

Actinide-Catalyzed Intermolecular Addition of Alcohols to Carbodiimides

Rami J. Batrice,[†] Christos E. Kefalidis,[‡] Laurent Maron,[‡] Moris S. Eisen^{†,*}

[†]Schulich Faculty of Chemistry, Technion – Israel Institute of Technology, Haifa 3200008, Israel.
[‡]LPCNO, CNRS, & INSA, Université Paul Sabatier, 135 Avenue de Rangueil, Toulouse 31077, France.

*E-mail: chmoris@tx.technion.ac.il

Supplementary Information

Experimental Section

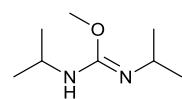
All manipulations of air-sensitive materials were performed with the rigorous exclusion of oxygen and moisture in flamed Schlenk-type glassware or J-Young Teflon valve-sealed NMR tubes on a dual manifold Schlenk line interfaced to a high vacuum (10^{-5} Torr) line, or in a nitrogen-filled Innovative Technologies glovebox with a medium-capacity recirculator (1 – 2 ppm of O₂). Argon and nitrogen were purified by passage through MnO oxygen-removal column and a Davison 4 Å molecular sieve column. Hydrocarbon solvents benzene-d₆ (Cambridge Isotopes), toluene (Bio-Lab), and diethyl ether (BioLab) were distilled under vacuum from Na/K alloy. 1,3-diisopropylcarbodiimide was distilled from sodium bicarbonate under nitrogen atmosphere, and 1,3-di-p-tolylcarbodiimide was dried under vacuum (10^{-6}) for 12 hours on a high vacuum line. Methanol and ethanol were dried using sodium (Na) metal, distilled, and stored over 4 Å molecular sieves. Isopropanol and *tert*-butanol were refluxed over CaH₂, distilled, and stored over 4 Å molecular sieves. The actinide complexes U[N(SiMe₃)₂]₃ (**1**)¹ and [(Me₃Si)₂N]₂An[κ²-(N,C)-CH₂Si(CH₃)₂N(SiMe₃)] (An = U (**2**), Th (**3**))² were prepared according to published procedures. All the aforementioned reagents were stored in an inert atmosphere glovebox prior to use. *O*-deuterated alcohols were prepared by quenching the corresponding metal-alkoxide (NaOEt or KO^tBu) with excess D₂O at reduced temperature, followed by fractional distillation, degassing, and storing over 4 Å molecular sieves.

NMR spectra were recorded on Bruker Avance 300, Bruker Avance III 400, or Bruker Avance 500 spectrometers on crude reaction mixtures. Chemical shifts for ¹H and ¹³C NMR are referenced to internal protiosolvent and reported relative to tetramethylsilane. *J*-values are reported for ¹H NMR coupling constants in the unit of Hertz (Hz).

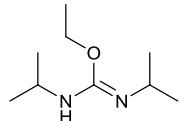
General Procedure for the Catalytic Addition of Alcohols to Carbodiimides

In a typical experiment, approximately 5 mg of desired catalyst in 600 µL of C₆D₆ was transferred to a J. Young Teflon sealed NMR tube, followed by the addition of carbodiimide (100 equiv.) and alcohol (100 equiv.). Samples were then placed in an oil bath preheated to 75 °C, and the reaction progress monitored at regular intervals using ¹H NMR spectroscopy for up to 24 hours. After completion of the reaction, crude mixtures were analysed using ¹H, ¹³C, and 2D NMR (when needed) spectroscopy as well as mass spectrometry. Known compounds were compared to previous literature.

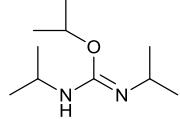
Characterization Data



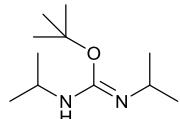
N,N'-diisopropyl-O-methylisourea: The insertion of methanol (5.7 µL, 140 µmol) into diisopropylcarbodiimide (21.9 µL, 140 µmol) was carried out following the general procedure described. ¹H NMR (300 MHz, C₆D₆) δ 3.80 – 3.68 (m, 1H), 3.66 (s, 3H), 3.11 (m, 1H), 2.35 (bs, 1H), 1.22 (d, *J* = 6.2 Hz, 6H), 0.90 (d, *J* = 6.4 Hz, 6H). ¹³C NMR (101 MHz, C₆D₆) δ 151.97, 52.56, 50.09, 46.56, 43.49, 23.92. MS (APCI+): m/z 159.1495 (M + H)*



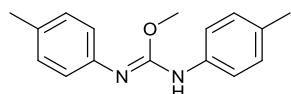
N,N'-diisopropyl-O-ethylisourea: The insertion of ethanol (8.2 μ L, 140 μ mol) into diisopropylcarbodiimide (21.9 μ L, 140 μ mol) was carried out following the general procedure described. ^1H NMR (400 MHz, CDCl_3) δ 4.07 (q, J = 7.1 Hz, 2H), 3.83 – 3.71 (m, 1H), 3.40 (bs, 1H), 3.21 – 3.09 (m, 1H), 1.24 (t, J = 7.0 Hz, 3H), 1.12 (d, J = 6.4 Hz, 6H), 1.09 (d, J = 6.4 Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 151.92, 60.78, 46.28, 43.42, 24.47, 24.06, 14.53. MS (APCI+): m/z 173.1658 ($M + H$)*



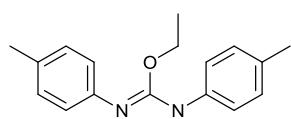
N,N'-diisopropyl-O-isopropylisourea: The insertion of isopropanol (10.7 μ L, 140 μ mol) into diisopropylcarbodiimide (21.9 μ L, 140 μ mol) was carried out following the general procedure described. ^1H NMR (300 MHz, C_6D_6) δ 5.33 (hept, J = 6.2 Hz, 1H), 3.86 – 3.60 (m, 1H), 3.20 (bs, 1H), 3.13 (m, 1H), 1.21 (d, J = 6.2 Hz, 12H), 0.92 (d, J = 6.4 Hz, 6H). ^{13}C NMR (101 MHz, C_6D_6) δ 150.40, 66.58, 46.52, 43.33, 24.91, 23.92, 22.20. MS (ESI+): m/z 187.1850 ($M + H$)*



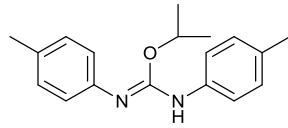
N,N'-diisopropyl-O-tert-butylisourea:³ The insertion of isopropanol (13.3 μ L, 140 μ mol) into diisopropylcarbodiimide (21.9 μ L, 140 μ mol) was carried out following the general procedure described. ^1H NMR (300 MHz, C_6D_6) δ 5.55 (bs, 1H), 3.75 – 3.58 (m, 1H), 3.18 – 3.04 (m, 1H), 1.57 (s, 9H), 1.17 (d, J = 6.4 Hz, 6H), 0.92 (d, J = 6.4 Hz, 6H). ^{13}C NMR (101 MHz, C_6D_6) δ 154.70, 72.75, 48.18, 40.20, 29.62, 22.92, 20.69. MS (APCI+): m/z 201.1962 ($M + H$)*



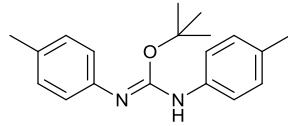
N,N'-di-p-tolyl-O-methylisourea: The insertion of methanol (8.5 μ L, 209 μ mol) into di-p-tolylcarbodiimide (46.4 mg, 209 μ mol) was carried out following the general procedure described. See Figure S1. ^1H NMR (500 MHz, C_6D_6) δ 7.03 (m, 4H), 6.84 (m, 2H), 6.74 (m, 2H), 5.87 (bs, 1H), 3.74 (s, 3H), 2.17 (s, 3H), 2.06 (s, 3H). ^{13}C NMR (126 MHz, C_6D_6) δ 150.74, 146.37, 136.68, 132.49, 132.07, 130.70, 129.56, 122.94, 121.10, 53.66, 20.86, 20.68. MS (APCI+): m/z 255.1507 ($M + H$)*



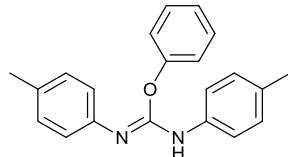
N,N'-di-p-tolyl-O-ethylisourea: The insertion of ethanol (12.2 μ L, 209 μ mol) into di-p-tolylcarbodiimide (46.4 mg, 209 μ mol) was carried out following the general procedure described. ^1H NMR (300 MHz, C_6D_6) δ 7.06 – 7.00 (m, 4H), 6.88 – 6.74 (m, 4H), 5.88 (bs, 1H), 4.37 (q, J = 7.1 Hz, 2H), 2.17 (s, 3H), 2.05 (s, 3H), 1.13 (t, J = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, C_6D_6) δ 150.15, 146.51, 136.86, 132.28, 131.98, 130.70, 129.56, 122.97, 120.90, 62.69, 20.86, 20.69, 14.39. MS (APCI+): m/z 269.1668 ($M + H$)*



N,N'-di-p-tolyl-O-isopropylisourea: The insertion of isopropanol (16.0 μ L, 209 μ mol) into di-*p*-tolylcarbodiimide (46.4 mg, 209 μ mol) was carried out following the general procedure described. ^1H NMR (500 MHz, C_6D_6) δ 7.03 (d, J = 7.9 Hz, 1H), 6.87 – 6.75 (m, 1H), 5.89 (s, 1H), 5.54 – 5.44 (m, 1H), 2.16 (s, 1H), 2.05 (s, 1H), 1.26 (d, J = 6.2 Hz, 2H). ^{13}C NMR (126 MHz, C_6D_6) δ 149.60, 146.61, 136.98, 132.15, 131.90, 130.69, 129.55, 122.96, 120.82, 69.64, 21.99, 20.86, 20.68. MS (APCI+): m/z 283.1808 ($M + \text{H}$)*



N,N'-di-p-tolyl-O-tert-butylisourea: The insertion of *tert*-butanol (33.2 μ L, 350 μ mol) and 1,3-di-*p*-tolylcarbodiimide (55 μ L, 350 μ mol) was carried out following the general procedure described. δ_{H} (300 MHz, C_6D_6) 7.11 – 6.92 (4 H, m), 6.90 – 6.73 (4 H, m), 5.85 (1 H, bs), 2.17 (3 H, s), 2.06 (3 H, s), 1.60 (9 H, s). ^{13}C NMR (75 MHz, C_6D_6) δ 148.64, 145.08, 131.83, 130.12, 129.66, 122.79, 120.98, 120.79, 118.65, 81.26, 28.51, 28.40, 20.79. MS (APCI+): m/z 295.0716 ($M + \text{H}$)*



N,N'-di-p-tolyl-O-phenylisourea: The insertion of phenol (19.7 mg, 350 μ mol) and 1,3-di-*p*-tolylcarbodiimide (55 μ L, 350 μ mol) was carried out following the general procedure described. ^1H NMR (500 MHz, C_6D_6) δ 7.26 (bs, 1H), 7.02 (m, 4H), 6.81 (d, J = 8.0 Hz, 4H), 6.75 (m, 1H), 6.67 (m, 2H), 6.63 (d, J = 8.0 Hz, 2H), 2.01 (s, 3H), 1.96 (s, 3H). ^{13}C NMR (126 MHz, C_6D_6) δ 156.99, 144.83, 144.10, 136.96, 131.83, 129.68, 129.46, 129.11, 122.37, 121.81, 120.42, 120.17, 115.75, 20.86, 20.78. MS (ESI+): m/z 317.1604 ($M + \text{H}$)*

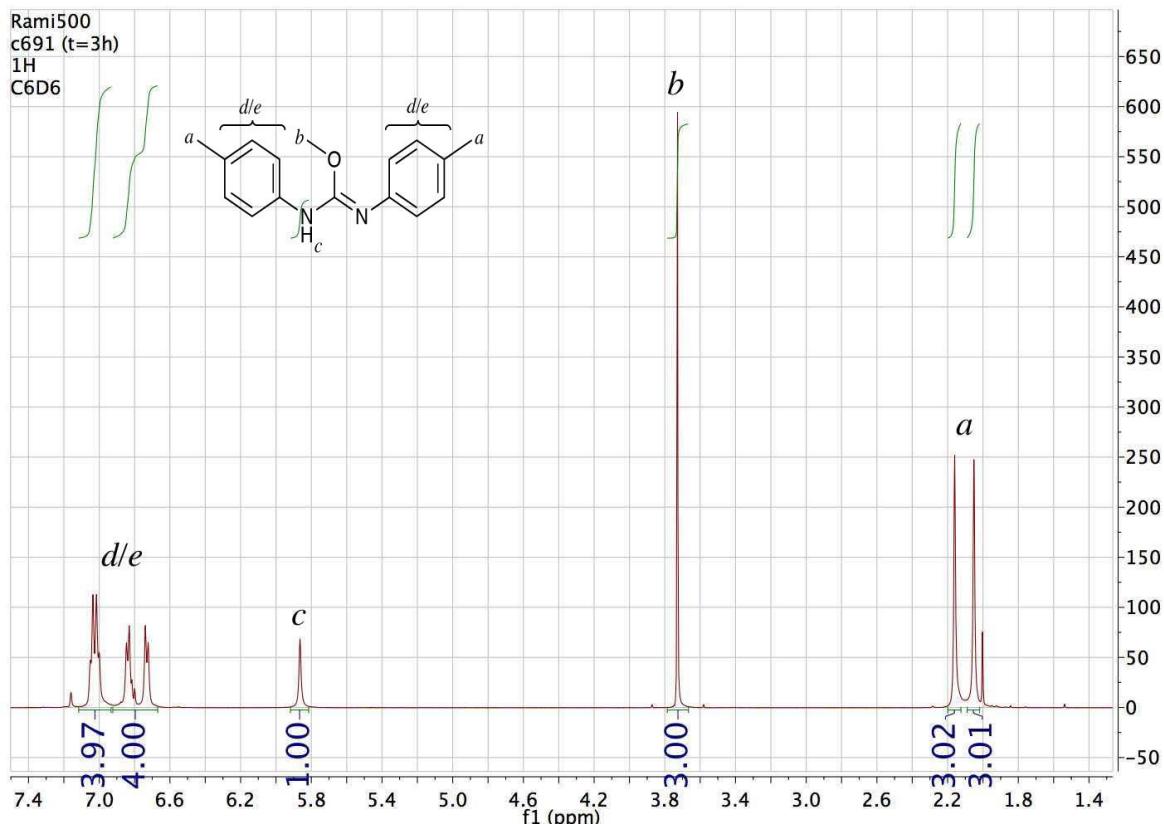


Figure S1: Representative sample of actinide-catalyzed addition of alcohols to carbodiimides. Reaction shown is thorium (**3**) mediated addition of methanol to 1,3-di-*p*-tolylcarbodiimide.

Preparative scale reaction of *tert*-butanol insertion into 1,3-di-*p*-tolylcarbodiimide

In an inert atmosphere glovebox, a Schlenk tube with stir bar and Teflon stopper was added 0.50 g 1,3-di-*p*-tolylcarbodiimide (2.25 mmol). A solution of catalyst **3** (30 mg, 42.1 μ mol, 2 mol%) in 10 mL of toluene was added to the solids, followed by the immediate addition of 215 μ L *tert*-butanol (167 mg, 2.25 mmol). The tube was sealed, removed from the glovebox, and immediately placed in an oil bath preheated to 75 °C with stirring for 24 hours. After completion of the reaction, the solvent was removed *in vacuo*. A yellow viscous liquid remained which was dissolved in 10 mL dichloromethane, filtered through a plug of Celite to remove the catalyst, loaded in a separatory funnel with 20 mL of distilled water, and the organics separated then evaporated to dryness. The oil was then dissolved in *n*-hexane, filtered through a plug of Celite, and evaporated under vacuum, leaving a white waxy solid (0.56 g, 85% isolated yield).

Activation Studies of Precatalysts (1-3)

In an inert atmosphere glovebox, a stock solution of the respective precatalyst was prepared in C₆D₆. An aliquot of the stock solution was transferred to a J-Young Teflon valve-sealed NMR tube, followed by the addition of four equivalents of alcohol. The tube was then sealed, shaken, and heated to 75 °C for 20 minutes, followed by acquiring a ¹H NMR spectrum of the mixture. It was revealed that complete displacement of the amides occurs to form an actinide-alkoxide complex. Attempts to isolate and crystallize these complexes was unsuccessful. In an attempt to elucidate the identity of precatalyst (**1**) after activation, four equivalents of diisopropylcarbodiimide was added, followed by heating and acquisition of the NMR spectrum (Figure S2).

