
C	-4.00870	3.21520	-0.27610
C	-4.54010	2.99030	-1.70560
C	-3.37260	2.31120	-2.43430
H	-1.97070	2.74040	0.43760
H	-2.95210	1.32210	-0.01960
H	-3.76060	4.26840	-0.11410
H	-4.71990	2.90810	0.49420
H	-4.81470	3.93490	-2.18140
H	-5.41970	2.34140	-1.71300
H	-3.12410	2.75350	-3.40110
H	-3.55550	1.23740	-2.56640
Pd	-0.62040	-0.22030	-0.48630
Pd	1.93120	-1.24120	-1.31620
Pd	1.54660	0.74680	0.44010
Pd	-0.33080	1.68350	-2.20390
C	0.57350	2.32380	1.14230
C	0.56590	3.48290	0.35550
C	-0.09080	4.63290	0.79330
C	-0.74280	4.64390	2.02670
C	-0.72260	3.49890	2.81990
C	-0.06730	2.34240	2.38340
H	1.06920	3.48620	-0.60850
H	-0.09180	5.52090	0.16540
H	-1.25650	5.53850	2.36850
H	-1.22350	3.49550	3.78500
H	-0.07150	1.45900	3.01550
C	3.54850	1.48610	0.12940
C	3.41310	1.31120	1.49750
C	3.26120	2.43130	2.45410
O	3.17540	2.28920	3.65790
O	3.27590	3.62770	1.85550
C	3.01690	4.73830	2.71020
H	3.99960	0.70500	-0.47670
H	3.48380	2.47420	-0.31690
H	3.70560	0.37420	1.96260
H	2.98550	5.61290	2.06040
H	2.05940	4.61580	3.22150
H	3.81230	4.85030	3.45230
I	1.82630	0.70900	-3.08650
C	-1.01380	-1.69730	0.77980
N	-2.27000	-2.11270	1.11310
C	-2.24220	-3.27420	1.86790
C	-0.94080	-3.62180	1.99060
N	-0.20810	-2.65630	1.31790
C	-3.46850	-1.39980	0.78360
C	-4.00590	-0.55230	1.76900
C	-5.18710	0.13230	1.47540
C	-5.80010	-0.00540	0.23750
C	-5.24670	-0.84690	-0.71920
C	-4.07960	-1.57860	-0.47220
C	1.20400	-2.69050	1.10920
C	2.06030	-2.37920	2.15050
C	3.44780	-2.33300	1.86810
C	3.92370	-2.55400	0.59570
C	3.04830	-2.93020	-0.45690
C	1.65090	-3.06200	-0.20810
H	-3.14320	-3.74850	2.22340
H	-0.47050	-4.45850	2.48280
C	-3.35310	-0.38730	3.12690
H	-5.62610	0.78480	2.22390
H	-6.71670	0.53590	0.01960
H	-5.73720	-0.96260	-1.68230
C	-3.59970	-2.49720	-1.58760
C	1.56150	-2.10570	3.55420

	H 4.14090 -2.09210 2.66940 H 4.99050 -2.49740 0.39570 H 3.48060 -3.37690 -1.34950 C 0.77030 -3.98090 -1.05010 C 0.88210 -5.41450 -0.52260 C 1.06600 -3.94460 -2.54570 C 1.99650 -0.73510 4.06190 C 2.01300 -3.21740 4.50400 C -4.06590 -1.24520 4.17590 C -3.30790 1.07380 3.57020 C -2.45020 -1.89610 -2.39780 C -3.29310 -3.93320 -1.16310 H -2.31910 -0.73730 3.04790 H -4.45540 -2.55980 -2.27150 H 0.46750 -2.11130 3.53110 H -0.26260 -3.64550 -0.91810 H 0.19510 -6.07670 -1.06110 H 1.89990 -5.79710 -0.66200 H 0.64510 -5.47820 0.54380 H 0.36000 -4.59230 -3.07700 H 0.96600 -2.92950 -2.94960 H 2.07550 -4.30460 -2.77380 H 1.67600 0.05790 3.38220 H 1.56060 -0.53800 5.04760 H 3.08380 -0.66280 4.16330 H 1.61910 -3.04350 5.51140 H 1.66560 -4.20000 4.16730 H 3.10590 -3.25600 4.57530 H -3.57460 -1.14400 5.14980 H -5.10930 -0.92950 4.28970 H -4.06400 -2.30530 3.90490 H -2.70740 1.16700 4.48130 H -2.85990 1.70890 2.80180 H -4.30650 1.46180 3.79820 H -1.52710 -1.81970 -1.80070 H -2.22020 -2.52810 -3.26310 H -2.69540 -0.89480 -2.76510 H -3.17720 -4.55660 -2.05630 H -2.36970 -4.01420 -0.58640 H -4.10580 -4.35600 -0.56330
TS-Vb-Pd_4 E = -2738.145406, E+ZPE = -2737.257584, H = -2737.198453, G = -2737.354856	