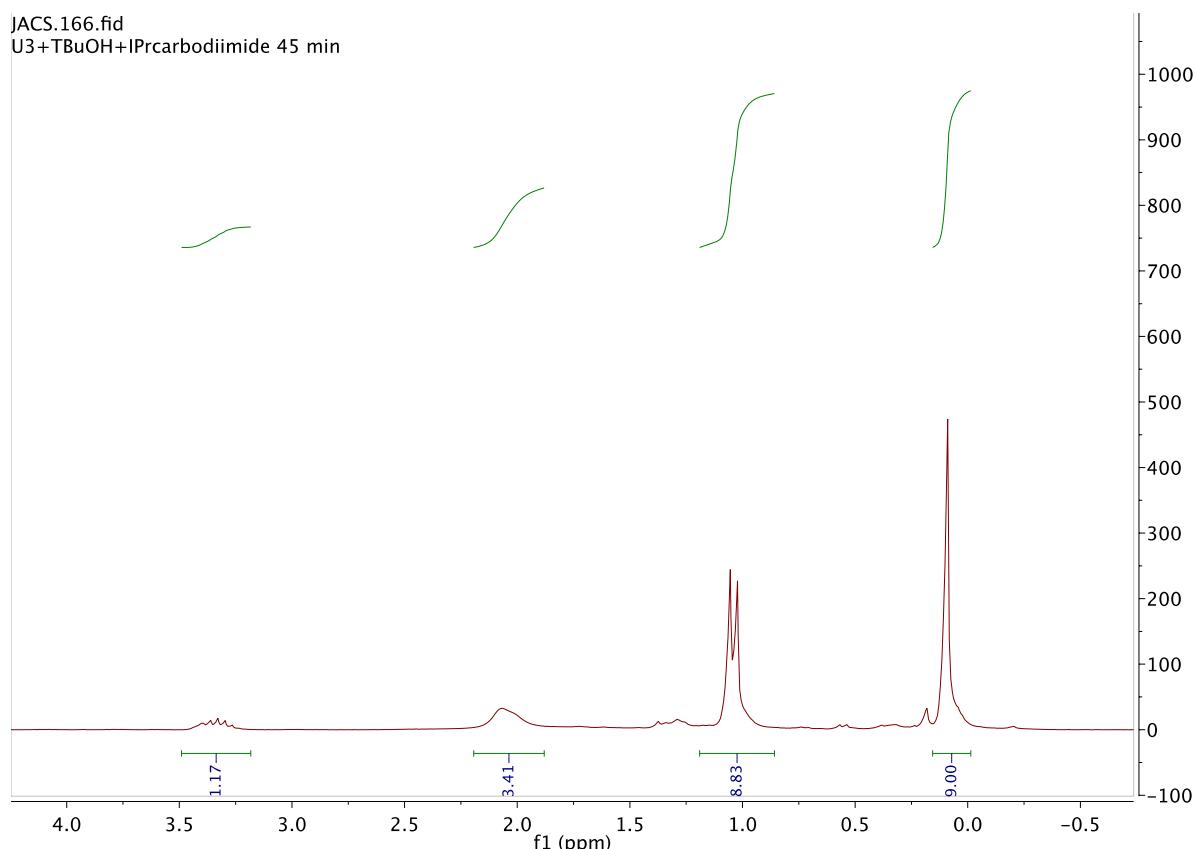


Figure S2: ¹H NMR spectrum of complex 1 after addition of ^tBuOH and DIC, and heating to 75 °C.

Unfortunately, this spectrum, as well as fluorescence studies, did not allow for conclusive assignment of the metal oxidation state and identity of the complex after activation.

Kinetic studies of alcohol insertion into diisopropylcarbodiimide

In a typical experiment, an NMR sample was prepared as described above in the presence of 100 μ L of mesitylene as internal standard ($\delta = 6.70$ and 2.15 ppm). Experiments for reagent-order determination were performed at variable concentrations of catalyst, alcohol, and carbodiimide, spanning one order of magnitude concentration differences while keeping the other reagent concentration constant. The sample tube was inserted into the probe of the Bruker Avance 300 spectrometer which had been previously set to the desired temperature ($T = 75 \pm 0.1$ °C; checked with ethylene glycol temperature standard). Data were acquired every five minutes up to one and one-half hours. Reaction rates were determined by least-squares fit of product concentration versus time, and the collective rate data plotted to determine reagent orders (Figures S3 – S5).

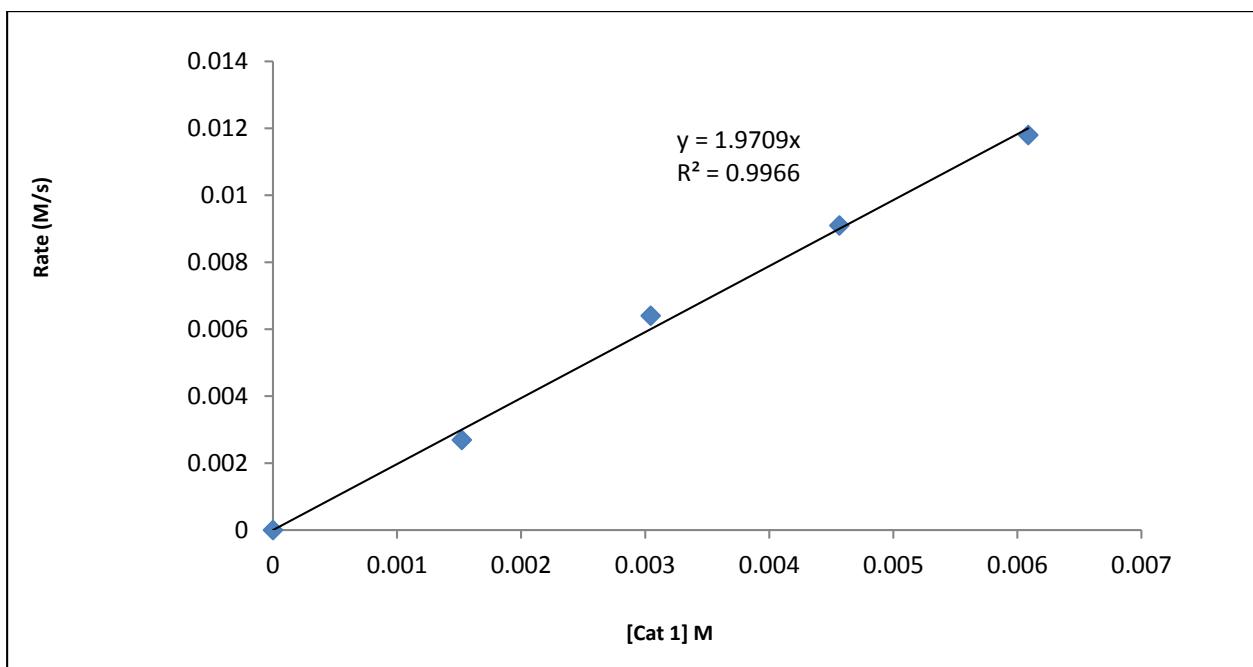


Figure S3: Plot of reaction rate as a function of precatalyst **1** concentration.

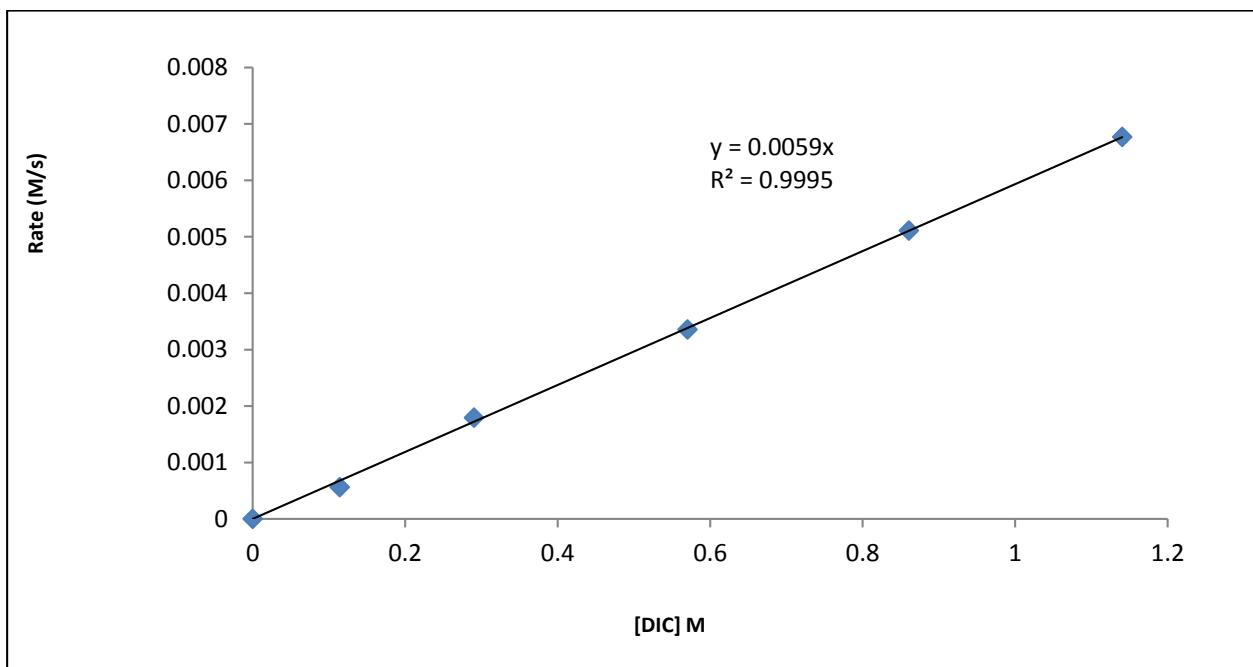


Figure S4: Plot of reaction rate as a function of diisopropylcarbodiimide concentration.

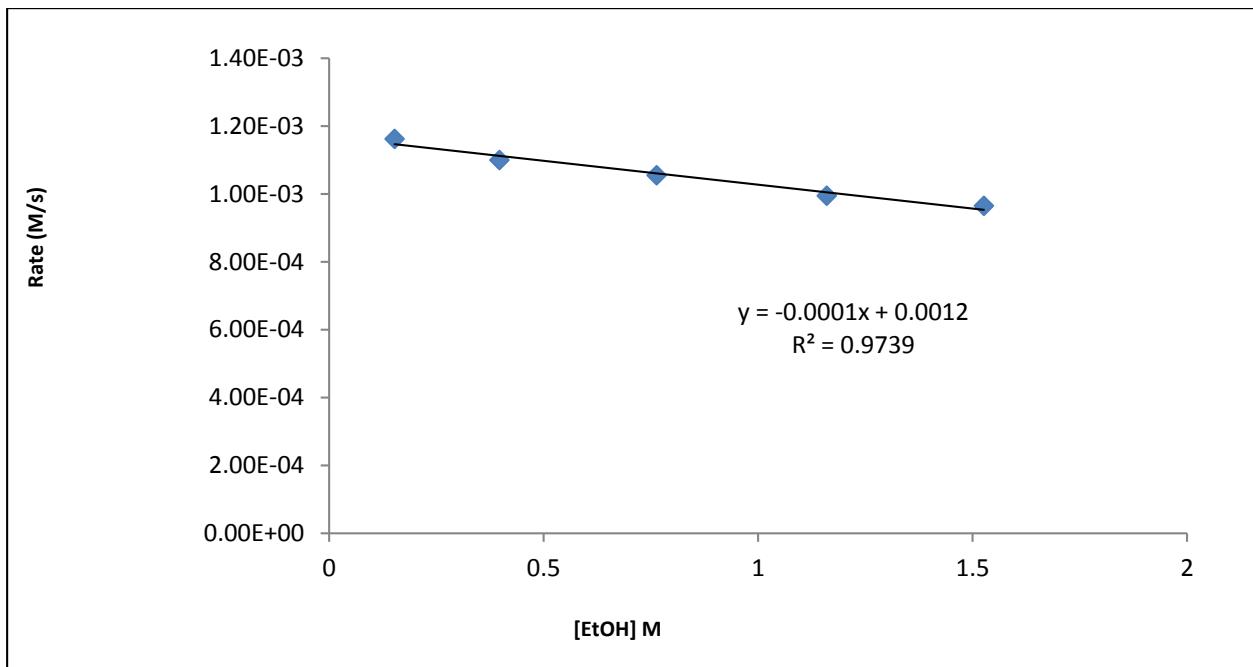
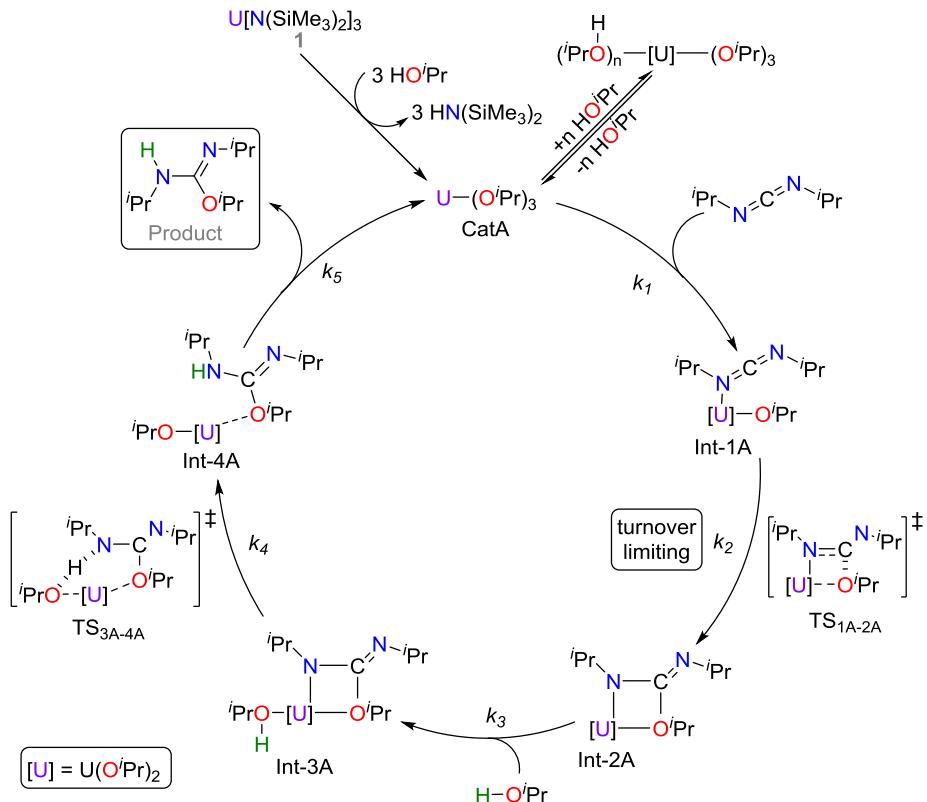


Figure S5: Plot of reaction rate as a function of alcohol concentration.

Discussion of Kinetic Rate Law

According to the kinetic and thermodynamic data obtained, the following mechanism is proposed:



Since the first step of the cycle is turnover limiting (k_1), and the remaining steps of the catalytic cycle are rapid (k_2-k_5), we can assume a steady-state approximation for this reaction, giving the rate equation:

$$\frac{\partial P}{\partial T} = k_1 [Cat_A] [DIC].$$

In describing the formation of the active catalyst, protonolysis of the amide starting material (Cat_A) is rapid and irreversible, however we must consider the equilibrium of alcohol coordination/decoordination, which is described by the following equilibrium expression:

$$K_{eq} = \frac{[satCat_A]}{[ROH][Cat_A]}$$

In studying the relationship between the active catalysts (Cat_A) and the alcohol-saturated complex (satCat_A), we can see that the sum of these two species is the total amount of **1** used in the reaction: [Cat_A] + [satCat_A] = [**1**]. By substituting Cat_A from the equilibrium expression into the rate equation, we see that the kinetic rate law for this reaction is:

$$\frac{\partial P}{\partial T} = \frac{k_1 [DIC][\mathbf{1}]}{(1 + K_{eq}[ROH])}$$

From this equation, we can see that if [ROH] is large, we see inverse-first order behavior, however when [ROH] is small, we see nearly zero-order behavior in alcohol.

Thermodynamic studies of aniline insertion into diisopropylcarbodiimide

Activation parameters (ΔH^\ddagger and ΔS^\ddagger) were calculated from acquired kinetic data using Eyring plots. In a typical experiment, an NMR sample was prepared as described above in the presence of 100 μL of mesitylene as internal standard ($\delta = 6.70$ and 2.15 ppm). The sample tube was inserted into the probe of the Bruker Avance 300 spectrometer which had been previously set to the desired temperature over the range of 35 – 75 °C ($T \pm 0.1$ °C; checked with ethylene glycol temperature standard). Data were acquired five minutes up to one and one-half hours. Reaction rates were determined by least-squares fit of product concentration versus time. Eyring plots were generated in the usual manner (Figures S6 – S8), and the ΔH^\ddagger and ΔS^\ddagger values for activation calculated from the slope and intercept of the least-squares fit, respectively.

Eyring plots of actinide-mediated carbodiimide insertion into alcohols

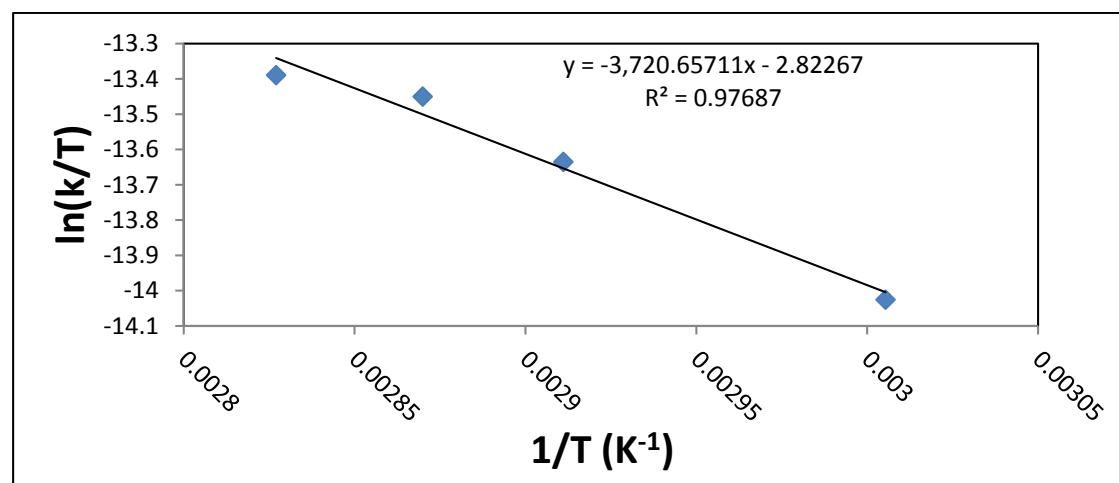


Figure S6: Eyring plot of ethanol addition to diisopropylcarbodiimide mediated by complex 1.

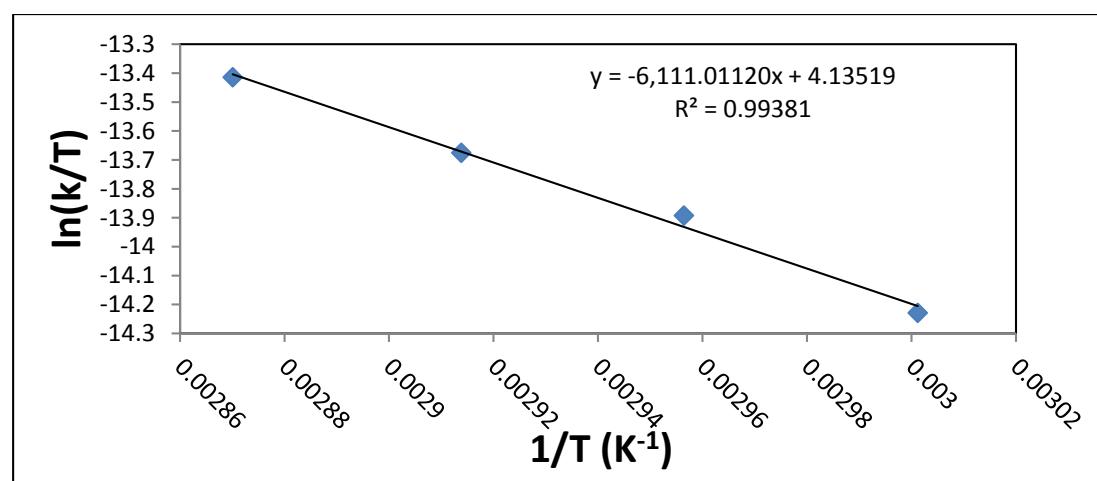


Figure S7: Eyring plot of *tert*-butanol addition to diisopropylcarbodiimide mediated by complex 2.

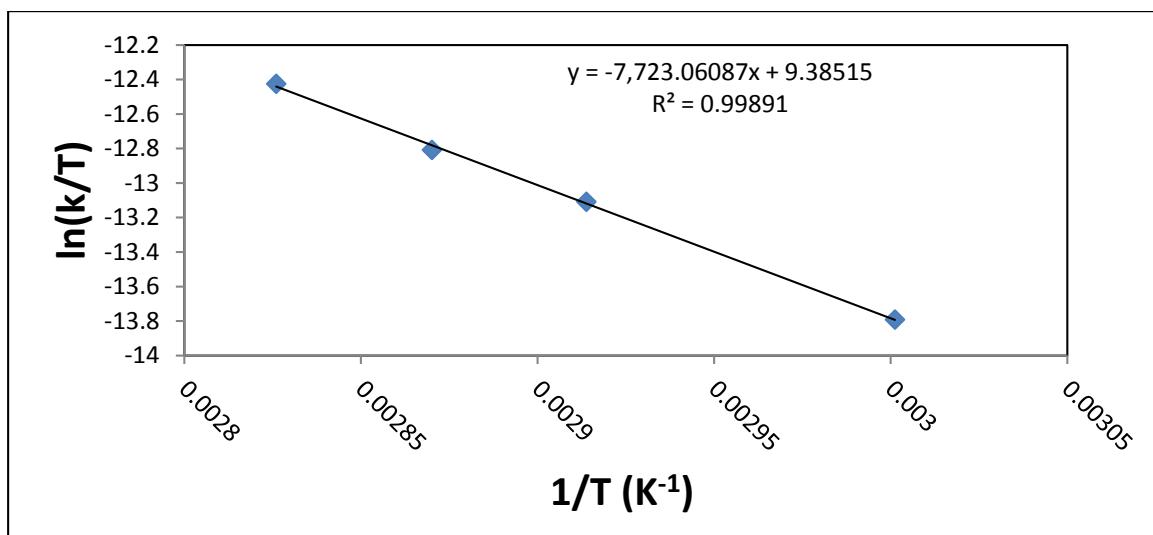


Figure S8: Eyring plot of ethanol addition to diisopropylcarbodiimide mediated by complex **3**.

Computational Details

All the structures reported in this study were fully optimised with the Becke's 3-parameter hybrid functional combined with the non-local correlation functional provided by Perdew/Wang (denoted as B3PW91).⁴ The choice of the basis set for **Cat_A**, which preserves a fixed oxidation state (III) throughout the catalytic process, is the quasi-relativistic energy-consistent 5f-in-core RECP (Relativistic Effective Core Potential), augmented by a *f* polarization function, in combination with its adapted basis set.⁵ The analogous 5f-in-core RECPs (augmented by a *f* polarization function) are used for the fixed oxidation states (IV) of the corresponding U and Th catalytic systems, **Cat_B** and **Cat_C** respectively.⁶ In addition, for the silicon atoms the quasi-relativistic energy-adjusted ab-initio pseudopotential is used, along with its corresponding energy-optimized valence basis set,⁷ augmented by a *d* polarization function.⁸ For the rest of the atoms the 6-31G(d,p) basis set is used.⁹ In all computations no constrains are imposed on the geometry. All stationary points have been identified for minimum (number of imaginary frequencies Nimag=0) or transition states (Nimag=1). Intrinsic Reaction Paths (IRPs) are traced from the various transition structures to verify the reactant to product linkage.¹⁰ Enthalpy energies are obtained at T=298.15K within the harmonic approximation. GAUSSIAN09 program suite is used in all calculations.¹¹ Finally, for the 3D representation of the structures the Cylview graphical program is used.¹²

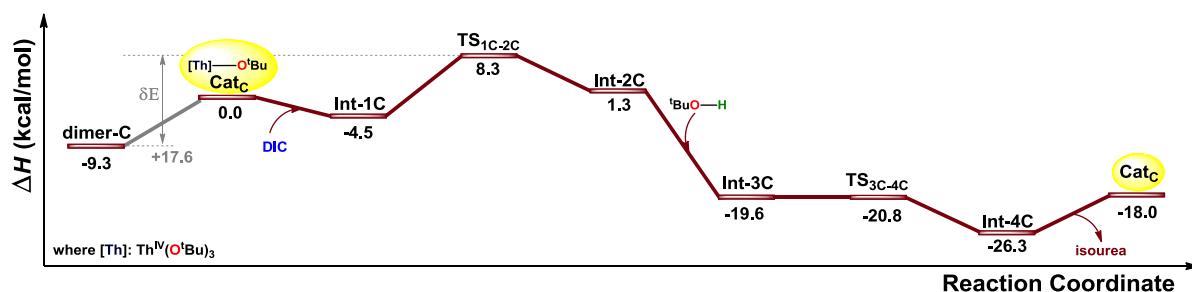


Figure S9: Plausible reaction profile of ^tBuOH addition to DIC mediated by complex **3**.

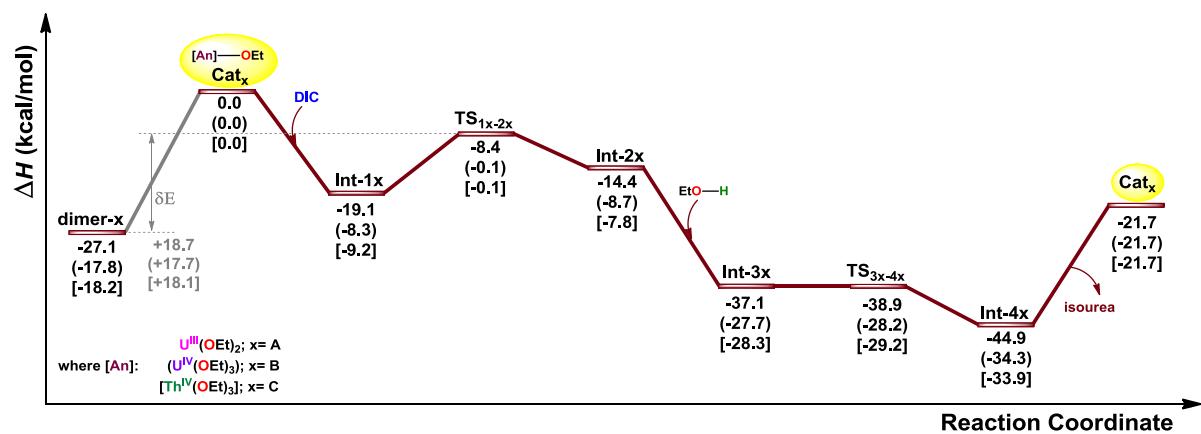


Figure S10: Plausible reaction profile of EtOH addition to DIC mediated by complex 1, 2 and 3.

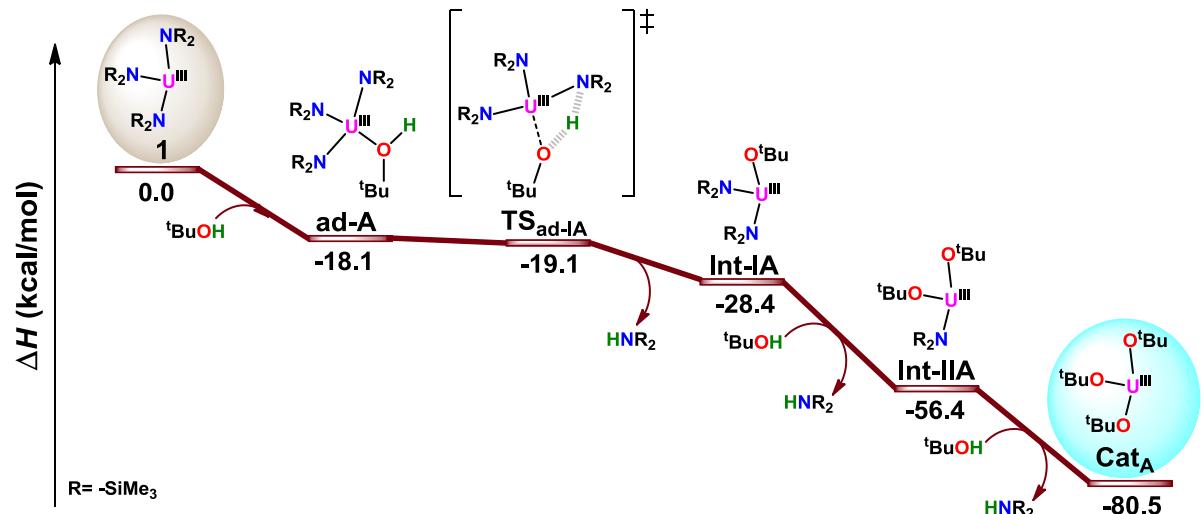


Figure S11: Enthalpy energy profile for the formation model catalyst **Cat_A** by consecutive additions of ^tBuOH at complex 1.

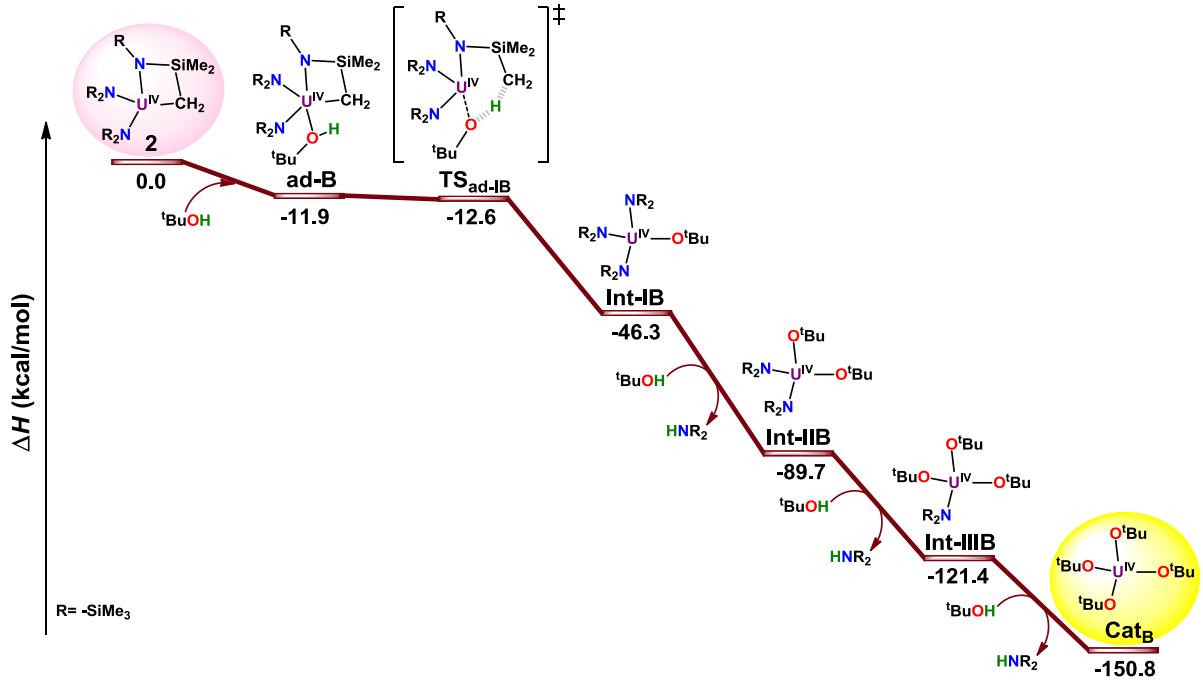


Figure S12: Enthalpy energy profile for the formation model catalyst **Cat_B** by consecutive additions of $t\text{BuOH}$ at complex **2**.

Enthalpy energies in a.u. along with Cartesian coordinates of the optimized structures.

pre-Cat_A				
H= -937.364609 au				
U	0.12983200	1.00653100	0.09761600	
Si	0.53143100	3.86079500	1.87807700	
Si	2.09898100	1.55733100	3.20189400	
Si	-3.24161000	0.51977500	1.56756100	
Si	-2.83489300	0.64385600	-1.49381800	
Si	0.98374700	-2.54450500	-0.52665300	
Si	2.87322700	-0.27320700	-1.43423100	
N	1.01991900	2.19372400	1.97643600	
N	-2.23465900	0.64203300	0.13852800	
N	1.43462200	-0.85582200	-0.64874200	
C	3.08037100	-0.86214400	-3.23678400	
H	2.19061100	-0.61961400	-3.83245600	
H	3.95425400	-0.38329500	-3.69993700	
H	3.22893700	-1.94974100	-3.27308500	
C	4.49847800	-0.62188900	-0.50292800	
H	4.68877400	-1.70088900	-0.44470400	
H	5.34734100	-0.14981700	-1.01747100	
H	4.44997500	-0.22890700	0.52045000	
C	2.72742900	1.65884700	-1.51798400	
H	1.87881800	2.01714500	-2.12874600	
H	2.72666600	2.14815600	-0.52913400	
H	3.62840500	2.02516100	-2.03092100	
C	-1.35635000	1.14487400	-2.64774200	
H	-0.53462400	0.40919700	-2.67647600	
H	-1.75744000	1.17872400	-3.67118300	
H	-0.96235700	2.15952200	-2.45691700	
C	-4.20898000	1.92397100	-1.82740800	
H	-4.46572300	1.94323200	-2.89567200	
H	-5.11609100	1.66909000	-1.26337200	
H	-3.89065300	2.92998300	-1.52442700	
C	-3.42709200	-1.04920500	-2.13515400	
H	-4.30061700	-1.39492600	-1.56823100	
H	-3.70748400	-0.98625500	-3.19602600	
H	-2.63377000	-1.79963100	-2.02854200	
C	-2.11717300	0.17024600	3.07193600	
H	-1.65287200	-0.82240900	2.99334400	
H	-1.32322900	0.92487300	3.17008600	
H	-2.71362500	0.19026800	3.99480400	
C	-4.52218400	-0.89242300	1.45237400	
H	-5.07175400	-0.98005600	2.40004800	
H	-5.25195200	-0.70429500	0.65311600	
H	-4.02687800	-1.85083200	1.24931600	
C	-4.19651000	2.13338200	1.93351400	
H	-4.80371700	2.01801000	2.84244800	
H	-3.50068600	2.96800300	2.09050800	
H	-4.86514400	2.39635000	1.10400000	
C	-0.36835300	4.09094300	0.17508200	
H	-0.65643700	5.15021600	0.10970200	
H	0.28263100	3.91152500	-0.69980100	
H	-1.30852900	3.52094100	0.08161300	
C	-0.73095600	4.40863800	3.19614000	
H	-0.29521400	4.34770100	4.20127700	
H	-1.04764900	5.44636500	3.01999500	
H	-1.61945500	3.76522000	3.17054000	
C	1.97305500	5.10960400	1.87396000	
H	2.69577700	4.87154100	1.08251500	
H	1.59573800	6.12856900	1.70999700	
H	2.50260000	5.09319600	2.83593200	
C	1.97581600	-0.34804100	3.18791400	
H	0.97204500	-0.67689500	3.49046200	
H	2.19773400	-0.76052100	2.19321400	
H	2.69885400	-0.77449300	3.89713300	