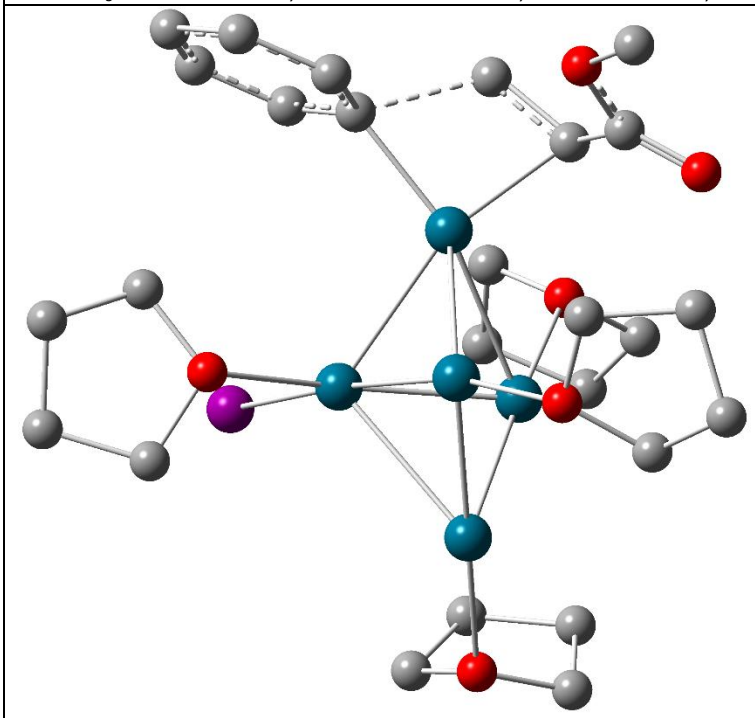


O	-2.46680	-3.08480	-0.19750
C	-2.90990	-2.73220	-1.51910
C	-4.43840	-2.85290	-1.48080
C	-4.77120	-2.97510	0.01880
C	-3.47110	-2.57660	0.69340
H	-2.42180	-3.41860	-2.21240
H	-2.58560	-1.70680	-1.73270
H	-4.78760	-3.72600	-2.03730
H	-4.89630	-1.96360	-1.92050
H	-5.02600	-4.00670	0.27860
H	-5.59900	-2.32930	0.32020
H	-3.30040	-3.02410	1.67400
H	-3.36410	-1.48510	0.76130
Pd	-0.73910	-0.31490	0.26800
Pd	1.74990	-0.31170	1.70250
Pd	1.59370	-0.42060	-0.89270
Pd	-0.41330	-2.90890	0.39370
C	1.01940	-0.77610	-2.85490
C	0.10840	-1.82170	-3.06410
C	-0.76800	-1.78320	-4.14540
C	-0.74330	-0.70960	-5.03440
C	0.16130	0.33310	-4.83250
C	1.04640	0.29570	-3.76050
H	0.09380	-2.66190	-2.37080
H	-1.46850	-2.60010	-4.29830
H	-1.42090	-0.68770	-5.88330
H	0.19180	1.17050	-5.52500
H	1.79210	1.07470	-3.64510
I	1.92040	-2.89700	1.35170
C	-1.15950	1.60520	0.49390
N	-2.40730	2.16710	0.49220
C	-2.39930	3.44540	1.02600
C	-1.11900	3.71120	1.37030
N	-0.37920	2.58910	1.03710
C	-3.59240	1.55420	-0.02840
C	-3.80370	1.61640	-1.42200
C	-4.99460	1.09110	-1.92380
C	-5.94780	0.53610	-1.07630
C	-5.71020	0.48240	0.28760
C	-4.52800	0.98340	0.84880
C	1.02930	2.46030	1.23470
C	1.89660	3.03260	0.31490
C	3.28060	2.81090	0.49180
C	3.75180	2.01780	1.51420
C	2.86730	1.47200	2.47350
C	1.47020	1.72990	2.38730
H	-3.29580	4.04030	1.10150
H	-0.67020	4.58270	1.81870
C	-2.78820	2.25980	-2.34950
H	-5.18530	1.11960	-2.99110
H	-6.87290	0.13850	-1.48450
H	-6.45170	0.04230	0.94980
C	-4.42380	0.88910	2.36480
C	1.39110	3.87560	-0.83830
H	3.98120	3.24060	-0.21650
H	4.81610	1.82610	1.60530
H	3.28380	1.06910	3.39350
C	0.57310	1.65280	3.61660
C	0.68690	2.95910	4.40790
C	0.85180	0.45950	4.52550
C	2.15420	3.61750	-2.13470
C	1.44970	5.36460	-0.48330
C	-2.89730	3.78860	-2.32430
C	-2.90340	1.77030	-3.78870
C	-3.03750	0.68220	2.96750
C	-5.11980	2.08500	3.02430

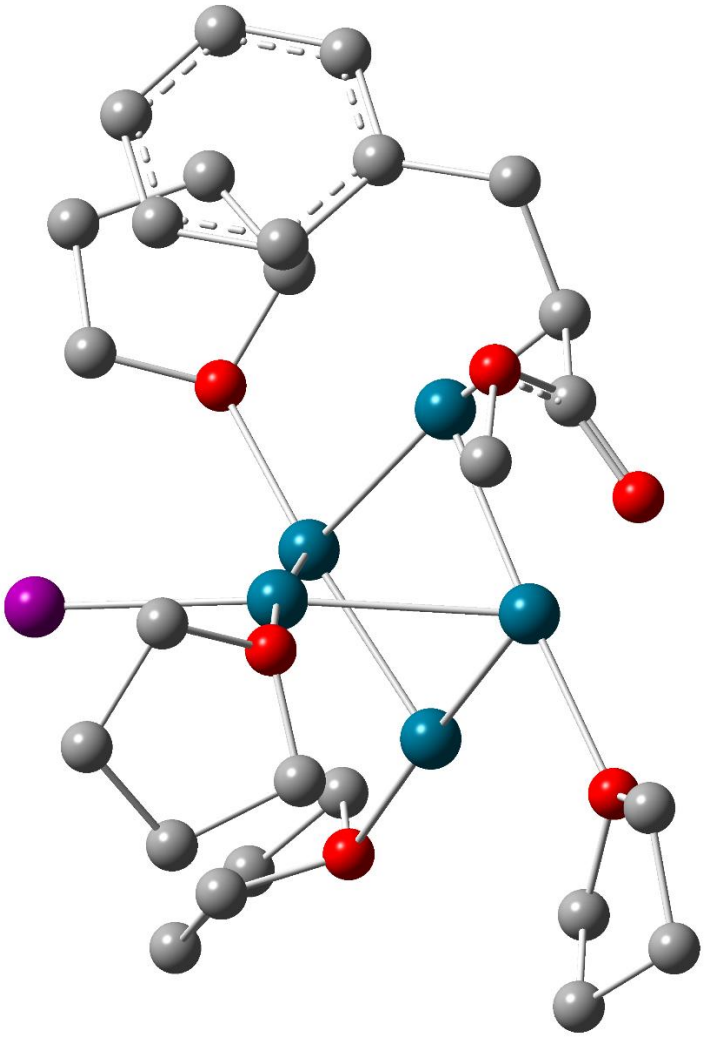
	H -1.79270 1.97870 -1.98610 H -5.01330 -0.00080 2.62120 H 0.34320 3.60650 -1.01040 H -0.45400 1.55510 3.25690 H -0.01000 2.95870 5.25340 H 1.70120 3.08130 4.80540 H 0.46470 3.83250 3.78710 H 0.13730 0.45380 5.35590 H 0.74460 -0.49200 3.98810 H 1.85710 0.49650 4.95940 H 2.25760 2.54690 -2.32180 H 1.62540 4.07050 -2.98000 H 3.15790 4.05460 -2.10460 H 1.06620 5.97160 -1.31110 H 0.86120 5.59830 0.40860 H 2.48390 5.67270 -0.29070 H -2.14150 4.22910 -2.98410 H -3.88360 4.10840 -2.68040 H -2.74760 4.20310 -1.32470 H -2.06490 2.15860 -4.37350 H -2.87500 0.67900 -3.85040 H -3.82460 2.12310 -4.26650 H -2.46790 1.61430 2.99430 H -3.14380 0.33700 4.00170 H -2.44630 -0.06120 2.42020 H -5.15640 1.95020 4.11090 H -4.57830 3.01490 2.82130 H -6.14540 2.20330 2.66050 C 2.81250 -1.49330 -2.47440 C 3.55460 -0.94430 -1.37900 C 4.48090 0.18330 -1.57020 O 5.41430 0.43570 -0.83300 O 4.21710 0.89950 -2.68170 C 5.14220 1.94630 -2.96210 H 2.56540 -2.54930 -2.40020 H 3.10760 -1.17970 -3.46940 H 3.84530 -1.59720 -0.56140 H 6.13530 1.53640 -3.16850 H 4.75910 2.45620 -3.84630 H 5.21410 2.64320 -2.12430
VIb E =, E+ZPE =, H =, G =	
IVa-Pd_5 E = -2403.842033, E+ZPE = -2403.171911, H = -2403.121772, G = -2403.267158	



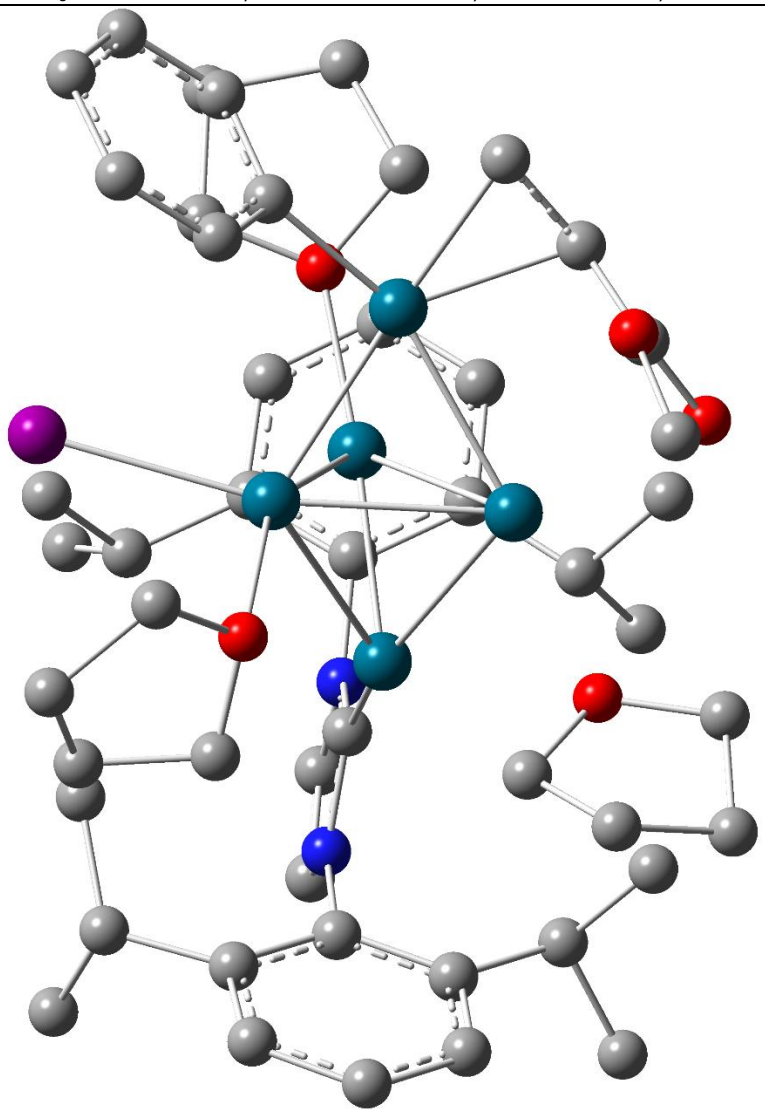
I	-2.00360	-2.18980	1.62760
Pd	0.10880	-0.95540	-1.46680
Pd	-0.22450	-0.29380	0.98530
Pd	1.33260	1.47090	-0.38040
Pd	2.15530	-0.95040	-0.08230
Pd	-1.30110	1.49330	-0.46830
C	-3.15030	1.26980	0.28960
C	-3.26930	1.54290	1.65770
C	-4.44090	1.21720	2.34170
C	-5.51120	0.63260	1.66600
C	-5.40850	0.39170	0.29810
C	-4.23970	0.72340	-0.39030
H	-2.43380	1.97560	2.20320
H	-4.51190	1.41600	3.40860
H	-6.42130	0.37500	2.20090
H	-6.24110	-0.05440	-0.24130
H	-4.18470	0.53790	-1.45930
C	-2.32050	3.18610	-1.31220
C	-0.99000	3.15260	-1.75000
C	0.11680	3.82700	-1.05640
O	1.30260	3.65260	-1.36050
O	-0.26200	4.65230	-0.07960
C	0.79310	5.17500	0.73070
H	-3.11000	2.88010	-1.99150
H	-2.61500	3.84500	-0.50180
H	-0.72400	2.75740	-2.72670
H	0.30700	5.80040	1.47890
H	1.33680	4.35850	1.21570
H	1.48720	5.77000	0.13270
O	2.95580	-2.99400	-0.21470
C	2.10220	-3.96830	0.41990
C	1.06700	-4.35010	-0.63490
C	1.74420	-3.98130	-1.97250
C	3.12410	-3.48440	-1.55670
H	1.68230	-3.50720	1.31530
H	2.72780	-4.82440	0.70530
H	0.15310	-3.76610	-0.49220
H	0.81410	-5.41130	-0.56970
H	1.18810	-3.17670	-2.46880
H	1.81570	-4.82510	-2.66360
H	3.51930	-2.66680	-2.16200
H	3.85560	-4.30330	-1.52910
O	3.67310	1.89660	-0.15140
C	4.33660	1.72930	-1.41960
C	5.27320	0.55240	-1.22940
C	5.70380	0.74160	0.22240
C	4.40700	1.19980	0.87010
H	4.88730	2.65020	-1.65170
H	3.57090	1.56950	-2.18310
H	6.10420	0.55630	-1.93940
H	4.71500	-0.38680	-1.33960
H	6.46910	1.52240	0.29400
H	6.09480	-0.16830	0.68510
H	4.54640	1.87510	1.72000
H	3.80300	0.34020	1.20430
O	-1.58610	-1.16720	-2.78180
C	-2.06450	-0.08880	-3.59830
C	-3.16900	-0.73230	-4.41170
C	-3.83030	-1.66840	-3.39080
C	-2.72080	-1.96670	-2.37500
H	-1.21740	0.27740	-4.18200
H	-2.43770	0.71820	-2.95430
H	-2.73550	-1.30220	-5.23970
H	-3.86300	0.00380	-4.82520
H	-4.21170	-2.58000	-3.85650
H	-4.66940	-1.17100	-2.89630