C	1.65991500	2.15707800	4.96109500	H	-1.76724400	4.90879700	0.44585500
H	1.79583500	3.24262700	5.06031700	H	-1.16689300	4.00100100	-0.93139400
H	0.61691300	1.91510500	5.20300900	H	-5.09131100	3.69570300	4.35971100
H	2.31016500	1.66556300	5.69820800	H	-4.20781000	5.00173000	5.15285600
C	3.92465000	2.01915900	2.87898200	H	1.60528100	5.38238600	5.24522900
H	4.57262700	1.57242500	3.64633800	H	2.54178800	4.98719300	3.80288900
H	4.25190900	1.65071700	1.89795800	H	2.91895900	-0.03288000	-0.79147000
H	4.06624200	3.10737800	2.90105900	H	2.03079700	-1.33886200	-1.57936900
C	0.30296100	-3.24462600	-2.16817400	H	-4.68353600	-1.40805400	-0.05774200
H	-0.58974400	-2.69122800	-2.48767500	H	-3.92627400	-1.53913900	-1.64571200
H	1.05139000	-3.17777900	-2.96795300				
H	0.02475800	-4.30071400	-2.04395500				
C	2.43218900	-3.66544100	0.01371200				
H	3.22630600	-3.68494200	-0.74504100				
H	2.86607800	-3.31453600	0.95894300				
H	2.07485300	-4.69475000	0.15722000				
C	-0.39975100	-2.70711800	0.77992800				
H	-0.76913600	-3.74189500	0.80495400				
H	-0.02370400	-2.45950100	1.78217200				
H	-1.25286500	-2.05217800	0.55044900				
dimer-A (EtOH)							
<i>H= -989.913284 au</i>							
O	-0.70023800	0.78792900	2.79293000				
U	-1.02384900	0.51717600	0.39492400				
O	-2.74188800	-0.74707000	-0.16345600				
O	0.87477500	0.07573800	-0.63268400				
C	-3.73079300	-1.64088000	-0.56409200				
C	-3.35405600	-3.08860400	-0.26664400				
H	-2.43124600	-3.36067800	-0.79069200				
H	-3.18966500	-3.22859000	0.80749900				
H	-4.14419100	-3.77921000	-0.58390200				
C	2.00679200	-0.25507800	-1.37188300				
C	2.06818400	0.50168600	-2.69470200				
H	1.19527100	0.26541400	-3.31334600				
H	2.07736600	1.58257300	-2.51654100				
H	2.96913300	0.24056500	-3.26211700				
O	-1.46439700	2.88493600	0.78728500				
U	-1.14387500	3.15531600	3.18548500				
O	-3.04642500	3.59010100	4.20827900				
O	0.56616700	4.42887800	3.74816400				
C	-4.18160500	3.91829600	4.94380400				
C	-4.24675400	3.15941400	6.26523600				
H	-3.37645600	3.39599500	6.88742800				
H	-5.15015300	3.41839900	6.82972600				
H	-4.25373100	2.07880200	6.08535900				
C	1.54978700	5.33059700	4.14402200				
C	1.29787300	6.73219800	3.59787600				
H	1.27304200	6.71728600	2.50268400				
H	0.33609700	7.11630900	3.95556500				
H	2.08291400	7.42972300	3.91256300				
C	-1.85659800	3.93953400	-0.07526000				
C	-3.28657200	3.77500600	-0.56961500				
H	-3.40445100	2.84540400	-1.13888600				
H	-3.98583000	3.74377600	0.27202400				
H	-3.57204200	4.60605100	-1.22376400				
C	-0.30824000	-0.26852400	3.65311900				
C	1.11757200	-0.09898900	4.15769700				
H	1.82216900	-0.06029700	3.32085100				
H	1.22684700	0.82850100	4.73216300				
H	1.40303700	-0.93152900	4.80993500				
H	-1.00323900	-0.33764900	4.50433700				
H	-0.38871900	-1.23589000	3.12685800				
Cat_A (EtOH)							
<i>H= -494.913388 au</i>							
U	0.98692500	2.51761500	-0.53975400				
C	4.75813000	0.47502000	-1.39226900				
H	5.16913900	1.42973100	-1.73812200				
H	4.74170300	0.48965200	-0.29735500				
H	5.43340100	-0.32571600	-1.71589700				
C	-2.12411500	0.20020400	-2.48974000				
H	-1.22533400	-0.40710800	-2.64044600				
H	-3.00087900	-0.44785700	-2.60501200				
H	-2.15453300	0.96078700	-3.27744700				
C	0.29860900	1.32101500	3.50259900				
H	-0.54894000	2.01420600	3.48330600				
H	0.02578200	0.43775900	2.91506600				
H	0.46212200	1.00533300	4.53971000				
O	2.48192100	1.28270400	-1.54923400				
O	1.35775500	2.41508600	1.61424000				
O	-0.99952400	1.69610600	-0.95169400				
C	-2.10046000	0.85802700	-1.11436100				
C	3.35182000	0.26876800	-1.94429500				
C	1.54412200	1.98490600	2.92606300				
H	-2.10684000	0.07369400	-0.33860000				
H	-3.03191600	1.43290800	-0.97433700				
H	3.40019700	0.22253100	-3.04573400				
H	2.97549300	-0.71391400	-1.61337600				
H	1.81969600	2.84345000	3.56229300				
H	2.38986400	1.27843200	2.98351000				
Int-1A (EtOH)							
<i>H= -879.261157 au</i>							
N	-0.93848800	2.23361100	0.51992600				
C	-0.91041600	2.52780300	1.73128500				
N	-0.72347500	2.81666900	2.88744700				
O	0.87305200	-1.00591200	1.80774600				
C	1.44443300	-1.83855700	2.76151400				
C	2.44662800	-2.82009500	2.15961000				
H	3.25588000	-2.28011400	1.65590300				
H	2.89022900	-3.46301200	2.92942200				
H	1.95586200	-3.46382000	1.42085000				
U	0.25533100	-0.12712000	-0.14855900				
O	-1.42626300	-1.23464400	-1.08671700				
O	1.90264400	0.20868500	-1.59157700				
C	-2.25498900	-2.18223600	-1.67333900				
C	-1.97697500	-3.59438000	-1.16589300				
H	-0.94551400	-3.88699800	-1.39245100				
H	-2.11116300	-3.64318900	-0.07983900				
H	-2.64862000	-4.32674700	-1.62986000				
C	2.93305500	0.16533400	-2.52096800				
C	2.47349100	-0.37063000	-3.87428800				
H	2.07982400	-1.38752900	-3.76977000				
H	1.67495600	0.25767900	-4.28369900				

H 3.29839900 -0.39348800 -4.59673100
 C -1.28304500 2.31187300 4.14648900
 C -1.61826200 3.49643400 5.04527800
 C -0.26103200 1.36576600 4.77306500
 H -2.20148800 1.75234400 3.92518500
 H -2.35156600 4.15744800 4.57460200
 H -2.03589000 3.13807600 5.99070900
 H -0.71795200 4.07902600 5.26229600
 H -0.01583100 0.54673700 4.09134400
 H 0.66050400 1.90460900 5.01348700
 H -0.66774200 0.94457000 5.69761500
 C -1.79079900 2.96776500 -0.46065300
 C -1.64252000 2.29616300 -1.81963500
 C -1.40884900 4.44438400 -0.49819900
 H -2.83331200 2.86982000 -0.13058900
 H -1.93254700 1.23887000 -1.78404300
 H -2.28464000 2.78962200 -2.55484300
 H -0.60924400 2.37188300 -2.18003000
 H -1.52521400 4.91505700 0.48319700
 H -0.36826400 4.56393300 -0.81601000
 H -2.04795100 4.97916500 -1.20754200
 H 1.96167500 -1.24160100 3.53534900
 H 0.66490300 -2.41371500 3.29420200
 H 3.36033800 1.17413700 -2.66627700
 H 3.76486100 -0.46299100 -2.15453400
 H -2.14344500 -2.17236700 -2.77274800
 H -3.31486200 -1.93930500 -1.47462500

TS_{1A-2A} (EtOH)

H= -879.244091 au

N -1.09944900 2.52925000 0.94635400
 C -0.94830700 2.38786700 2.21671700
 N -0.98047000 2.89729700 3.33440100
 O -0.27261500 0.54405700 2.25152600
 C 0.73582300 0.31397400 3.20225300
 C 1.94723200 -0.39384200 2.60350000
 H 2.39761700 0.19679300 1.79701100
 H 2.71953900 -0.56337600 3.36205800
 H 1.66905400 -1.37659500 2.20050600
 U -0.39281700 0.33440300 -0.12166000
 O -2.09019300 -0.77437800 -1.00872000
 O 1.49590400 0.44175200 -1.26547600
 C -3.12188100 -1.53938000 -1.54198500
 C -3.63830100 -2.57905700 -0.55191400
 H -2.83538000 -3.26699100 -0.26429300
 H -4.00739200 -2.09137900 0.35684900
 H -4.45582300 -3.16935200 -0.98246100
 C 2.53798300 0.41351700 -2.18647900
 C 2.04023200 0.28471500 -3.62289500
 H 1.46110400 -0.63697400 -3.74727600
 H 1.39088800 1.12895500 -3.88064600
 H 2.87341600 0.26525700 -4.33530000
 C -1.43692100 2.37945500 4.61191600
 C -2.94042500 2.62608500 4.76299200
 C -0.64463700 3.03683500 5.73890100
 H -1.26300700 1.29531000 4.63280500
 H -3.50065100 2.12535800 3.96770100
 H -3.29578600 2.24260700 5.72526600
 H -3.15996200 3.69769100 4.71715000
 H 0.42637400 2.84386100 5.62979500
 H -0.79555900 4.12120400 5.73001000
 H -0.96785900 2.65100300 6.71083400

C -1.85628100 3.71824700 0.50052200
 C -2.40010100 3.44622800 -0.89787800
 C -0.96627500 4.95959800 0.53686700
 H -2.70191500 3.87402400 1.18566300
 H -3.04821300 2.56315000 -0.90949000
 H -2.98427000 4.29673000 -1.26225800
 H -1.57777500 3.28994500 -1.60911200
 H -0.58995700 5.13184600 1.54891900
 H -0.10974700 4.83550400 -0.13451300
 H -1.52577600 5.84694100 0.22158600
 H 1.05662000 1.27192400 3.64118500
 H 0.33714300 -0.29329000 4.03196200
 H 3.14896200 1.32902300 -2.10029700
 H 3.21968700 -0.42728900 -1.96869400
 H -2.78924600 -2.05475000 -2.46021300
 H -3.96221900 -0.89063800 -1.84547500

Int-2A (EtOH)

H= -879.253606 au

N -0.55910400 1.39450400 0.54148800
 C -0.42521400 1.23501400 1.86908600
 N -0.78850700 2.00063300 2.81801800
 O 0.20775200 -0.07377800 2.08396800
 C 1.50459800 -0.02725500 2.71054900
 C 2.34229100 -1.18900000 2.20970100
 H 2.58204400 -1.09417700 1.14200400
 H 3.29696600 -1.22003200 2.74394000
 H 1.83787900 -2.14495500 2.39508700
 U 0.02438200 -0.77135700 -0.43163100
 O -1.63556500 -1.67154800 -1.56165200
 O 1.95410100 -0.63759800 -1.47915500
 C -2.65989700 -2.20803000 -2.33924100
 C -3.06340300 -3.60044300 -1.86614600
 H -2.21117500 -4.28689700 -1.92029100
 H -3.40860900 -3.56707700 -0.82701900
 H -3.87176900 -4.01051900 -2.48252400
 C 2.97729300 -0.49802100 -2.41535700
 C 2.47146000 -0.61153000 -3.84911300
 H 1.99720600 -1.58522400 -4.01349700
 H 1.72860800 0.16650400 -4.05736900
 H 3.28994700 -0.50255900 -4.57007100
 C -0.81498200 1.61783200 4.21431100
 C -2.25158500 1.76243100 4.72792000
 C 0.13681100 2.50902500 5.01777400
 H -0.52162000 0.56510700 4.36102900
 H -2.92930900 1.11206700 4.16658800
 H -2.32000400 1.49956200 5.78969900
 H -2.59357400 2.79450200 4.60009200
 H 1.17121800 2.39565900 4.67732100
 H -0.14063900 3.56022300 4.88843300
 H 0.09804400 2.26890600 6.08610100
 C -1.25236700 2.59669600 0.08834300
 C -1.74909700 2.37022800 -1.33787000
 C -0.34494500 3.82679600 0.17300500
 H -2.11703400 2.77202900 0.74625200
 H -2.42804300 1.51148200 -1.39392200
 H -2.28682900 3.24634400 -1.71409200
 H -0.90484800 2.19373300 -2.01964200
 H -0.01313500 3.97415200 1.20357400
 H 0.53494800 3.69745800 -0.46786000
 H -0.87634500 4.72922800 -0.15018100
 H 1.98156100 0.92985300 2.47148600
 H 1.37982800 -0.08339600 3.79671400

H 3.48085000 0.47506000 -2.28615900
 H 3.74976500 -1.26770200 -2.24607500
 H -2.35082300 -2.26431300 -3.39673700
 H -3.54538200 -1.55069400 -2.31107000

Int-3A (EtOH)

H= -1034.178253 au

N -1.07642700 0.99036700 1.59885600
 C -0.53023600 -0.02839800 2.29398500
 N -0.64716400 -0.34507100 3.52262500
 O 0.21777400 -0.84256400 1.33558300
 C 1.63387900 -0.99109500 1.57733600
 C 2.40739300 0.28869700 1.32111000
 H 2.04080000 1.09996200 1.95737700
 H 3.46601500 0.13113000 1.55320600
 H 2.33343500 0.58039600 0.26812400
 U -0.70317400 0.21064800 -0.84025300
 O -2.51859900 -0.57072200 -1.81943700
 O 1.19632200 -0.17486100 -1.92486900
 C -3.57774100 -1.17631700 -2.48935500
 C -3.92338800 -2.54061500 -1.90141500
 H -4.19632000 -2.44392700 -0.84510000
 H -4.76445000 -3.00178300 -2.43250900
 H -3.06442000 -3.21742000 -1.96969600
 C 2.30796900 -0.60403000 -2.64141100
 C 2.06966100 -1.93901900 -3.34009700
 H 1.82306000 -2.71660500 -2.60852300
 H 1.23309200 -1.85968400 -4.04253400
 H 2.95688100 -2.26294300 -3.89692500
 C -0.27687200 -1.62846700 4.08667300
 C -1.53785000 -2.29711400 4.64614400
 C 0.75589000 -1.42630200 5.19987700
 H 0.14131400 -2.31315100 3.33145100
 H -2.27267500 -2.46435700 3.85284800
 H -1.29975800 -3.26438500 5.10321600
 H -1.99884300 -1.65740600 5.40599900
 H 1.67210600 -0.96150500 4.82008700
 H 0.34674600 -0.76298500 5.96890800
 H 1.02336300 -2.37902200 5.66966000
 C -2.13717600 1.78445300 2.24378200
 C -1.61653500 2.62988000 3.41222900
 C -3.35918300 0.95472100 2.65077500
 H -2.47468000 2.48419700 1.46328000
 H -0.78248100 3.26690200 3.09433100
 H -2.40741300 3.28145700 3.80053600
 H -1.26377600 1.97944400 4.21553200
 H -3.73699100 0.37837700 1.79924000
 H -3.10207800 0.26264000 3.45502700
 H -4.16484400 1.61043500 2.99912200
 H -0.36539000 2.48078300 0.56748300
 C 0.45861700 3.85827300 -0.68700300
 C 0.51988400 4.03996400 -2.18820600
 H 0.97641500 3.16787200 -2.66678300
 H -0.48248400 4.18508200 -2.60245300
 H 1.12202100 4.91879100 -2.43743700
 O -0.35418100 2.71793700 -0.39275200
 H 1.78277600 -1.33677100 2.60202200
 H 1.95360900 -1.78616400 0.89814300
 H 1.46510900 3.71048500 -0.27542100
 H 0.01889100 4.74102300 -0.20610800
 H 3.18503200 -0.70157200 -1.97522700
 H 2.58886500 0.14802500 -3.39969000
 H -4.47345500 -0.53288500 -2.44655700

H -3.33909400 -1.29890300 -3.56026200

TS_{3A-4A} (EtOH)

H= -1034.181219 au

N -1.09619100 1.10414000 1.59497600
 C -0.44107500 0.16332800 2.31603200
 N -0.61379400 -0.19792600 3.52268400
 O 0.48764100 -0.48627600 1.40904500
 C 1.86985500 -0.61193800 1.80920300
 C 2.76481600 0.21770500 0.90915000
 H 2.54102000 1.28379300 1.01291300
 H 3.81363300 0.06210900 1.18321600
 H 2.63952400 -0.06843400 -0.14098300
 U -0.49666700 0.17798400 -0.92159100
 O -2.40366700 -0.43449100 -1.82584700
 O 1.20243000 -0.51314400 -2.15582700
 C -3.54931000 -0.91331500 -2.45561600
 C -3.94676200 -2.29552300 -1.94806600
 H -4.13738600 -2.26737700 -0.86977400
 H -4.85365500 -2.65676100 -2.44695200
 H -3.14417000 -3.01786100 -2.13337600
 C 2.15624700 -1.08274700 -2.99452200
 C 1.78566000 -2.50219900 -3.41136400
 H 1.68573500 -3.14670500 -2.53085700
 H 0.82919300 -2.50722300 -3.94478700
 H 2.54823500 -2.93691300 -4.06823400
 C -0.10934700 -1.42803200 4.10227300
 C -1.30098800 -2.32052500 4.46727300
 C 0.71946400 -1.10795000 5.34918800
 H 0.51853900 -1.99873000 3.39971000
 H -1.88695300 -2.57096200 3.57767800
 H -0.96241200 -3.25455800 4.92946600
 H -1.95941500 -1.80261300 5.17217500
 H 1.59102900 -0.49036700 5.10757300
 H 0.11038000 -0.55019500 6.06781200
 H 1.07388300 -2.02506800 5.83170600
 C -2.33092800 1.69734000 2.13800600
 C -2.07869700 2.57453100 3.36883400
 C -3.43180100 0.66491700 2.38922600
 H -2.68458500 2.35787100 1.33254200
 H -1.32242900 3.33761500 3.15446000
 H -2.99965900 3.08704400 3.66854000
 H -1.72576900 1.96334900 4.20230400
 H -3.62324000 0.07610600 1.48563400
 H -3.14905000 -0.01168300 3.19868000
 H -4.36456000 1.16661100 2.66850700
 H -0.45307900 2.06109800 0.76777500
 C 0.30588800 3.84960000 -0.22667600
 C 0.75146500 4.24343000 -1.62266700
 H 1.58116800 3.61259000 -1.95756300
 H -0.07213700 4.13922400 -2.33670000
 C 1.08575700 5.28588700 -1.64140300
 O -0.11485600 2.49890400 -0.20684300
 H 1.95369500 -0.29231000 2.85056800
 H 2.12911700 -1.67461600 1.75346400
 H 1.13352600 3.98983100 0.48400300
 H -0.51847500 4.49912100 0.10132900
 H 3.14321200 -1.10184600 -2.49786000
 H 2.28476600 -0.46581000 -3.90027600
 H -4.39132900 -0.21825900 -2.29581200
 H -3.39505000 -0.96407400 -3.54720000

Int-4A (EtOH)