	H -2.38560 -3.00640 -2.37970 H -2.99880 -1.68780 -1.35480 O 0.03510 0.80110 3.06050 C -0.32390 0.02020 4.20620 C 0.84360 -0.94640 4.41210 C 2.02720 -0.23820 3.71490 C 1.42480 1.08660 3.25960 H -1.27890 -0.46290 3.99410 H -0.43830 0.69780 5.06420 H 0.62850 -1.90660 3.93440 H 1.02730 -1.12770 5.47430 H 2.35380 -0.81190 2.83920 H 2.88810 -0.09110 4.37250 H 1.81590 1.46620 2.31270 H 1.51680 1.85810 4.03850
TS-Va-Pd_5 E = -2403.829070, E+ZPE = -2403.158216, H = -2403.108632, G = -2403.251371	
	O 2.41830 -3.43310 -1.36850 C 3.61010 -2.75780 -0.91820 C 3.54650 -2.80120 0.60650 C 2.60240 -3.98630 0.90640 C 2.28270 -4.54940 -0.47320 H 3.59940 -1.75100 -1.33840 H 4.47520 -3.31200 -1.30590 H 3.12320 -1.86620 0.98600 H 4.54140 -2.93210 1.03940 H 1.68340 -3.62540 1.38430 H 3.05360 -4.74270 1.55390 H 1.27230 -4.94570 -0.58590 H 3.01060 -5.31600 -0.77290 Pd 0.29950 -1.34420 0.94480 Pd 0.91450 0.56880 -0.67620 Pd -1.27680 -0.53670 -1.38600 Pd 0.66450 -2.11550 -1.44110 Pd -1.14040 0.90210 0.89260 C -1.39780 2.92380 1.08940 C -2.35370 3.50870 0.24430 C -2.16450 4.80610 -0.22320 C -1.04290 5.54060 0.16670 C -0.10590 4.96760 1.02510 C -0.28150 3.66760 1.49580 H -3.24300 2.94880 -0.03120 H -2.90200 5.24870 -0.88790 H -0.90460 6.55650 -0.19210 H 0.77050 5.53150 1.33350 H 0.45100 3.22940 2.16760 C -2.18540 1.88670 2.61420 C -2.47770 0.50160 2.38840 C -3.78350 0.05610 1.85810 O -4.16050 -1.10050 1.86230 O -4.52870 1.07300 1.39190 C -5.84230 0.73140 0.95160 H -1.45500 2.11370 3.38650 H -3.01970 2.57840 2.57900 H -1.96330 -0.25440 2.97710 H -6.33170 1.67750 0.71940 H -5.80750 0.10240 0.05980 H -6.38950 0.20700 1.73910 I 3.38910 1.46080 0.27040 O -2.90780 -1.83410 -2.13330 C -4.23040 -1.26330 -2.01860 C -5.08390 -2.32070 -1.33310 C -4.37040 -3.61470 -1.71960 C -2.91760 -3.19030 -1.64010 H -4.58140 -1.03450 -3.03120 H -4.15460 -0.32900 -1.45150 H -6.12540 -2.28260 -1.66250

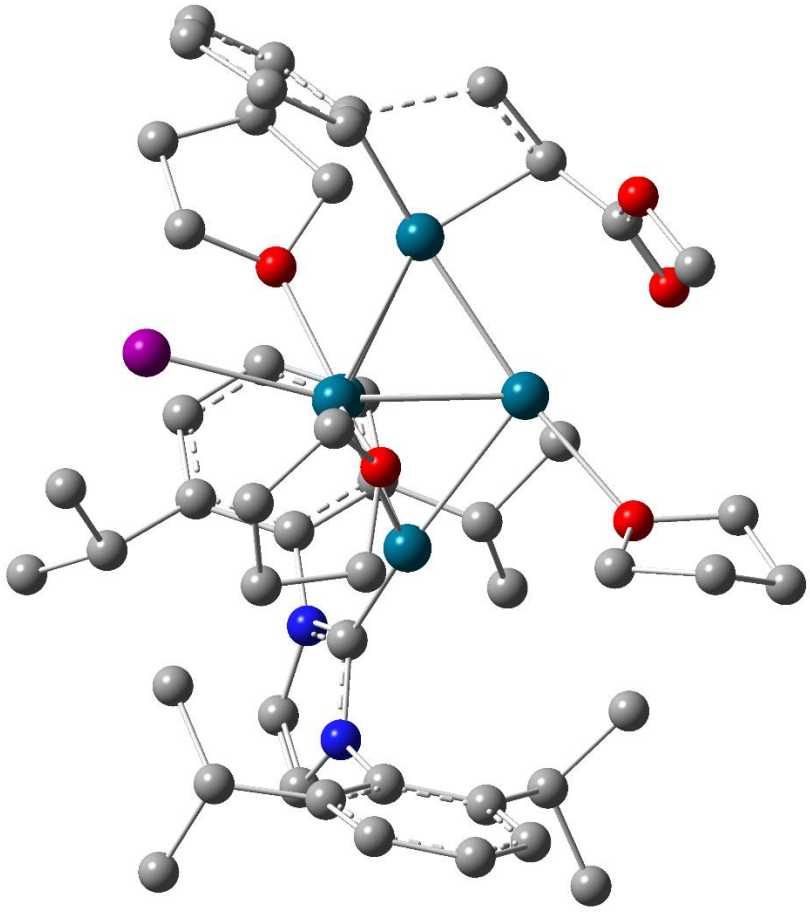
	H -5.05260 -2.18160 -0.24770 H -4.62850 -3.91210 -2.74210 H -4.59370 -4.44650 -1.04690 H -2.23600 -3.77050 -2.26710 H -2.54650 -3.19770 -0.60810 O 0.34950 -0.85880 3.15280 C 0.68750 -1.97340 3.99070 C 2.20520 -1.91270 4.17630 C 2.56690 -0.45740 3.81120 C 1.21710 0.20610 3.57150 H 0.32210 -2.87930 3.50050 H 0.16200 -1.85420 4.94780 H 2.71150 -2.61680 3.51160 H 2.47910 -2.16650 5.20350 H 3.16110 -0.42130 2.89420 H 3.12810 0.05110 4.59890 H 1.22280 0.95590 2.77840 H 0.80800 0.63960 4.49530 O 0.88250 2.01660 -2.31800 C 0.83690 3.42020 -2.01000 C 1.30580 4.09410 -3.28270 C 2.41180 3.14080 -3.73390 C 1.84950 1.77370 -3.36480 H 1.51340 3.62890 -1.17310 H -0.18760 3.65190 -1.71460 H 1.66160 5.11230 -3.10500 H 0.49540 4.12930 -4.01950 H 3.32700 3.33640 -3.16540 H 2.64400 3.21420 -4.79940 H 2.61160 1.08530 -2.98810 H 1.31360 1.29740 -4.19290
VIa E = -2403.889318, E+ZPE = -2403.216142, H = -2403.166705, G = -2403.308643	