H= -1034.190808 au

N	-0.66954900	0.96499200	1.87151100
C	0.06509800	-0.00189600	2.52082800
N	-0.18002100	-0.46645700	3.67046000
O	1.03878600	-0.46407100	1.60989000
C	2.42109600	-0.56768300	2.04118800
C	3.30831700	0.18977600	1.07579300
H	3.07528200	1.25821600	1.08216700
H	4.35640600	0.06286400	1.36606800
H	3.18993900	-0.18855500	0.05397200
U	0.10367100	0.02801600	-0.87760100
O	-1.83847500	-0.45637400	-1.81861200
O	1.81443600	-0.77034900	-2.03978800
C	-3.00519600	-0.72698800	-2.52267800
C	-3.56125800	-2.11070700	-2.19867300
H	-3.78262300	-2.19315000	-1.12875000
H	-4.48393600	-2.31203300	-2.75602500
H	-2.83026400	-2.88565000	-2.45394500
C	2.71069200	-1.28779100	-2.96830100
C	2.30807200	-2.67856100	-3.44962000
H	2.25442200	-3.37501600	-2.60538300
H	1.32196900	-2.64816400	-3.92549200
H	3.02809300	-3.07490300	-4.17556100
C	0.38449500	-1.70273100	4.18695800
C	-0.75957700	-2.69551500	4.41335600
C	1.12265500	-1.41540500	5.49560800
H	1.08783200	-2.16568500	3.47878600
H	-1.28103100	-2.91349800	3.47647500
H	-0.37688700	-3.63771700	4.81973300
H	-1.48699700	-2.28278400	5.11959800
H	1.95942500	-0.72632700	5.34283200
H	0.44090600	-0.95550100	6.21785500
H	1.51653900	-2.34004900	5.92957900
C	-1.91434800	1.53511200	2.41839400
C	-1.68264600	2.34223900	3.69748900
C	-2.99665600	0.47120600	2.58289700
H	-2.24100800	2.22497700	1.63083400
H	-0.93276700	3.12396800	3.53718800
H	-2.61322400	2.82845600	4.00818600
H	-1.34125200	1.68919800	4.50365400
H	-3.14878400	-0.07458500	1.64644000
H	-2.73140500	-0.23802900	3.36959500
H	-3.94289300	0.94925800	2.85433200
H	-0.12513400	1.64304400	1.31521600
C	0.65993700	3.56069200	-0.81327800
C	1.02033200	3.72085300	-2.28642000
H	1.91045000	3.13041000	-2.53032100
H	0.19666900	3.37472400	-2.92152300
H	1.22475900	4.76821800	-2.53782800
O	0.39608200	2.23520600	-0.47141700
H	2.49030700	-0.16860900	3.05683700
H	2.68026600	-1.63083600	2.06756400
H	1.48958400	3.95749700	-0.20101700
H	-0.21409800	4.19885900	-0.59134900
H	3.72532800	-1.34220000	-2.53341000
H	2.79345700	-0.61851900	-3.84243200
H	-3.77893000	0.02846700	-2.29705600
H	-2.82657500	-0.66340100	-3.61067500

U	0.16052800	0.67549600	0.34366600
Si	0.37553500	3.84719500	1.97043300
Si	2.41099700	1.75914400	2.89974500
Si	-3.12858900	0.55719300	1.13334600
Si	-2.74051500	1.02279500	-1.88776400
Si	1.66001800	-1.60332900	-1.07563100
Si	2.66822000	1.12343400	-2.38748000
N	1.04781800	2.21189300	1.86636100
N	-2.07786600	0.84835400	-0.25487800
N	1.62463200	0.17723800	-1.32816000
C	2.37470300	0.72891700	-4.22093800
H	1.33349000	0.90125100	-4.50929900
H	3.00763700	1.36345200	-4.85187100
H	2.61826000	-0.31347100	-4.45014900
C	4.51507600	0.85325600	-2.03531900
H	4.84529500	-0.15009500	-2.31891300
H	5.11130800	1.57183000	-2.60940100
H	4.74814000	0.99596300	-0.97553200
C	2.31145000	2.96835300	-2.10706700
H	1.28920300	3.23483400	-2.39518300
H	2.46389600	3.24761800	-1.05851800
H	2.98937400	3.58180100	-2.71096000
C	-1.44083300	1.87299300	-2.97464700
H	-0.50714800	1.30087500	-3.00272600
H	-1.80392400	1.95728100	-4.00492900
H	-1.22031900	2.88475200	-2.61792600
C	-4.31651500	2.08113700	-1.93880100
H	-4.62524300	2.22487200	-2.98064700
H	-5.15210500	1.60632800	-1.41449400
H	-4.15484000	3.06949400	-1.49762700
C	-3.15123200	-0.65637200	-2.67160000
H	-3.93142800	-1.18354800	-2.11427100
H	-3.50668700	-0.52218400	-3.69967000
H	-2.27076100	-1.30575300	-2.70505200
C	-1.99828100	0.11378200	2.61740000
H	-1.45193300	-0.82795000	2.47447100
H	-1.29176100	0.90171900	2.91428500
H	-2.64517300	-0.03801900	3.48920500
C	-4.30924400	-0.90638400	0.89521300
H	-4.85818100	-1.10488200	1.82265500
H	-5.04806500	-0.70518500	0.11298700
H	-3.76482600	-1.81516000	0.62097700
C	-4.14709500	2.06725000	1.66019000
H	-4.68285600	1.85468400	2.59246300
H	-3.51128600	2.94149800	1.82971100
H	-4.88959500	2.33691100	0.90411500
C	-0.64415500	4.19731000	0.40145800
H	-1.12040700	5.17966100	0.50123600
H	-0.00672900	4.23948100	-0.48866000
H	-1.44584900	3.47155600	0.22192900
C	-0.77970100	4.06988700	3.46152900
H	-0.24572400	3.95046400	4.40860100
H	-1.22145800	5.07297400	3.45177700
H	-1.60043100	3.34584900	3.44886100
C	1.70073800	5.20410200	2.06154800
H	2.39075600	5.14740600	1.21410800
H	1.21750600	6.18757700	2.03464100
H	2.28914500	5.15411900	2.98292500
C	2.59956400	-0.13362800	2.88800400
H	1.71744200	-0.65273700	3.27739500
H	2.82901600	-0.54064300	1.89725100
H	3.44337600	-0.39951200	3.53536400
C	2.17306200	2.26417400	4.71532200

pre-Cat_B

H= -942.447023 au

H 2.15590000 3.35036000 4.84982500
 H 1.24254600 1.85707000 5.12340600
 H 3.00232200 1.87402400 5.31669800
 C 4.06289800 2.47150100 2.29596300
 H 4.88711100 2.09408200 2.91212900
 H 4.25916100 2.17926300 1.25936900
 H 4.08249700 3.56357500 2.34512200
 C 0.96470200 -2.54542300 -2.56677800
 H -0.05051700 -2.21498200 -2.80578800
 H 1.58190800 -2.40080700 -3.45945700
 H 0.92859000 -3.61910400 -2.35134900
 C 3.40045100 -2.26974000 -0.71801300
 H 4.03165900 -2.24245600 -1.61163400
 H 3.90843200 -1.70628600 0.06993500
 H 3.32565600 -3.31382800 -0.39425400
 C 0.54224200 -1.73086700 0.46001100
 H 1.06312100 -2.20343200 1.29802600
 H -0.37646100 -2.29579900 0.25493600

dimer-B (EtOH)

H= -1310.038493 au

O -0.30199500 1.28592000 2.47675100
 O -1.92646600 2.64764800 0.94395200
 U -1.24789400 3.39207900 3.11575900
 C -2.76399500 3.45182300 0.11152000
 C -4.18105600 2.90842000 0.04495200
 H -4.19796800 1.89935500 -0.38070000
 H -4.62328700 2.87033800 1.04492100
 H -4.80869100 3.54897200 -0.58449900
 C 0.53173800 0.47478700 3.30537500
 C 1.94263200 1.02923300 3.40468700
 H 2.40001400 1.09217200 2.41289400
 H 1.94392100 2.02876000 3.85258900
 H 2.56648800 0.38076600 4.02978100
 U -0.96830200 0.55181100 0.29704100
 O -1.18501500 1.18219200 -1.74698800
 O -2.45941500 -0.92961700 0.67552500
 O 0.91568500 -0.46739800 0.11215000
 O -3.12151200 4.42848600 3.31667300
 O 0.24939900 4.86006300 2.71444700
 O -1.00325900 2.78200600 5.16246600
 C -3.32218800 -2.02985900 0.66889600
 C -4.18048700 -2.07007000 1.92541600
 H -4.78618100 -1.16187000 2.00599200
 H -4.85484500 -2.93365800 1.90941900
 H -3.55131300 -2.14126800 2.81841700
 C 2.19197500 -0.98719700 -0.10884800
 C 2.21434700 -1.94768700 -1.29034000
 H 3.22126200 -2.35028000 -1.44908800
 H 1.53204800 -2.78579600 -1.11563700
 H 1.89892000 -1.43679800 -2.20555600
 C -1.09437800 1.61494500 -3.07108300
 C -4.36540700 4.98785800 3.61191400
 C 1.13822300 5.93943900 2.70332800
 C 2.18903200 5.78289700 1.61312800
 H 1.71482600 5.72339300 0.62825700
 H 2.87935800 6.63391400 1.61226500
 H 2.77027600 4.86841500 1.76816300
 C -1.04348500 2.33209000 6.48309500
 C -2.31495500 1.54860900 6.78380000
 H -3.19872100 2.17227100 6.61435100
 H -2.38890200 0.66835600 6.13605700
 H -2.32982200 1.20782700 7.82523300

H -2.32551600 3.49452200 -0.89332200
 H -2.78609000 4.47810000 0.50490400
 H 0.07956100 0.40791100 4.30283800
 H 0.56997000 -0.54364000 2.89288000
 H -0.16555500 1.69810200 6.68779200
 H -0.97296700 3.19207100 7.16724000
 H -4.85314100 4.41495200 4.41712400
 H 1.63339200 6.02452800 3.68326500
 H 0.58188100 6.87676300 2.54721500
 H 2.54058000 -1.51172900 0.79541800
 H 2.90708900 -0.16826500 -0.28995300
 H -0.04779100 1.56055200 -3.41133900
 H -1.39089100 2.67446900 -3.14136700
 H -2.73882600 -2.96068700 0.59106600
 H -3.97135900 -1.98824000 -0.21970200
 C -1.97161300 0.78342000 -3.99721100
 H -1.89084400 1.13427300 -5.03235000
 H -1.67199400 -0.26900400 -3.96561500
 H -3.02106300 0.84759500 -3.69252800
 C -4.24153300 6.44626400 4.03235000
 H -5.22476000 6.87407800 4.25900300
 H -3.61295400 6.53550900 4.92423900
 H -3.78398800 7.03815300 3.23307700
 H -5.02574000 4.91628500 2.73245500

Cat_B (EtOH)

H= -654.990954 au

C 3.73213000 0.75789500 -3.54137800
 H 3.99203100 1.82058300 -3.49808800
 H 4.51341900 0.23544100 -4.10475800
 H 2.78968500 0.65863900 -4.08988900
 C -2.31383500 0.77193000 -2.71877200
 H -1.54691900 0.23107500 -3.28287200
 H -3.29384100 0.36998800 -2.99940300
 H -2.27736200 1.82543900 -3.01488500
 C 1.48107300 0.04742200 3.50373100
 H 0.48687100 -0.32961600 3.24229800
 H 2.22585300 -0.55089200 2.96871600
 H 1.63175500 -0.09875800 4.57922200
 O 2.60746300 0.83984700 -1.40153700
 O 1.41845400 1.72552400 1.76287100
 O -0.82966400 1.13687000 -0.84468100
 C -2.07505900 0.62959000 -1.22172400
 C 3.59653700 0.18359200 -2.13766700
 C 1.60936400 1.51812500 3.13084800
 O 1.18806900 3.99381000 -0.88006900
 C 1.21392200 5.36161300 -1.16173600
 C 0.26031400 6.14163000 -0.26689700
 H -0.76828600 5.79254700 -0.40493800
 H 0.52795000 6.00965400 0.78658500
 H 0.29305000 7.21223500 -0.49817000
 H 4.56161700 0.26218100 -1.61287500
 H 3.35938900 -0.89005500 -2.20024600
 H 2.23769300 5.74659800 -1.03278400
 H 0.94682600 5.52672400 -2.21733200
 H 2.60424100 1.88737700 3.42537200
 H 0.87400800 2.10791500 3.70034100
 H -2.14375900 -0.43218000 -0.93724000
 U 1.09602000 1.92450000 -0.34396600

Int-1B (EtOH)

H= -1039.321514	au		
N	-0.29174200	2.16353900	0.46726100
C	-0.71202400	2.29997600	1.62912300
N	-0.99483000	2.41304700	2.80120700
O	1.20550600	-0.20393100	1.95536600
C	1.83812200	-0.03529800	3.18475800
C	3.35271100	0.05927200	3.04482200
H	3.62922900	0.91537400	2.42002300
H	3.83266100	0.18065100	4.02289700
H	3.75084100	-0.84727300	2.57713900
U	0.45028800	-0.47242000	-0.04688400
O	-1.69681900	-0.78401500	-0.07016400
O	1.35598800	0.41491200	-1.82071600
C	-2.22064100	2.06013000	3.52112700
C	-3.32413200	1.55507700	2.59680100
C	-2.65330300	3.25689100	4.36416300
H	-1.92438500	1.24990800	4.19971200
H	-2.97243000	0.72034300	1.98269900
H	-4.18336400	1.21600100	3.18366200
H	-3.66532500	2.35572000	1.93071800
H	-1.83733300	3.59513600	5.00807600
H	-2.95488300	4.09202300	3.72352600
H	-3.50475000	2.98396300	4.99467100
C	-0.41109100	3.28179300	-0.51005000
C	-1.17176800	2.79848000	-1.73914800
C	0.99054100	3.77468000	-0.85332400
H	-0.97475700	4.09673800	-0.03593600
H	-2.16377600	2.42585900	-1.46898900
H	-1.29293900	3.62144300	-2.45090000
H	-0.61402500	1.99498500	-2.23021100
H	1.50586900	4.14777100	0.03657000
H	1.57324500	2.95283200	-1.27869500
H	0.93598500	4.58637700	-1.58612700
O	1.11390600	-2.47976800	-0.37048200
C	1.61618100	-3.77659500	-0.45299800
C	0.50853400	-4.80342900	-0.65085300
H	0.92065100	-5.81707700	-0.71497200
H	-0.19851100	-4.77066700	0.18427800
H	-0.04452000	-4.59776900	-1.57301100
C	2.10557600	0.54666500	-2.98967800
C	3.59618800	0.34298800	-2.74627600
H	4.16707000	0.46272700	-3.67436400
H	3.97072700	1.07012700	-2.01782900
H	3.78720300	-0.66129600	-2.35394100
C	-2.92696700	-1.33373200	-0.42825000
C	-3.00007500	-1.68036700	-1.91073000
H	-2.84300500	-0.78585700	-2.52309700
H	-2.22865700	-2.41274900	-2.17148200
H	-3.97643100	-2.10574500	-2.17033800
H	1.58833000	-0.87806800	3.85028800
H	1.45853700	0.87544400	3.67550700
H	2.17978100	-4.01866100	0.46262300
H	1.94430600	1.54835000	-3.42379900
H	1.75972600	-0.17666500	-3.74630000
H	2.33093300	-3.84562100	-1.28908000
H	-3.12192600	-2.24132500	0.16660600
H	-3.73563100	-0.62431800	-0.18348300
N	-1.48777900	3.05680700	3.04524400
O	-0.70283700	0.58302700	2.35740800
C	0.08951800	0.38901500	3.50741900
C	1.57959000	0.54868300	3.23051800
H	1.79815600	1.55877000	2.86633700
H	2.16955200	0.38568000	4.13928800
H	1.91431000	-0.17845400	2.48138700
U	-0.36154100	0.03138600	0.10986700
O	-2.19845000	-0.60644800	-0.78034800
O	0.97762200	0.74851000	-1.41135300
C	-2.39183600	2.75168000	4.14354300
C	-3.80747900	3.21477200	3.79003500
C	-1.88591200	3.42045000	5.41886900
H	-2.41264500	1.66307000	4.28977100
H	-4.17065300	2.70977000	2.89000900
H	-4.49885800	2.99209200	4.60967500
H	-3.82278600	4.29447800	3.60958000
H	-0.87746900	3.07870600	5.66943300
H	-1.85147700	4.50733000	5.29180200
H	-2.54705700	3.19152000	6.26052000
C	-1.45441300	3.59243500	-0.00648000
C	-1.81317000	3.16085900	-1.42417800
C	-0.35780000	4.65614800	0.01104400
H	-2.34919700	4.00607300	0.47938200
H	-2.62304200	2.42459200	-1.41915100
H	-2.13721100	4.02132900	-2.01798600
H	-0.94382000	2.71369000	-1.91978100
H	-0.12573600	4.95458900	1.03749900
H	0.55551600	4.26905400	-0.45263300
H	-0.67474200	5.54718500	-0.54176800
O	0.67697200	-1.76390300	0.67025600
C	1.38977200	-2.89367400	1.07126700
C	0.50725600	-4.13394000	1.11850900
H	1.08188800	-5.01189700	1.43500800
H	-0.31883100	-3.99069100	1.82253000
H	0.08118600	-4.33915400	0.13128500
C	2.00154600	1.13828400	-2.27540200
C	1.99503900	0.32311000	-3.56181400
H	2.80083700	0.64232800	-4.23265100
H	2.13085900	-0.74056900	-3.34153600
H	1.04171900	0.44314300	-4.08643100
C	-3.26248100	-1.25220500	-1.41406000
C	-2.80691300	-2.06676400	-2.61720000
H	-2.32182200	-1.42249400	-3.35764200
H	-2.09001600	-2.83587200	-2.31164300
H	-3.65752500	-2.56299100	-3.09815400
H	-0.11615800	-0.61142800	3.91464100
H	-0.21141200	1.11680500	4.27375100
H	1.83374100	-2.72402900	2.06613000
H	2.97861200	1.02864500	-1.77765500
H	1.89440000	2.20771200	-2.51986700
H	2.22978600	-3.06664000	0.37961300
H	-3.77557700	-1.91167300	-0.69640500
H	-4.00278300	-0.50342800	-1.73695900

Int-2B (EtOH)

H= -1039.322152 au

N	-0.34418900	1.72889500	0.23907400
C	-0.65583200	1.53561000	1.54029300
N	-1.09168400	2.38022000	2.38357700
O	-0.46169700	0.12298500	1.78543900
C	0.44637900	-0.24132600	2.85034900
C	1.84491500	0.31033500	2.65234800

H	1.83789400	1.40293400	2.60580300	O	-1.73072300	0.98073100	-1.63881700
H	2.47698100	0.01172500	3.49508300	O	1.48409800	-0.15483100	-2.06674300
H	2.29695400	-0.08712200	1.73836800	C	1.29920400	-1.63594800	4.18358200
U	0.02983500	-0.44042500	-0.71762300	C	0.45359100	-2.83141200	4.63704200
O	-1.84196400	-1.21857000	-1.37379700	C	2.07748200	-1.05162100	5.36540600
O	1.15210100	0.03486800	-2.46945300	H	2.01894200	-2.01609800	3.44263100
C	-1.69253200	2.04589400	3.66009400	H	-0.09288000	-3.26095000	3.79218300
C	-3.11528300	2.61515700	3.67905600	H	1.08492500	-3.61382600	5.07310700
C	-0.86156000	2.63962000	4.80112300	H	-0.27695500	-2.51501900	5.38883600
H	-1.77865300	0.95730300	3.80883300	H	2.71244400	-0.21483700	5.05569100
H	-3.71530300	2.17976100	2.87445500	H	1.38025400	-0.67445200	6.12055700
H	-3.61100900	2.40394300	4.63333800	H	2.71573600	-1.81071200	5.83039400
H	-3.08817000	3.69954100	3.53086800	C	-1.85857100	0.72305500	2.40798000
H	0.15189300	2.22504400	4.81864200	C	-1.73777900	1.67070000	3.60574700
H	-0.77273200	3.72285800	4.66947100	C	-2.61820700	-0.55640600	2.77237000
H	-1.32822900	2.44501900	5.77289200	H	-2.44990600	1.24202200	1.63892800
C	-0.60290100	3.05983200	-0.31050300	H	-1.24973200	2.60803300	3.31532600
C	-0.88105200	2.95204700	-1.80838100	H	-2.72924800	1.91638100	4.00218200
C	0.56309200	4.00683200	-0.01824900	H	-1.14587800	1.20343400	4.39583700
H	-1.49387100	3.46223800	0.19162800	H	-2.70386200	-1.21662400	1.90295000
H	-1.76081200	2.32666100	-2.00227100	H	-2.10225300	-1.09622300	3.56911900
H	-1.07524900	3.93899500	-2.24046100	H	-3.62965700	-0.31198100	3.11510100
H	-0.02474000	2.51980800	-2.34040100	H	0.16226900	2.00334100	1.03826800
H	0.72491600	4.07771700	1.06048400	C	-0.00131200	3.60211400	-0.19113500
H	1.48330300	3.64383100	-0.49062700	C	0.55402400	4.00373400	-1.54037400
H	0.35679800	5.01336000	-0.39961600	H	1.64585700	4.06094400	-1.50927900
O	1.21238000	-1.99398000	0.18516700	H	0.26355000	3.27759800	-2.30496900
C	1.93711200	-3.06262200	0.71394200	H	0.16426900	4.98387600	-1.83234900
C	1.10779100	-4.33822400	0.78291300	O	0.54986800	2.33472100	0.18210400
H	1.69307800	-5.16371600	1.20342800	O	-0.91863100	-2.04989300	-0.68721200
H	0.22264000	-4.19030200	1.41035800	C	-1.46876200	-3.33022000	-0.76931100
H	0.76993800	-4.63115900	-0.21631300	C	-0.51413500	-4.31627800	-1.42887700
C	2.00328200	0.25733700	-3.55582100	H	-0.96133200	-5.31530100	-1.48435100
C	3.46992600	0.19466600	-3.15231200	H	-0.26819300	-3.99210400	-2.44517000
H	4.12055700	0.37257200	-4.01582800	H	0.41805700	-4.38771000	-0.85932500
H	3.69299600	0.95254800	-2.39408900	C	2.51302000	-0.22628200	-3.00498700
H	3.71294600	-0.78821600	-2.73587800	C	2.05456700	0.22689000	-4.38503600
C	-2.98425900	-1.79272000	-1.94062300	H	2.87379600	0.16492400	-5.11047100
C	-2.66235500	-2.56792700	-3.21047300	H	1.23130800	-0.40103400	-4.74060900
H	-2.21267800	-1.90916000	-3.96049400	H	1.70258600	1.26296800	-4.35140600
H	-1.95649900	-3.37797400	-2.99914900	C	-2.77904400	1.47696000	-2.41625300
H	-3.56967300	-3.00763600	-3.63954100	C	-3.83913800	0.41954600	-2.69313100
H	0.44813700	-1.33334700	2.83823000	H	-4.26372500	0.04593900	-1.75596900
H	0.02612100	0.09207000	3.80152100	H	-4.65300800	0.83281400	-3.29971800
H	2.29849800	-2.80686500	1.72433300	H	-3.40512900	-0.42865000	-3.23208900
H	1.78326700	1.24199400	-3.99673900	H	3.26068900	-1.34727600	1.78676200
H	1.80229800	-0.49015700	-4.33834800	H	0.26679900	4.34335300	0.57299700
H	2.83414000	-3.24091900	0.10019600	H	-1.09579200	3.53431800	-0.23393300
H	-3.45753000	-2.46318700	-1.20709200	H	2.82926300	0.06592700	2.76755900
H	-3.71670900	-1.00249700	-2.16541100	H	-1.72509000	-3.68540700	0.24086100

Int-3B (EtOH)

H= -1194.240951 au

N	-0.56022500	0.46658200	1.76047900
C	0.38505100	-0.24601400	2.42308800
N	0.41213400	-0.62979600	3.63385700
O	1.39007200	-0.55713000	1.42867700
C	2.78116900	-0.36258200	1.76311700
C	3.45654300	0.54462700	0.75505100
H	2.98591600	1.53126900	0.73840200
H	4.51182800	0.66384300	1.02318000
H	3.40447400	0.12250400	-0.25189200
U	-0.14167300	-0.06516900	-0.65597900

TS_{3B-4B} (EtOH)

H= -1194.241752 au

N	-1.05153400	0.66771900	1.80618700
C	-0.08718900	-0.11937700	2.37262800
N	-0.07531900	-0.64844900	3.52445000
O	0.90124700	-0.30705800	1.35478000
C	2.29611200	-0.10873200	1.67942500

C	2.90876800	0.93242400	0.76556600	N	-0.54569400	0.86422100	2.49387200
H	2.41397100	1.89845700	0.88985100	C	0.41589400	-0.09064200	2.46462400
H	3.97266700	1.04398500	1.00037500	N	0.63648500	-0.94975400	3.37292400
H	2.81618900	0.63305200	-0.28229500	O	1.11361600	-0.01066800	1.23017200
U	-0.61540900	0.16002900	-0.77163300	C	2.48505100	0.46469100	1.32414300
O	-2.19399700	1.01724100	-1.92474100	C	2.56937700	1.90767400	1.77904300
O	1.04822300	-0.04902800	-2.11087800	H	2.20290100	2.02983100	2.80235000
C	0.83560800	-1.69331800	3.95412300	H	3.61509800	2.23170900	1.75494000
C	0.01237200	-2.94362400	4.28142100	H	1.98694500	2.55735600	1.12052200
C	1.61183700	-1.22431300	5.18724400	U	-0.20702900	0.32347500	-1.07814400
H	1.55404100	-1.97318100	3.16901300	O	-1.19520200	0.81562600	-2.90243000
H	-0.53174600	-3.29226600	3.39882300	O	1.79844600	0.03343600	-1.83334100
H	0.66003000	-3.75563400	4.63008000	C	1.54507700	-2.06917200	3.20243000
H	-0.71824900	-2.72043600	5.06566100	C	0.75085400	-3.36987400	3.35449600
H	2.22671400	-0.34532000	4.96754100	C	2.65440400	-1.98937200	4.25498400
H	0.91375000	-0.94830600	5.98409400	H	2.00385200	-2.07819500	2.20137500
H	2.26928500	-2.01667600	5.56044900	H	-0.03245600	-3.43690800	2.59404100
C	-2.34750500	0.85416800	2.48258000	H	1.40663100	-4.24148200	3.25136000
C	-2.22118800	1.63753600	3.79245800	H	0.27316100	-3.40934900	4.33906800
C	-3.11568700	-0.45579500	2.66792100	H	3.23906600	-1.06909900	4.15249200
H	-2.92545100	1.47597600	1.78298100	H	2.21796300	-1.99308200	5.25911100
H	-1.71034200	2.59219900	3.62747800	H	3.33779500	-2.84113800	4.17076300
H	-3.21363400	1.85160300	4.20406100	C	-1.53898300	1.02448400	3.55605700
H	-1.65157500	1.06092300	4.52432200	C	-0.89657900	1.42402200	4.88757500
H	-3.20048400	-0.99339800	1.71793300	C	-2.43970400	-0.20438000	3.69691100
H	-2.60889000	-1.10096600	3.38875900	H	-2.16161900	1.86024700	3.21364500
H	-4.12664600	-0.25097600	3.03590100	H	-0.30710800	2.33970300	4.77538300
H	-0.57959900	1.76307500	1.18955500	H	-1.66854300	1.60639500	5.64255100
C	-0.56021100	3.69942400	0.09571600	H	-0.24000600	0.62606700	5.24231100
C	-0.04926400	4.24348600	-1.22653700	H	-2.91533600	-0.44603200	2.74172900
H	1.04084200	4.16442100	-1.28096400	H	-1.85772400	-1.06783200	4.02624900
H	-0.47870400	3.68485400	-2.06412200	H	-3.22614400	-0.01056900	4.43379100
H	-0.32437500	5.29732800	-1.34274900	H	-0.52834600	1.54778700	1.73282200
O	-0.18070600	2.34550700	0.25982100	C	-0.94657000	3.58510400	-0.17889300
O	-1.37447500	-1.83301200	-0.60737200	C	-0.31914200	4.23925900	-1.40315500
C	-1.97216400	-3.08333200	-0.44520900	H	0.77349400	4.23791900	-1.32449900
C	-1.06880200	-4.20792500	-0.93349200	H	-0.59776800	3.69524600	-2.31202300
H	-1.55075500	-5.18303100	-0.79905700	H	-0.65178600	5.27792300	-1.51050600
H	-0.83826300	-4.08112500	-1.99608300	O	-0.54236800	2.24968900	-0.02136000
H	-0.12525200	-4.21041100	-0.37837500	O	-1.34779800	-1.39406500	-0.48179900
C	2.02861800	-0.42520100	-3.03131100	C	-2.15053000	-2.49479600	-0.18070400
C	1.62235300	-0.09425700	-4.46085800	C	-1.62275600	-3.77570300	-0.81390500
H	2.40692400	-0.38744000	-5.16770500	H	-2.26357300	-4.62923300	-0.56481600
H	0.70202800	-0.62217700	-4.73091800	H	-1.58817700	-3.67954300	-1.90410500
H	1.44372800	0.98011900	-4.56990400	H	-0.60997700	-3.99137900	-0.45824600
C	-3.21498800	1.44354000	-2.77619400	C	2.88830000	-0.31781900	-2.63223100
C	-4.28678100	0.37784300	-2.96125900	C	2.67384700	-1.64357500	-3.35097100
H	-4.74256100	0.11906500	-2.00021400	H	3.54395500	-1.90477800	-3.96396200
H	-5.07682200	0.73210300	-3.63313200	H	2.50887400	-2.45015300	-2.62881300
H	-3.85361600	-0.53224800	-3.38818900	H	1.79863200	-1.58756000	-4.00700900
H	2.80065300	-1.07498500	1.57292800	C	-1.83815300	1.05842700	-4.11718900
H	-0.14882900	4.29097800	0.92677600	C	-3.13853300	0.27583600	-4.23997600
H	-1.65557200	3.79928200	0.13832500	H	-3.82790800	0.54766100	-3.43421400
H	2.35972900	0.19896200	2.72625600	H	-3.62957700	0.48183400	-5.19784700
H	-2.21709000	-3.24418100	0.61656500	H	-2.94767300	-0.80007000	-4.17520100
H	-2.92555400	-3.11153800	-0.99634400	H	2.86578000	0.34009100	0.30851300
H	-3.67343000	2.35915100	-2.37037600	H	-0.67028900	4.15812200	0.72113700
H	2.97489900	0.08785900	-2.79342500	H	-2.04429600	3.64246600	-0.25893700
H	2.22727500	-1.50552900	-2.94632100	H	3.03626600	-0.19888600	1.99540500
H	-2.79116100	1.71249200	-3.75658600	H	-2.20842000	-2.62256400	0.91167200
				H	-3.17916700	-2.31158300	-0.53040300
				H	-2.04719500	2.13567900	-4.21375000
				H	3.07883000	0.47461600	-3.37349100

Int-4B (EtOH)

H= -1194.251345 au

H 3.79654300 -0.38570700 -2.01002800
H -1.16781000 0.79322900 -4.94972500

pre-Cat_c

H= -940.840765 au

Th 0.16242500 0.67607700 0.34585700
Si 0.38779800 3.88082500 1.95052200
Si 2.38794900 1.76694400 2.90891100
Si -3.12583400 0.55442600 1.15247800
Si -2.76515600 1.00814500 -1.87350400
Si 1.66903700 -1.61294800 -1.10368900
Si 2.68668700 1.12234200 -2.37386700
N 1.04686100 2.24152100 1.86090200
N -2.09320500 0.84671600 -0.24496800
N 1.64110500 0.17402700 -1.32016100
C 2.40054800 0.74316300 -4.21177700
H 1.35827600 0.90948900 -4.50009600
H 3.02899900 1.38939900 -4.83530600
H 2.65323500 -0.29468900 -4.45097700
C 4.53379600 0.85882200 -2.01758900
H 4.86840600 -0.14156400 -2.30666800
H 5.12991700 1.58331600 -2.58426000
H 4.76213600 0.99438400 -0.95579400
C 2.32048400 2.96556100 -2.08580700
H 1.29932000 3.22906900 -2.38152900
H 2.46310400 3.24164900 -1.03487900
H 2.99983400 3.58557200 -2.68132000
C -1.45652400 1.83536200 -2.96970100
H -0.52666700 1.25572700 -2.99277400
H -1.81721400 1.91081700 -4.00149800
H -1.22762100 2.84976100 -2.62559300
C -4.33304100 2.07746700 -1.92947100
H -4.64926900 2.21286200 -2.97011000
H -5.16716600 1.61292700 -1.39352600
H -4.16195100 3.06883900 -1.49865800
C -3.18554300 -0.67704900 -2.63870200
H -3.97812600 -1.18763100 -2.08336500
H -3.52636600 -0.55576000 -3.67325300
H -2.31132100 -1.33576500 -2.64923400
C -1.96170900 0.12467700 2.61878500
H -1.40303200 -0.81021800 2.47007800
H -1.26662900 0.92451900 2.91321100
H -2.59465100 -0.04116700 3.49803600
C -4.29996500 -0.91802100 0.94241900
H -4.83407900 -1.11566200 1.87861700
H -5.05129900 -0.72416100 0.17012400
H -3.75399100 -1.82433700 0.66344900
C -4.14355000 2.05926400 1.69397700
H -4.66110700 1.84888500 2.63691100
H -3.51039300 2.93865900 1.84578100
H -4.90139000 2.31958400 0.94967700
C -0.63420500 4.21122000 0.37749600
H -1.11497000 5.19225800 0.46744000
H 0.00104400 4.24758900 -0.51442600
H -1.43549600 3.48210900 0.20647900
C -0.76745600 4.12794400 3.43780100
H -0.23471500 4.01987900 4.38699700
H -1.20676400 5.13187700 3.41429800
H -1.58995300 3.40569500 3.43411600
C 1.72202700 5.22926100 2.02638700
H 2.42008000 5.14889200 1.18750800
H 1.24998600 6.21721000 1.97670500
H 2.30062600 5.18972600 2.95473900

C 2.53893300 -0.13048500 2.85693800
H 1.63886800 -0.64547700 3.21037800
H 2.79162500 -0.52198300 1.86477700
H 3.35866900 -0.42911700 3.52068000
C 2.13148900 2.24723800 4.72794600
H 2.13215600 3.33226600 4.87358800
H 1.18667000 1.85384700 5.11596200
H 2.94354700 1.83541800 5.33818800
C 4.05981500 2.46066100 2.34134200
H 4.86788900 2.06830900 2.96935600
H 4.27062500 2.17363200 1.30617900
H 4.09193500 3.55213000 2.39908000
C 1.00164900 -2.52017800 -2.62992000
H 0.00057300 -2.16629400 -2.89458500
H 1.64753100 -2.37706900 -3.50234100
H 0.93741300 -3.59566000 -2.43043000
C 3.40416600 -2.28527600 -0.73059300
H 4.05314000 -2.23704200 -1.61047600
H 3.89528300 -1.73842700 0.07960000
H 3.32593700 -3.33629200 -0.43084500
C 0.52975700 -1.76368000 0.40969700
H 1.02503000 -2.29807100 1.22619100
H -0.39837300 -2.29748100 0.16129400

dimer-C (EtOH)

H= -1306.854051 au

O -0.27241300 1.29830400 2.45451100
O -1.90536900 2.68054200 0.90007800
C -2.71878600 3.51001100 0.07010500
C -4.14146100 2.98609100 -0.02977700
H -4.16277500 1.98285400 -0.46885600
H -4.60295000 2.94046500 0.96117200
H -4.74964500 3.64276400 -0.66171400
C 0.55198100 0.47309000 3.27764900
C 1.96602700 1.01801400 3.38832100
H 2.42938300 1.08343700 2.39932900
H 1.97121500 2.01559600 3.84066400
H 2.58270100 0.36256600 4.01327200
O -1.07813600 1.22909500 -1.82064700
O -2.39825300 -0.89458400 0.57660900
O 0.98445500 -0.44410800 0.04553100
O -3.15169400 4.43870000 3.31008500
O 0.22846200 4.87023000 2.76710900
O -1.07176000 2.76705500 5.17551000
C -3.29169800 -1.97009800 0.61944900
C -4.09589800 -1.97799900 1.91204000
H -4.67365200 -1.05337100 2.01065100
H -4.79306500 -2.82317600 1.93351000
H -3.43087900 -2.05913600 2.77795700
C 2.23395700 -1.02510300 -0.18714400
C 2.12706700 -2.26019500 -1.07113000
H 3.11309700 -2.70692600 -1.24240800
H 1.48492400 -3.01276200 -0.60218800
H 1.69369600 -1.99999100 -2.04215400
C -1.02265700 1.62429400 -3.16030400
C -4.38957100 5.04024300 3.55178200
C 1.13323900 5.93646100 2.72588800
C 1.95182100 5.92630700 1.44244700
H 1.29748800 6.00762900 0.56845100
H 2.65776800 6.76421000 1.42268100
H 2.52120600 4.99517400 1.35729700
C -1.09271900 2.36224600 6.51317300
C -2.33649800 1.54726500 6.84320200