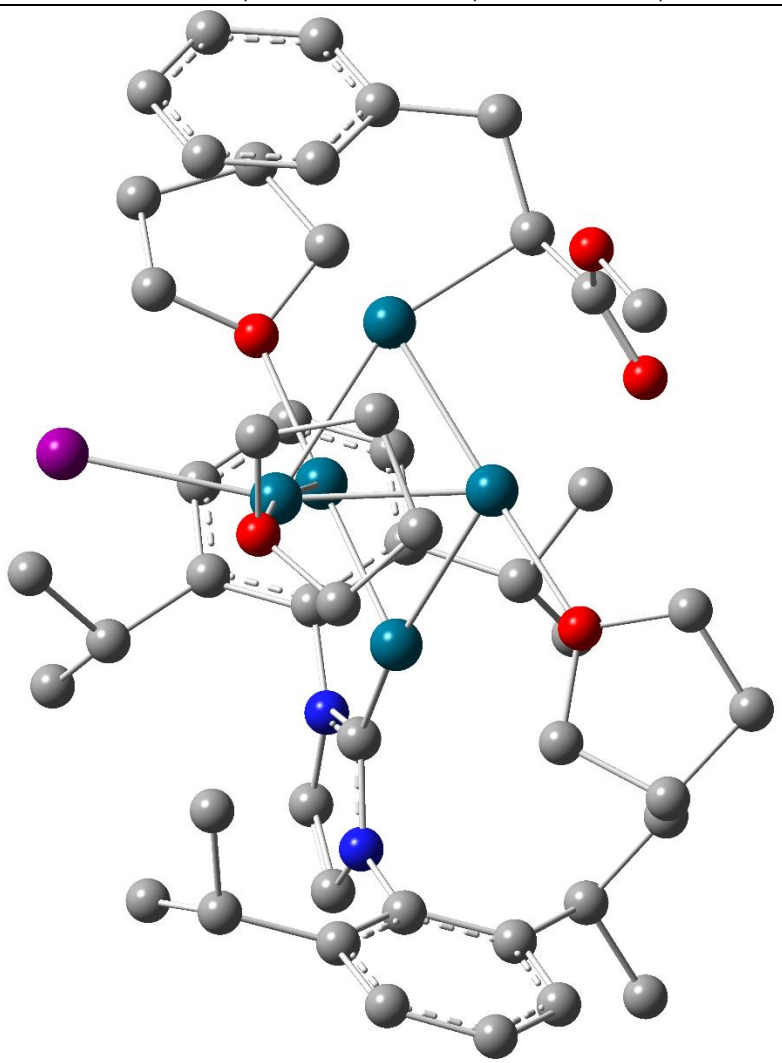
O	-1.71880	-3.51680	1.29960
C	-1.65210	-4.12850	-0.00070
C	-1.50670	-5.61390	0.29720
C	-0.75230	-5.64090	1.64390
C	-0.70150	-4.17150	2.07110
H	-0.78090	-3.72780	-0.53670
H	-2.56070	-3.85450	-0.54020
H	-0.96690	-6.12880	-0.50110
H	-2.49070	-6.08010	0.39720
H	0.25740	-6.04700	1.54390
H	-1.28570	-6.24710	2.38030
H	0.27250	-3.71600	1.82480
H	-0.92080	-3.99110	3.12490
Pd	0.89110	-1.42230	0.84750
Pd	-0.26600	-0.02390	-0.90740
Pd	-1.46370	1.20410	1.14720
Pd	-1.56180	-1.30430	1.21170
Pd	1.05200	1.18730	1.25270
C	3.21510	2.98460	0.40080
C	2.71320	2.36670	-0.75580
C	3.54640	1.60680	-1.57600
C	4.89820	1.46560	-1.26740
C	5.41090	2.08250	-0.12760
C	4.57230	2.82660	0.70110
H	1.67010	2.50390	-1.02750
H	3.13190	1.12560	-2.45780
H	5.54770	0.88100	-1.91310
H	6.46400	1.98050	0.12120
H	4.97630	3.29960	1.59370
C	2.32810	3.83330	1.28980
C	0.98490	3.20790	1.65700
C	-0.20440	3.62450	0.92760
O	-1.37260	3.48480	1.34400
O	0.03320	4.18880	-0.26670
C	-1.11420	4.43660	-1.07760
H	2.87720	4.04190	2.21310
H	2.16820	4.80320	0.79930
H	0.77080	3.22480	2.72940
H	-0.73160	4.87860	-1.99860
H	-1.62870	3.49730	-1.29550
H	-1.79940	5.13240	-0.58680
I	0.82570	-1.58650	-2.70210
O	-3.68660	1.20070	1.19880
C	-4.42900	2.32120	0.68100
C	-5.86430	1.83430	0.59490
C	-5.67700	0.35550	0.26020
C	-4.46820	-0.00600	1.10660
H	-4.02960	2.58580	-0.30500
H	-4.28120	3.16400	1.35910
H	-6.43980	2.37860	-0.15810
H	-6.36500	1.94680	1.56270
H	-5.44900	0.23120	-0.80420
H	-6.54690	-0.26000	0.50140
H	-3.84090	-0.78980	0.65570
H	-4.75000	-0.31150	2.12100
O	3.08570	-1.73390	0.90650
C	3.83510	-0.73060	1.60900
C	5.27390	-1.21300	1.51020
C	5.31490	-1.94670	0.15410
C	3.84610	-2.03330	-0.27510
H	3.44120	-0.67750	2.62590
H	3.69620	0.23880	1.11220
H	5.49690	-1.90240	2.32950
H	5.97940	-0.38050	1.56370
H	5.75990	-2.93930	0.25820
H	5.89550	-1.39520	-0.58960