H	-3.24096400	2.13543500	6.65681000
H	-2.38249900	0.64505300	6.22380700
H	-2.33779500	1.23952600	7.89497500
H	-2.26471100	3.56873300	-0.92748400
H	-2.73587800	4.53099700	0.47977000
H	0.09594700	0.39605300	4.27302000
H	0.58716700	-0.54268900	2.85640300
H	-0.19333900	1.76584600	6.73521200
H	-1.04993200	3.24709400	7.16696500
H	-5.05500300	4.33257000	4.07198800
H	1.80869100	5.88359000	3.59400500
H	0.58828400	6.88986900	2.80747700
H	2.69989600	-1.30098100	0.77260800
H	2.90570800	-0.29192700	-0.66186600
H	0.01702500	1.57302600	-3.52068100
H	-1.33433600	2.67740400	-3.25251400
H	-2.73843700	-2.91751900	0.52438300
H	-3.97754600	-1.91753900	-0.24050300
C	-1.90889400	0.75608200	-4.04293600
H	-1.85486200	1.07709100	-5.08943300
H	-1.59584200	-0.29150300	-3.98765400
H	-2.95246400	0.81669800	-3.71777000
C	-4.24891600	6.30785600	4.38358100
H	-5.22636500	6.76952300	4.56419700
H	-3.79074700	6.08183200	5.35179400
H	-3.61427600	7.03603500	3.86822200
H	-4.87817100	5.28304200	2.59437800
Th	-1.27828300	3.38941100	3.12353600
Th	-0.89561800	0.59352500	0.22951300

Cat_c (EtOH)

H= -653.398001 au

Th	1.10082400	1.91989700	-0.34343000
C	3.74143700	0.73965800	-3.55554800
H	3.99582700	1.80422500	-3.52654100
H	4.52291800	0.21474100	-4.11638500
H	2.79710000	0.62895100	-4.09870300
C	-2.33183200	0.78311000	-2.72799900
H	-1.56925000	0.24828800	-3.30369300
H	-3.31377400	0.38274000	-3.00410800
H	-2.29884800	1.83925900	-3.01512200
C	1.48895000	0.04415300	3.52777700
H	0.49789000	-0.34209600	3.26765300
H	2.23862200	-0.55245300	2.99757900
H	1.63935800	-0.09420900	4.60434800
O	2.62372300	0.84359100	-1.41195100
O	1.41545700	1.70870800	1.77323700
O	-0.82981100	1.13399300	-0.86419300
C	-2.07954800	0.62784800	-1.23450000
C	3.61464900	0.18231100	-2.14420700
C	1.60675900	1.51309300	3.14450700
O	1.18182900	4.00150700	-0.86752300
C	1.20817800	5.36930100	-1.15714100
C	0.25483600	6.15388600	-0.26604300
H	-0.77376700	5.80376800	-0.40175300
H	0.52275400	6.02714900	0.78806800
H	0.28683600	7.22343800	-0.50227400
H	4.58143200	0.27267100	-1.62454900
H	3.38340200	-0.89330700	-2.19246400
H	2.23192500	5.75493500	-1.03040300
H	0.94092400	5.52913200	-2.21344400
H	2.59847200	1.89169900	3.43769100
H	0.86653600	2.10136100	3.70916500

H	-2.14464800	-0.43642500	-0.95882700
H	-2.87104000	1.14688900	-0.67145500

Int-1C (EtOH)

H= -1037.72995 au

N	-0.27231900	2.18721400	0.45526900
C	-0.68599900	2.33149700	1.61883100
N	-0.96333400	2.45509400	2.79081900
O	1.15502000	-0.23370000	1.97459600
C	1.74099200	-0.12486800	3.23501800
C	3.25898400	-0.01610500	3.15484300
H	3.55190500	0.87263300	2.58533400
H	3.70418000	0.05666300	4.15394900
H	3.67894000	-0.89534000	2.65508300
Th	0.47272600	-0.47238900	-0.06794200
O	-1.66987600	-0.83183700	-0.12882500
O	1.36733800	0.38127900	-1.87555400
C	-2.18101500	2.10369900	3.52470600
C	-3.28956200	1.58304600	2.61516400
C	-2.61340400	3.30749400	4.35785500
H	-1.87518700	1.30253300	4.20963500
H	-2.94137500	0.73984100	2.01076500
H	-4.14371100	1.24983600	3.21262300
H	-3.63762600	2.37307100	1.94009200
H	-1.79404700	3.65707200	4.99129300
H	-2.92469400	4.13392700	3.71064000
H	-3.45812600	3.03691000	4.99830000
C	-0.40345600	3.29421800	-0.53309900
C	-1.16346500	2.79043800	-1.75446100
C	0.99341600	3.79310700	-0.88705200
H	-0.97138200	4.11053300	-0.06660500
H	-2.15220700	2.41382100	-1.47793000
H	-1.29231000	3.60323900	-2.47643100
H	-0.60105300	1.98503000	-2.23770000
H	1.51171200	4.17488000	-0.00262100
H	1.57970700	2.97312900	-1.31165300
H	0.93036900	4.59959000	-1.62487000
O	1.17968200	-2.47491400	-0.36426000
C	1.68100800	-3.77252200	-0.46288800
C	0.57217000	-4.79585800	-0.67116200
H	0.98212500	-5.80969700	-0.74602200
H	-0.13463000	-4.77022700	0.16446600
H	0.01898100	-4.57948200	-1.59085000
C	2.10772800	0.56854600	-3.04339500
C	3.60562900	0.41529900	-2.80721200
H	4.16993800	0.56889900	-3.73433800
H	3.95678900	1.14433700	-2.06879300
H	3.83284700	-0.58720600	-2.42987500
C	-2.93227900	-1.35257600	-0.41162000
C	-3.08230500	-1.74051900	-1.87787400
H	-2.92529900	-0.86994400	-2.52375100
H	-2.34522200	-2.50350500	-2.14915200
H	-4.08174300	-2.14239000	-2.08109300
H	1.47259600	-1.00104400	3.84790500
H	1.33874800	0.75880600	3.75641800
H	2.24497900	-4.02517700	0.44954200
H	1.90780000	1.57205500	-3.45701200
H	1.78679700	-0.15163900	-3.81372200
H	2.39499400	-3.83252900	-1.30019400
H	-3.12577400	-2.23565200	0.21936900
H	-3.70810400	-0.61204100	-0.15304500

TS_{1C-2C} (EtOH)

H= -1037.715573 au

N	-1.00532900	2.39597400	0.68306100
C	-1.15051200	2.40789200	1.96138600
N	-1.38761000	3.03898300	2.98911900
O	-0.64415400	0.57581000	2.27479600
C	0.19375700	0.39214900	3.39418600
C	1.67175300	0.37874000	3.02202600
H	1.96644900	1.33639700	2.57782200
H	2.29935500	0.21406700	3.90487600
H	1.88439800	-0.42410000	2.30647500
Th	-0.47101100	-0.03009500	-0.00161000
O	-2.40323500	-0.61492000	-0.71715700
O	0.74020200	0.59122900	-1.67040200
C	-2.23263400	2.71536200	4.12805300
C	-3.67645800	3.13103500	3.83379800
C	-1.69337000	3.41067900	5.37530200
H	-2.21450100	1.62787100	4.28467500
H	-4.06171200	2.60798100	2.95339600
H	-4.32478700	2.89315100	4.68389100
H	-3.73403800	4.20827500	3.64702500
H	-0.66591100	3.10011900	5.58654400
H	-1.69508200	4.49676800	5.23722800
H	-2.31184200	3.17182900	6.24619300
C	-1.48138400	3.59274500	-0.04424800
C	-1.92033700	3.17533800	-1.44368100
C	-0.37741600	4.64850600	-0.07881200
H	-2.34485800	4.01005300	0.49267300
H	-2.73884300	2.44963500	-1.39956100
H	-2.26466800	4.04251000	-2.01595300
H	-1.08470600	2.71978900	-1.98771000
H	-0.08574300	4.93411500	0.93598900
H	0.50565700	4.26037000	-0.59730700
H	-0.71791800	5.54769300	-0.60380600
O	0.53693300	-1.87208100	0.47566000
C	1.21788300	-3.06070700	0.75040600
C	0.28478500	-4.26387800	0.74287200
H	0.83331800	-5.18689100	0.96262600
H	-0.50241300	-4.14366400	1.49418600
H	-0.19307100	-4.37282300	-0.23599700
C	1.64229100	0.91464700	-2.68685000
C	3.08269100	0.92533800	-2.19196800
H	3.77533900	1.17717500	-3.00306400
H	3.21025700	1.66313700	-1.39262400
H	3.35938400	-0.05767500	-1.79719900
C	-3.57423500	-1.16897500	-1.24313100
C	-3.31583700	-1.93201000	-2.53506600
H	-2.88772300	-1.26961900	-3.29451200
H	-2.61225000	-2.75308200	-2.36257300
H	-4.24531400	-2.35523200	-2.93259300
H	-0.08132600	-0.54866800	3.89250700
H	0.01311800	1.20406100	4.11220100
H	1.71240000	-2.98809100	1.73272600
H	1.39125100	1.90274400	-3.10503600
H	1.54369500	0.19216200	-3.51216400
H	2.01736800	-3.20991000	0.00741300
H	-4.02952900	-1.84366300	-0.50132800
H	-4.30603600	-0.36744900	-1.42945700

Int-2C (EtOH)

H= -1037.727735 au

N	-0.34875200	1.74692200	0.25011500
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C	-0.65325100	1.55014200	1.55014100
N	-1.10218600	2.38377200	2.39841000
O	-0.43542100	0.13739800	1.79779100
C	0.49265300	-0.20366600	2.85127100
C	1.89147200	0.32662500	2.60106800
H	1.89378300	1.41728200	2.52159900
H	2.54373100	0.04655000	3.43471100
H	2.31825100	-0.10249800	1.68845900
Th	0.05118500	-0.44382700	-0.72775300
O	-1.82552400	-1.19624000	-1.41406000
O	1.21804000	0.02077400	-2.45871000
C	-1.69581000	2.03313000	3.67361000
C	-3.13755300	2.55293400	3.68712300
C	-0.88918200	2.65945500	4.81476000
H	-1.74507600	0.94274900	3.82697300
H	-3.72023600	2.09372800	2.88297100
H	-3.62817500	2.32879500	4.64115100
H	-3.14775100	3.63698600	3.53419000
H	0.13811000	2.28049500	4.83634300
H	-0.83714400	3.74453400	4.67862300
H	-1.35129400	2.45291500	5.78626700
C	-0.62743300	3.07332400	-0.29758300
C	-0.88378400	2.95727700	-1.79916700
C	0.51640600	4.04332100	0.00646000
H	-1.53242600	3.46007100	0.19218200
H	-1.74888900	2.31451800	-2.00321700
H	-1.09056600	3.93826100	-2.23891400
H	-0.01127700	2.54077700	-2.31844200
H	0.66283100	4.11953700	1.08701000
H	1.44911400	3.69570600	-0.45303700
H	0.29663400	5.04498900	-0.38032200
O	1.19848200	-2.04255500	0.15189200
C	1.92201500	-3.10172700	0.70660100
C	1.08342900	-4.36769700	0.81979200
H	1.66622100	-5.18612100	1.25721000
H	0.20614000	-4.19494500	1.45194700
H	0.73274500	-4.68541100	-0.16732900
C	2.05605500	0.22243900	-3.56184500
C	3.52679000	0.17771100	-3.17186400
H	4.16810700	0.33874800	-4.04558400
H	3.75275700	0.95442700	-2.43386100
H	3.77946100	-0.79371200	-2.73474500
C	-2.99160500	-1.75094200	-1.95610900
C	-2.70707200	-2.54558200	-3.22261100
H	-2.25648100	-1.90405400	-3.98691800
H	-2.01442400	-3.36774800	-3.01435000
H	-3.63003300	-2.97095700	-3.63229100
H	0.48312700	-1.29580300	2.87694200
H	0.10147800	0.16569600	3.80155300
H	2.29426100	-2.81854300	1.70534700
H	1.82510400	1.19488300	-4.02310500
H	1.85132600	-0.54486900	-4.32376200
H	2.81141600	-3.30358100	0.08954300
H	-3.46692000	-2.40332500	-1.20795500
H	-3.70985500	-0.94689800	-2.17670700

Int-3C (EtOH)

H= -1192.648925 au

N	-0.55858800	0.48019100	1.77622200
C	0.37958500	-0.23657700	2.44220400
N	0.40246900	-0.62200600	3.65305100
O	1.38913700	-0.55659800	1.45187200
C	2.77829600	-0.35867300	1.78885200

C	3.45833800	0.52525100	0.76272000	N	-1.05138300	0.67095500	1.80696300
H	2.99018400	1.51262800	0.72454300	C	-0.10150400	-0.11420200	2.39486400
H	4.51356700	0.64822300	1.02916800	N	-0.10215900	-0.62519100	3.55562400
H	3.40856500	0.08188600	-0.23581400	O	0.89744000	-0.33209700	1.38937600
Th	-0.12152500	-0.06959700	-0.67657900	C	2.28862700	-0.13345300	1.72584300
O	-1.71902000	0.94861100	-1.68456900	C	2.91864600	0.87376700	0.78568300
O	1.49599100	-0.17164900	-2.10183600	H	2.42766600	1.84605300	0.87200100
C	1.28382200	-1.63387900	4.20091600	H	3.98032200	0.98841100	1.02866900
C	0.43239700	-2.82657100	4.65093000	H	2.83863500	0.54045100	-0.25335800
C	2.06460500	-1.05666500	5.38463000	Th	-0.58589700	0.10799600	-0.79255500
H	2.00215700	-2.01561300	3.45937400	O	-2.17630500	0.92881500	-1.96246300
H	-0.11538300	-3.25158300	3.80461100	O	1.07549200	-0.08638500	-2.14482400
H	1.05961200	-3.61299200	5.08579100	C	0.79279400	-1.67513400	4.00515300
H	-0.29738300	-2.50848800	5.40277000	C	-0.04710800	-2.91226100	4.34053600
H	2.70395600	-0.22246100	5.07707700	C	1.56501600	-1.20082000	5.23881300
H	1.36907900	-0.67776900	6.14050500	H	1.51438400	-1.97271200	3.22941700
H	2.69881400	-1.82015100	5.84802800	H	-0.58819500	-3.26498500	3.45766600
C	-1.85366100	0.74900200	2.42387600	H	0.58816900	-3.72754500	4.70413200
C	-1.72704900	1.69592200	3.62166300	H	-0.78144500	-2.67124600	5.11600100
C	-2.62467700	-0.52388300	2.78755700	H	2.19174200	-0.33169900	5.01340000
H	-2.44080500	1.27266500	1.65423800	H	0.86417500	-0.90726800	6.02693800
H	-1.23087900	2.62907400	3.33154000	H	2.21036800	-1.99620900	5.62654100
H	-2.71675600	1.94996400	4.01734000	C	-2.34855700	0.88327500	2.47201500
H	-1.13951500	1.22387400	4.41221500	C	-2.22375200	1.68649100	3.77001900
H	-2.71556700	-1.18299700	1.91761700	C	-3.13227100	-0.41531600	2.67370100
H	-2.11313000	-1.06856700	3.58383400	H	-2.91563100	1.49941000	1.75845900
H	-3.63426400	-0.27165100	3.13018200	H	-1.70108300	2.63260500	3.59310200
H	0.16331500	1.98694500	1.05046900	H	-3.21658000	1.91822800	4.17112400
C	0.01141900	3.62362700	-0.13589000	H	-1.66543500	1.11576800	4.51515200
C	0.52405900	4.03515800	-1.49922100	H	-3.21602500	-0.96866600	1.73238400
H	1.61725700	4.07112500	-1.50785900	H	-2.63740700	-1.05362500	3.40875500
H	0.19122700	3.32653900	-2.26324300	H	-4.14395300	-0.19440900	3.03030500
H	0.14352000	5.02696700	-1.76245600	H	-0.56795800	1.75935600	1.16235600
O	0.54926000	2.34087400	0.19823700	C	-0.50080000	3.70010300	0.09951600
O	-0.88539000	-2.06254000	-0.71088100	C	-0.03305800	4.23476200	-1.24244500
C	-1.42475300	-3.34943900	-0.79994500	H	1.04909400	4.11255600	-1.35084000
C	-0.45709100	-4.32505300	-1.45549200	H	-0.52467500	3.70055200	-2.06171800
H	-0.89439100	-5.32812500	-1.51629300	H	-0.27009900	5.29977800	-1.33842900
H	-0.20752800	-3.99638200	-2.46948500	O	-0.17566900	2.32932900	0.22992000
H	0.47203200	-4.38932400	-0.88003000	O	-1.32198100	-1.89738100	-0.64798200
C	2.49831300	-0.26988200	-3.06976000	C	-1.90372700	-3.16465600	-0.55348500
C	2.02090700	0.21649200	-4.43165400	C	-0.97273100	-4.25315000	-1.06984800
H	2.81801700	0.13461100	-5.17936400	H	-1.44211100	-5.24024600	-0.98942400
H	1.16672200	-0.37719500	-4.77294300	H	-0.72075800	-4.07619700	-2.12037900
H	1.70724700	1.26394500	-4.37678700	H	-0.04171100	-4.26664800	-0.49408900
C	-2.76910000	1.45382000	-2.45721200	C	2.05677000	-0.39206300	-3.09266100
C	-3.85040100	0.41084700	-2.70440400	C	1.61745900	-0.02529300	-4.50344500
H	-4.27084000	0.06046400	-1.75642400	H	2.40051100	-0.26502700	-5.23176300
H	-4.66398300	0.82747500	-3.30904800	H	0.71202700	-0.57549500	-4.77939500
H	-3.43682800	-0.45374200	-3.23325100	H	1.39968700	1.04530400	-4.57132900
H	3.25727500	-1.34291200	1.83563400	C	-3.20653700	1.35393800	-2.80654700
H	0.32146700	4.34860700	0.62810700	C	-4.40817500	0.42041300	-2.75423100
H	-1.08535100	3.57940100	-0.13809200	H	-4.81167300	0.36853400	-1.73785600
H	2.82405600	0.09114000	2.78426400	H	-5.20334700	0.76980700	-3.42257600
H	-1.68425600	-3.70856300	0.20772700	H	-4.12196500	-0.59131300	-3.05836800
H	-2.36290600	-3.31636600	-1.37525300	H	2.78942900	-1.10517800	1.65714400
H	-3.21174000	2.32677800	-1.95166000	H	-0.02396500	4.26541300	0.91387100
H	3.37679500	0.31989900	-2.75995400	H	-1.58737300	3.84560800	0.19755000
H	2.83506600	-1.31557900	-3.15150600	H	2.34163000	0.20747800	2.76303900
H	-2.37888400	1.81445700	-3.42202700	H	-2.16754400	-3.37312000	0.49506400
				H	-2.84485000	-3.18231500	-1.12521700
				H	-3.51853000	2.37106900	-2.52189200
				H	2.98694000	0.14632700	-2.84849800