	H 3.53170 -3.01980 -0.62040 H 3.60390 -1.29340 -1.04530 O -1.42960 1.28550 -2.28640 C -1.02370 1.51180 -3.64740 C -1.86580 0.56410 -4.51430 C -2.87370 -0.05180 -3.52730 C -2.80810 0.89630 -2.34520 H 0.05010 1.32660 -3.69940 H -1.22150 2.56460 -3.88570 H -1.24470 -0.20640 -4.97720 H -2.37090 1.12050 -5.30860 H -2.54150 -1.04620 -3.21340 H -3.88260 -0.13300 -3.94000 H -3.05690 0.45670 -1.37790 H -3.41940 1.79520 -2.51310
IVb-Pd_5 E = -3330.523908, E+ZPE = -3329.396966, H = -3329.322616, G = -3329.516360	
	I 2.03370 0.89090 3.00840 O -1.49780 -3.16960 -1.29580 C -1.81710 -3.80460 -0.04590 C -2.16580 -5.24120 -0.39820 C -2.75510 -5.08750 -1.79870 C -1.85840 -4.01700 -2.39690 H -2.67280 -3.27960 0.39840 H -0.95460 -3.70310 0.61640 H -2.85850 -5.68720 0.32030 H -1.26010 -5.85740 -0.43190 H -3.78940 -4.73130 -1.73690 H -2.74200 -6.01200 -2.38190 H -2.34980 -3.39940 -3.15440 H -0.94640 -4.44120 -2.83050 O 2.14430 2.42960 -1.28950 C 3.02040 2.17030 -2.38760 C 3.94680 3.37620 -2.40930 C 4.03360 3.79590 -0.92770 C 2.94330 2.97770 -0.22920 H 2.40050 2.05430 -3.27880 H 3.56490 1.23670 -2.19800 H 3.50780 4.17710 -3.01080 H 4.92120 3.12710 -2.83740 H 3.86050 4.86910 -0.81440 H 5.01210 3.56960 -0.49580 H 2.27420 3.56560 0.39780 H 3.35400 2.15700 0.36550 O 0.31560 -2.45580 2.40100 C 1.18360 -2.83420 3.48120 C 0.46860 -2.45720 4.78680 C -0.76860 -1.68490 4.31600 C -0.99620 -2.26040 2.93240 H 2.12230 -2.29340 3.34150 H 1.37890 -3.91220 3.41740 H 1.10750 -1.85160 5.43470 H 0.17740 -3.35630 5.33880 H -0.54560 -0.61680 4.23720 H -1.63160 -1.81870 4.97420 H -1.53030 -1.59470 2.24500 H -1.52630 -3.22440 2.98030 C -2.73010 1.33330 -0.05850 N -3.96660 1.26770 0.49570 C -4.67820 2.43690 0.28870 C -3.85500 3.26650 -0.39650 N -2.66400 2.57620 -0.59260 C -4.44230 0.03950 1.05350 C -4.99450 -0.89430 0.16060 C -5.37960 -2.13640 0.67170 C -5.21560 -2.42990 2.01950 C -4.67570 -1.48020 2.88030

	C -4.27530 -0.21990 2.42460 C -1.52000 3.13720 -1.24980 C -1.18470 2.68580 -2.54830 C -0.20170 3.40660 -3.23990 C 0.41330 4.51320 -2.67000 C 0.08260 4.91790 -1.38090 C -0.88820 4.24220 -0.64190 H -5.69220 2.56310 0.63450 H -3.99460 4.27410 -0.75650 C -5.17250 -0.59200 -1.31440 H -5.80480 -2.87910 0.00220 H -5.51130 -3.40220 2.40390 H -4.55710 -1.71340 3.93550 C -3.76210 0.77200 3.45670 C -1.97290 1.58890 -3.24080 H 0.06520 3.10280 -4.24720 H 1.16170 5.06360 -3.23290 H 0.58970 5.77020 -0.93790 C -1.21330 4.67050 0.77550 C -1.52600 6.16250 0.87370 C -0.08440 4.27010 1.72590 C -1.09930 0.67640 -4.09450 C -3.11320 2.20540 -4.05480 C -6.64720 -0.65340 -1.71440 C -4.32160 -1.52650 -2.17350 C -2.48130 1.53580 3.11520 C -4.87530 1.74360 3.86260 H -4.82510 0.42850 -1.50090 H -3.53630 0.15930 4.33810 H -2.41120 0.95710 -2.46280 H -2.10570 4.12830 1.09830 H -1.81700 6.41810 1.89810 H -0.65660 6.77730 0.61720 H -2.34710 6.44700 0.20700 H -0.36730 4.47800 2.76360 H 0.14340 3.20210 1.64280 H 0.83060 4.83360 1.51060 H -0.29510 0.24380 -3.48670 H -1.70180 -0.14840 -4.49020 H -0.65620 1.19800 -4.95010 H -3.72060 1.42010 -4.51830 H -3.77100 2.81410 -3.42500 H -2.72380 2.84740 -4.85370 H -6.76410 -0.38620 -2.77010 H -7.05740 -1.66010 -1.57820 H -7.25150 0.03960 -1.11960 H -4.40090 -1.24810 -3.23030 H -3.26700 -1.48200 -1.87920 H -4.65720 -2.56510 -2.07650 H -2.66890 2.36500 2.42810 H -2.06370 1.96290 4.03320 H -1.71620 0.89690 2.66350 H -4.54270 2.37110 4.69670 H -5.13920 2.40740 3.03260 H -5.77970 1.21140 4.17480 Pd 0.42710 1.23790 -0.80500 Pd 0.94970 -0.55820 1.01150 Pd 0.32200 -1.70660 -1.32890 Pd -1.47610 -0.13860 -0.06200 Pd 2.73840 -0.86500 -0.80660 C 4.38550 -0.62180 0.35140 C 4.54270 -1.55130 1.39070 C 5.56480 -1.41600 2.33020 C 6.46390 -0.35380 2.24250 C 6.34350 0.55550 1.19430 C 5.32260 0.41230 0.25190

	H 3.84500 -2.38140 1.48430 H 5.65370 -2.14010 3.13720 H 7.25740 -0.24380 2.97700 H 7.04780 1.38000 1.10420 H 5.26120 1.12830 -0.56470 C 4.24970 -1.51250 -2.15430 C 3.00180 -1.58130 -2.80080 C 2.17140 -2.78750 -2.84040 O 1.04370 -2.81900 -3.35450 O 2.74670 -3.87360 -2.30830 C 1.88500 -4.99370 -2.11640 H 4.93240 -0.70670 -2.40750 H 4.70860 -2.41420 -1.76110 H 2.67430 -0.79950 -3.48040 H 2.49790 -5.76160 -1.64420 H 1.05490 -4.71810 -1.45750 H 1.49410 -5.35950 -3.06900
TS-Vb-Pd_5 E = -3330.511983, E+ZPE = -3329.385366, H = -3329.310832, G = -3329.505540	
	I 2.09630 0.91200 3.02980 O -1.46290 -3.18080 -1.39010 C -1.79420 -3.87660 -0.17670 C -1.99590 -5.32690 -0.58350 C -2.52610 -5.18290 -2.00860 C -1.69940 -4.01960 -2.53080 H -2.71460 -3.43850 0.23200 H -0.98090 -3.72150 0.53600 H -2.67980 -5.85490 0.08610 H -1.03740 -5.85900 -0.58740 H -3.59040 -4.92270 -1.99310 H -2.40030 -6.08460 -2.61370 H -2.20960 -3.42060 -3.29140 H -0.73350 -4.34590 -2.93110 O 2.11970 2.47320 -1.26780 C 2.98000 2.23760 -2.38350 C 3.93540 3.42510 -2.38150 C 3.97080 3.87510 -0.90480 C 2.93770 2.98910 -0.20830 H 2.34870 2.16190 -3.27080 H 3.50450 1.28510 -2.23430 H 3.54980 4.22580 -3.01830 H 4.92090 3.14170 -2.76050 H 3.70530 4.93180 -0.81650 H 4.95770 3.74160 -0.45400 H 2.27610 3.51950 0.47550 H 3.39710 2.15240 0.32600 O 0.32740 -2.44040 2.41130 C 1.16840 -2.80710 3.51290 C 0.47660 -2.30660 4.79110 C -0.81320 -1.64880 4.28020 C -0.99850 -2.29650 2.92070 H 2.14240 -2.34430 3.33940 H 1.28630 -3.89900 3.51850 H 1.10350 -1.59270 5.33150 H 0.25600 -3.14320 5.46090 H -0.66500 -0.57260 4.15350 H -1.66780 -1.81130 4.94290 H -1.56040 -1.69170 2.20070 H -1.47200 -3.28730 3.00700 C -2.76890 1.29670 -0.08600 N -4.00850 1.22250 0.46240 C -4.73380 2.38070 0.24010 C -3.91730 3.21410 -0.44840 N -2.71690 2.53650 -0.63180 C -4.46990 -0.00160 1.04050 C -5.00120 -0.96260 0.16400 C -5.37390 -2.19880 0.69850

	C -5.21630 -2.46190 2.05320 C -4.69460 -1.48730 2.89720 C -4.30800 -0.23170 2.41770 C -1.57610 3.10480 -1.28780 C -1.22420 2.64230 -2.57750 C -0.24430 3.36680 -3.26960 C 0.35300 4.48750 -2.70850 C 0.00850 4.90160 -1.42620 C -0.95900 4.22170 -0.68680 H -5.75120 2.49800 0.57890 H -4.06840 4.21620 -0.81900 C -5.17390 -0.69530 -1.31840 H -5.78450 -2.96070 0.04160 H -5.50210 -3.42970 2.45600 H -4.57910 -1.69720 3.95750 C -3.81050 0.78590 3.43230 C -1.98800 1.52300 -3.26100 H 0.03470 3.05380 -4.27080 H 1.10020 5.03940 -3.27190 H 0.50420 5.76300 -0.98780 C -1.28980 4.65340 0.72830 C -1.60000 6.14590 0.82490 C -0.16420 4.25180 1.68290 C -1.09360 0.61810 -4.10170 C -3.13750 2.10760 -4.08550 C -6.64870 -0.75680 -1.71780 C -4.32790 -1.65520 -2.15430 C -2.53950 1.56030 3.07780 C -4.93690 1.74930 3.82020 H -4.81860 0.31780 -1.52840 H -3.57730 0.19230 4.32490 H -2.41510 0.89100 -2.47680 H -2.18440 4.11290 1.04810 H -1.89620 6.40210 1.84760 H -0.72800 6.75930 0.57350 H -2.41670 6.43210 0.15350 H -0.44800 4.46460 2.71940 H 0.06050 3.18270 1.60340 H 0.75280 4.81180 1.46660 H -0.28540 0.20400 -3.48580 H -1.68040 -0.22030 -4.49250 H -0.65530 1.13910 -4.96040 H -3.72750 1.30530 -4.54240 H -3.80970 2.70960 -3.46440 H -2.75850 2.74870 -4.89010 H -6.76370 -0.51750 -2.78050 H -7.06580 -1.75670 -1.55400 H -7.24850 -0.04370 -1.14240 H -4.40410 -1.39970 -3.21730 H -3.27330 -1.61180 -1.86070 H -4.67010 -2.68970 -2.03610 H -2.74010 2.37860 2.38140 H -2.12460 2.00370 3.98930 H -1.76880 0.92500 2.63040 H -4.61370 2.39590 4.64330 H -5.20880 2.39490 2.97850 H -5.83450 1.21080 4.14110 Pd 0.42050 1.23850 -0.79600 Pd 0.90420 -0.51690 1.08470 Pd 0.31250 -1.70190 -1.28760 Pd -1.48510 -0.15640 -0.08840 Pd 2.65770 -0.77160 -0.82100 C 4.57190 -0.71730 0.00930 C 4.71080 -1.65520 1.04440 C 5.53170 -1.38510 2.13570 C 6.24870 -0.18970 2.19870

	C 6.15520 0.72280 1.15000 C 5.33690 0.45350 0.05380 H 4.15450 -2.58880 1.00460 H 5.60840 -2.11010 2.94230 H 6.88710 0.02070 3.05200 H 6.72400 1.64910 1.18110 H 5.29040 1.16520 -0.76660 C 4.46590 -1.52060 -1.86660 C 3.22880 -1.62540 -2.59910 C 2.39300 -2.82360 -2.60980 O 1.30080 -2.88680 -3.19100 O 2.90910 -3.87100 -1.94460 C 1.99820 -4.93630 -1.68510 H 5.19220 -0.81910 -2.26760 H 4.90270 -2.44890 -1.51190 H 3.00470 -0.92500 -3.40060 H 2.55280 -5.66450 -1.09260 H 1.14190 -4.56050 -1.11470 H 1.64990 -5.39650 -2.61320
VIb-Pd5 E = -3330.571344, E+ZPE = -3329.441474, H = -3329.367627, G = -3329.558003	
	I 2.01340 1.06470 3.23440 O -1.47160 -3.46520 -0.50080 C -1.53820 -4.57280 -1.41530 C -2.97730 -4.59390 -1.88390 C -3.71390 -4.21920 -0.60070 C -2.78100 -3.19240 0.03310 H -1.28430 -5.49660 -0.87540 H -0.79720 -4.39810 -2.19570 H -3.27420 -5.56600 -2.28590 H -3.13190 -3.83210 -2.65610 H -3.81340 -5.09640 0.04800 H -4.71050 -3.80880 -0.77290 H -2.74260 -3.26500 1.12380 H -3.05170 -2.16310 -0.23850 O 2.18600 2.51730 -0.88450 C 2.96020 2.26870 -2.06130 C 4.01610 3.37370 -2.07810 C 4.05810 3.87520 -0.61870 C 3.11600 2.93290 0.12010 H 2.27630 2.27920 -2.91030 H 3.41530 1.27240 -1.97970 H 3.73070 4.17930 -2.75980 H 4.98060 2.98060 -2.40950 H 3.69530 4.90480 -0.55480 H 5.06300 3.84360 -0.19020 H 2.54500 3.39460 0.92500 H 3.63730 2.05230 0.51360 O 0.86320 -2.23820 2.89040 C -0.09860 -3.28570 2.70000 C 0.63420 -4.44270 2.00150 C 2.06790 -3.91850 1.83910 C 2.14730 -2.86670 2.92810 H -0.90550 -2.86480 2.10040 H -0.49020 -3.58480 3.68100 H 0.17020 -4.67290 1.04000 H 0.61210 -5.34400 2.62160 H 2.18330 -3.42440 0.86690 H 2.82890 -4.69750 1.93930 H 2.89770 -2.09030 2.76950 H 2.29900 -3.32110 3.91890 C -2.76300 1.36030 -0.03910 N -4.06170 1.34640 0.35990 C -4.67790 2.56700 0.13930 C -3.73950 3.37720 -0.39940 N -2.57470 2.62580 -0.49510 C -4.74980 0.15800 0.75550

	C -5.45570 -0.52470 -0.25320 C -6.15410 -1.67800 0.10500 C -6.13540 -2.14060 1.41590 C -5.42000 -1.45200 2.38590 C -4.71000 -0.28200 2.08810 C -1.36790 3.15880 -1.05690 C -0.99210 2.77070 -2.36710 C -0.01110 3.54160 -3.00610 C 0.56830 4.63570 -2.37950 C 0.20490 4.97570 -1.07970 C -0.76740 4.25270 -0.39270 H -5.71480 2.73660 0.38420 H -3.78020 4.40740 -0.71650 C -5.43410 -0.06990 -1.70140 H -6.71090 -2.22280 -0.65240 H -6.68280 -3.04050 1.68260 H -5.41070 -1.81710 3.41020 C -3.93320 0.35240 3.23300 C -1.73110 1.68990 -3.13370 H 0.27640 3.28780 -4.02210 H 1.31350 5.22680 -2.90450 H 0.68120 5.82050 -0.58990 C -1.15260 4.64360 1.01960 C -1.72170 6.06170 1.07290 C 0.03480 4.48330 1.96760 C -0.78450 0.74280 -3.86580 C -2.74980 2.32430 -4.08320 C -6.84290 0.08400 -2.27310 C -4.58980 -1.02290 -2.55120 C -2.56450 -0.32140 3.38280 C -3.78450 1.87270 3.22920 H -4.95630 0.91260 -1.74920 H -4.51390 0.09870 4.12980 H -2.27500 1.08120 -2.40630 H -1.93050 3.95560 1.36320 H -2.04280 6.30400 2.09160 H -0.97140 6.80260 0.77530 H -2.58520 6.17540 0.40890 H -0.26380 4.72150 2.99440 H 0.40520 3.45350 1.95430 H 0.85900 5.15250 1.69530 H -0.08790 0.27930 -3.15720 H -1.35800 -0.05670 -4.34790 H -0.20820 1.25140 -4.64710 H -3.32440 1.54830 -4.60110 H -3.45560 2.96390 -3.54190 H -2.25360 2.93950 -4.84290 H -6.79320 0.47830 -3.29350 H -7.37190 -0.87410 -2.31550 H -7.44360 0.77390 -1.67130 H -4.56240 -0.68230 -3.59220 H -3.55890 -1.07090 -2.18340 H -5.00680 -2.03620 -2.54090 H -1.93310 -0.12970 2.50220 H -2.03790 0.07190 4.25930 H -2.66430 -1.40520 3.50220 H -3.44560 2.19430 4.21960 H -3.03830 2.21410 2.50780 H -4.73150 2.37980 3.01950 Pd 0.40780 1.33160 -0.47270 Pd 0.82240 -0.46670 1.37510 Pd 0.23440 -1.98100 -0.73500 Pd -1.51650 -0.13320 0.02800 Pd 2.41080 -0.72840 -0.73750 C 5.05430 -0.91880 -1.27800 C 4.73990 -1.31130 0.03930

	C 5.17570 -0.54640 1.12770 C 5.94290 0.59620 0.91950 C 6.28670 0.97160 -0.37940 C 5.83670 0.22550 -1.46620 H 4.22950 -2.25770 0.21230 H 4.91830 -0.85310 2.13700 H 6.27670 1.18770 1.76710 H 6.89920 1.85350 -0.54690 H 6.09350 0.52910 -2.47860 C 4.52830 -1.72720 -2.44580 C 3.00440 -1.73610 -2.45000 C 2.29440 -2.99010 -2.28780 O 1.09260 -3.16190 -2.57680 O 3.02550 -4.00120 -1.77520 C 2.31720 -5.20870 -1.51690 H 4.90200 -1.29210 -3.37880 H 4.91720 -2.74940 -2.38760 H 2.54120 -1.13800 -3.23740 H 3.03080 -5.87290 -1.02770 H 1.46220 -5.02930 -0.86050 H 1.96530 -5.66400 -2.44740

References

(S1) Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian, Inc., Wallingford CT, 2019.

(S2) C. Adamo and V. Barone, *J. Chem. Phys.*, 1999, **110**, 6158; https://doi.org/10.1063/1.478522.

(S3) S. Grimme, S. Ehrlich and L. Goerigk, *J. Comp. Chem*., 2011, **32**, 1456; https://doi.org/10.1002/jcc.21759.

(S4) F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297; https://doi.org/10.1039/B508541A.

(S5) G. A. Petersson and M. A. Al-Laham, *J. Chem. Phys.*, 1991, **94**, 6081; https://doi.org/10.1063/1.460447.

(S6) A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378; https://doi.org/10.1021/jp810292n.