TS_{3C-4C} (EtOH)

H= -1192.650271 au

H 2.29486900 -1.46664600 -3.04891100
H -2.83391800 1.41695600 -3.84076600

Int-4C (EtOH)

H= -1192.657775 au

N -0.63290400 0.68455000 2.01309400
C 0.37936600 -0.15007700 2.45721600
N 0.35868900 -0.82118400 3.52666600
O 1.34719400 -0.17229100 1.44333600
C 2.74088500 0.02026100 1.78700800
C 3.34150400 1.06976300 0.87667400
H 2.82474500 2.02582200 0.98920900
H 4.39978000 1.20554500 1.12266400
H 3.26646600 0.76031000 -0.16994600
Th -0.10605000 0.27242600 -0.86189700
O -1.64924700 0.79032400 -2.25093000
O 1.63535500 -0.02982900 -2.09352200
C 1.27956800 -1.90452300 3.82988100
C 0.46673100 -3.19091300 3.99860600
C 2.04678100 -1.57466200 5.11188600
H 2.00087400 -2.07456200 3.01733600
H -0.07261200 -3.43389100 3.07886200
H 1.12411600 -4.03180200 4.24398000
H -0.26512000 -3.07566700 4.80463600
H 2.65262700 -0.67007400 4.99799400
H 1.34602400 -1.40429300 5.93541100
H 2.71231300 -2.39902600 5.38763400
C -1.90993900 0.84989100 2.73128700
C -1.73802500 1.50556200 4.10307000
C -2.69146800 -0.45948100 2.79871300
H -2.47230100 1.54236100 2.09127700
H -1.21698100 2.46514400 4.01777400
H -2.71781300 1.69510600 4.55377900
H -1.16599500 0.85392200 4.76702200
H -2.78019500 -0.90812500 1.80493400
H -2.19729100 -1.17301400 3.46085900
H -3.69808900 -0.26800400 3.18325600
H -0.27582200 1.55848800 1.59241500
C 0.18203800 3.75555500 -0.11382900
C 0.41042900 4.25678300 -1.53477100
H 1.36235400 3.88163600 -1.92574500
H -0.38991500 3.90766200 -2.19539200
H 0.43313900 5.35226000 -1.57054600
O 0.14138800 2.36074000 -0.04325900
O -0.81660900 -1.73476200 -0.44884500
C -1.37791900 -2.98879500 -0.21751600
C -0.46585500 -4.11471800 -0.68981700
H -0.91821500 -5.09529200 -0.50100200
H -0.27319200 -4.02519500 -1.76376500
H 0.49645200 -4.07266700 -0.16899500
C 2.59272200 -0.41869800 -3.03308400
C 2.14185100 -0.13563200 -4.45980300
H 2.90843600 -0.44128600 -5.18115300
H 1.21994500 -0.68106400 -4.68654000
H 1.94665400 0.93284700 -4.59564000
C -2.63288300 1.07699800 -3.19785900
C -3.94447400 0.36690700 -2.88849300
H -4.32505600 0.67357100 -1.90850300
H -4.70557300 0.60217100 -3.64135600
H -3.79821500 -0.71770600 -2.87198700
H 3.25149200 -0.94124600 1.67259900
H 0.98464500 4.14491200 0.53717500
H -0.75840800 4.18671600 0.27116300

H 2.79465500 0.31758900 2.83827200
H -1.58775500 -3.11862200 0.85753600
H -2.34896800 -3.06742000 -0.73407500
H -2.80546700 2.16471700 -3.23638500
H 3.53879500 0.11305800 -2.83858500
H 2.81017200 -1.49371900 -2.92436500
H -2.28263500 0.77950300 -4.19883100

dimer-A (^tBuOH)

H= -1461.241935 au

O -0.66909300 0.79420600 2.73989800
U -0.90587200 0.51381800 0.32026700
O -2.61840100 -0.64888100 -0.46354300
O 1.04319200 0.12378200 -0.64840000
C -3.57233800 -1.50640300 -1.02830200
C -3.31228800 -1.63092000 -2.53653600
H -2.30703000 -2.02766500 -2.71464800
H -4.03520100 -2.29592400 -3.02269000
H -3.37926600 -0.64711100 -3.01352900
C -3.46129400 -2.88745900 -0.36593700
H -2.45879700 -3.30079900 -0.52170000
H -3.63384900 -2.80229900 0.71237100
H -4.19060400 -3.59634400 -0.77395600
C -4.97253700 -0.92489500 -0.78569500
H -5.15244700 -0.81253400 0.28850200
H -5.05535600 0.06380600 -1.24913500
H -5.75840000 -1.56529100 -1.20217400
C 2.20951400 -0.15711800 -1.37298800
C 1.88115400 -0.17184400 -2.87278500
H 1.12509500 -0.93504700 -3.08562200
H 1.48076300 0.80050600 -3.17966000
H 2.76577400 -0.38504600 -3.48358600
C 2.74755500 -1.52976700 -0.94409900
H 2.96201100 -1.53026500 0.12998300
H 2.00215800 -2.30672400 -1.14515900
H 3.66838100 -1.79241300 -1.47708100
C 3.25460500 0.92835900 -1.07735800
H 4.19103500 0.75312200 -1.61915100
H 2.86869300 1.91107500 -1.36850900
H 3.47730500 0.95515500 -0.00553500
O -1.44636600 2.86212400 0.70648700
U -1.20936000 3.14189000 3.12632400
O -3.15454200 3.53226700 4.10349000
O 0.50780800 4.29757500 3.90760500
C -4.31177300 3.81852500 4.84030900
C -3.96583000 3.83931200 6.33611600
H -3.20465700 4.60102500 6.53605000
H -4.84236400 4.05860000 6.95636000
H -3.56518000 2.86706500 6.64308500
C -4.85251700 5.19019700 4.41163200
H -4.10426900 5.96713100 4.60183100
H -5.07796600 5.18663700 3.33982100
H -5.76749400 5.45607200 4.95303200
C -5.36216600 2.73367500 4.56156000
H -5.59726200 2.70289400 3.49249200
H -4.97455600 1.75153800 4.85242400
H -6.29190500 2.91295500 5.11345700
C 1.48409600 5.13561900 4.46335300
C 1.68228300 4.76675300 5.94075400
H 0.74301500 4.89179200 6.49014600
H 1.99337900 3.72028400 6.02899300
H 2.44504200 5.39150900 6.41918000
C 1.02010700 6.59511200 4.35012100

H	0.86458300	6.85999900	3.29863300	H	2.52158900	-0.26553800	2.38264800
H	0.07201400	6.73144100	4.88132100	H	1.83523600	-0.40825700	4.01334300
H	1.75328900	7.29158400	4.77245800	C	0.26956700	1.89210700	3.90306000
C	2.80107800	4.94552800	3.69709500	H	0.12797900	2.97812600	3.91066600
H	3.60079900	5.58066100	4.09487800	H	-0.63550500	1.43320800	3.49186100
H	3.12667100	3.90202100	3.76130400	H	0.38717100	1.55429600	4.93888300
H	2.66080300	5.19213700	2.63937200	C	2.74930200	2.18963900	3.60426800
C	-1.93468600	3.83948800	-0.21157400	H	2.95898900	1.86307100	4.62906500
C	-3.43265900	3.60984800	-0.43875300	H	3.61436400	1.94258900	2.98000700
C	-1.70132400	5.23479800	0.38311200	H	2.63132800	3.27855200	3.60904400
C	-1.16564900	3.70622100	-1.53104300	O	2.51413100	1.26926400	-1.55324000
H	-3.61245700	2.60929000	-0.84695000	O	1.27444600	1.99292500	1.73531800
H	-3.97799100	3.68903800	0.50752000	O	-1.02090400	1.41521400	-0.96178700
H	-3.85083900	4.34200900	-1.13786700	C	-2.15244100	0.62049900	-1.20108500
H	-0.63850300	5.39056300	0.60112200	C	3.43047800	0.38425300	-2.14156500
H	-2.02118100	6.02769400	-0.30055200	C	1.48544400	1.52461400	3.04110900
H	-2.28487500	5.37081000	1.30528600				
H	-1.48326700	4.45509600	-2.26394700				
H	-0.09023000	3.82247800	-1.36319500				
H	-1.34061300	2.72217400	-1.98725400				
C	-0.16956100	-0.17877000	3.65687600				
C	1.32482000	0.07052500	3.88782100				
C	-0.94343800	-0.05915000	4.97476600				
C	-0.38197500	-1.57550900	3.05794900				
H	1.87273900	0.00037400	2.94232000				
H	1.49074200	1.07233000	4.29900700				
H	1.75117300	-0.65768600	4.58612100				
H	-2.01677400	-0.18904400	4.80378400				
H	-0.61765200	-0.80586300	5.70629200				
H	-0.78300500	0.92586300	5.43410900				
H	-0.05447800	-2.36572000	3.74110500				
H	-1.44170300	-1.74532800	2.83527900				
H	0.20744000	-1.70111500	2.13810100				
Cat_A (^tBuOH)							
<i>H= -1114.924459 au</i>							
<i>H= -730.576978 au</i>							
U	0.92637100	2.25931000	-0.41360100	U	-0.29616300	0.54437100	0.51404000
C	3.50119900	0.68018300	-3.64627300	O	-2.18965800	-0.39204100	-0.18528400
H	3.81967700	1.71505100	-3.81157200	O	1.26744300	0.55966800	-1.06856400
H	4.20813500	0.01803400	-4.15874000	C	-3.21542100	-1.25017600	-0.59071900
H	2.51426800	0.54964300	-4.10224500	C	-3.51212400	-1.01698900	-2.08013700
C	2.95994700	-1.05869000	-1.91371600	H	-2.61081500	-1.20073300	-2.67422300
H	1.96828700	-1.20611700	-2.35428600	H	-4.30881000	-1.67383900	-2.44858000
H	3.64632800	-1.78553400	-2.36250600	H	-3.82072100	0.02108500	-2.24492400
H	2.89290800	-1.26915100	-0.84099100	C	-2.78066300	-2.70773600	-0.37223900
C	4.80823700	0.59462400	-1.49866800	H	-1.87873200	-2.92235800	-0.95591800
H	5.13777700	1.62882900	-1.64450500	H	-2.55140700	-2.87669000	0.68540500
H	4.75354400	0.40320100	-0.42198900	H	-3.55903400	-3.41894200	-0.67241800
H	5.56504100	-0.07072000	-1.92932200	C	-4.47244300	-0.95558500	0.24270800
C	-2.09957900	0.09419200	-2.64192300	H	-4.26111000	-1.11213000	1.30590600
H	-1.19666700	-0.50713000	-2.79016100	H	-4.77584100	0.08805300	0.10576100
H	-2.97003700	-0.52730200	-2.88065700	H	-5.31410900	-1.59852100	-0.04003200
H	-2.07075000	0.93077100	-3.34810300	C	2.27342200	0.24412900	-1.98690000
C	-3.40619100	1.48441500	-1.00322500	C	1.87054300	0.76606200	-3.37468700
H	-4.32503200	0.91359800	-1.17838500	H	0.92132300	0.31507100	-3.68236800
H	-3.43468400	1.87711600	0.01865000	H	1.73775900	1.85300100	-3.34341700
H	-3.39245200	2.33302700	-1.69548900	H	2.62557800	0.53553600	-4.13525300
C	-2.16795200	-0.55439800	-0.21362500	C	2.45481000	-1.28055300	-2.04164300
H	-2.18275000	-0.18150400	0.81579300	H	2.72585600	-1.66241600	-1.05124100
H	-3.04474400	-1.19517700	-0.35991500	H	1.51829800	-1.75897000	-2.34842600
H	-1.27062800	-1.16900200	-0.34260400	H	3.23842600	-1.57686000	-2.74861400
C	1.66513200	0.00077600	3.01101200	C	3.58620600	0.90735700	-1.54242900
H	0.77205000	-0.47647000	2.59397300				

H	4.40936300	0.69527100	-2.23470000	H	1.64271200	1.03769400	-3.32583200
H	3.45664200	1.99352200	-1.48529700	H	2.78140600	-0.16483700	-3.96287000
H	3.87081000	0.54717900	-0.54811800	C	2.94233800	-1.71063700	-1.65571500
C	-1.91113600	3.76418800	4.50554700	H	3.27292100	-1.90682000	-0.63011200
C	-3.15429700	2.93575200	4.19890700	H	2.11828300	-2.39473100	-1.88621700
C	-2.24050600	5.18394000	4.96391100	H	3.77417300	-1.93696100	-2.33236800
H	-1.33701000	3.27096600	5.29922700	C	3.62822900	0.69942400	-1.45188300
H	-2.88772400	1.92118100	3.88881600	H	4.48297100	0.56192100	-2.12403200
H	-3.78431100	2.86136100	5.09023800	H	3.29211100	1.73859400	-1.52996000
H	-3.74679500	3.40138700	3.40380000	H	3.96734600	0.52958900	-0.42461700
H	-1.32788100	5.75197900	5.16113900	C	-1.48152600	3.16642300	4.59258500
H	-2.81964900	5.71284800	4.20008200	C	-2.88274100	2.55311100	4.56448200
H	-2.83393600	5.14988900	5.88200100	C	-1.46844200	4.53066000	5.28094600
C	-1.30420300	4.05515800	-0.10528500	H	-0.82066900	2.49660400	5.16224300
C	-1.48764100	3.21320300	-1.36131200	H	-2.86098200	1.56786300	4.09078600
C	-0.22771600	5.12283600	-0.27662000	H	-3.27564300	2.44249300	5.58073900
H	-2.25883800	4.53824100	0.14091700	H	-3.56748900	3.19539700	4.00059600
H	-2.24285800	2.43298800	-1.21612300	H	-0.45824300	4.94936900	5.29389900
H	-1.81648200	3.84337900	-2.19262000	H	-2.12009100	5.23291900	4.75099100
H	-0.54246700	2.74381400	-1.66386900	H	-1.82181400	4.44266300	6.31299800
H	-0.11338500	5.72394200	0.63060100	C	-1.34154800	3.77413500	0.32389800
H	0.73701200	4.66126300	-0.50894200	C	-1.79047900	3.39934700	-1.08496900
H	-0.49331900	5.79443100	-1.09908600	C	-0.27566000	4.86899200	0.30874500

TS_{1A-2A} (^tBuOH)

H= -1114.899304 au

N	-0.82893000	2.55885600	0.98668800
C	-0.81481500	2.58431800	2.28130400
N	-0.94116700	3.31158600	3.26286200
O	-0.42325700	0.72684700	2.57936000
C	0.55774800	0.19678800	3.46885500
C	-0.12886700	-0.32629800	4.73528600
H	0.59435800	-0.78018100	5.42173900
H	-0.64020200	0.47916000	5.26811900
H	-0.87616900	-1.08207500	4.47327200
C	1.23390100	-0.98998200	2.75483300
H	1.78466200	-0.66553400	1.86044900
H	1.96075300	-1.49306100	3.40090800
H	0.48733500	-1.74986700	2.47784400
C	1.62804100	1.23987800	3.80817100
H	1.19443900	2.10399900	4.31591100
H	2.39667800	0.80936600	4.45890100
H	2.11613700	1.59806100	2.89571900
U	-0.48622900	0.18633800	0.21887400
O	-2.31699000	-0.76338100	-0.59832800
O	1.41750100	-0.02684500	-0.89904100
C	-3.43974000	-1.42051800	-1.11550400
C	-3.66116400	-0.97626100	-2.56885700
H	-2.77994200	-1.21426000	-3.17396300
H	-4.53073900	-1.46880100	-3.01885900
H	-3.82138700	0.10638800	-2.61161400
C	-3.19970400	-2.93695900	-1.06756200
H	-2.31383600	-3.19667100	-1.65706800
H	-3.02954200	-3.25838200	-0.03406600
H	-4.05260600	-3.49959200	-1.46402900
C	-4.66883200	-1.06122200	-0.26730000
H	-4.50809200	-1.36135800	0.77366100
H	-4.83530900	0.02105800	-0.28642600
H	-5.57711100	-1.55498300	-0.63149500
C	2.47353100	-0.25427600	-1.79080200
C	1.98838500	0.00305000	-3.22527300
H	1.15124600	-0.66177600	-3.46446600

H	1.64271200	1.03769400	-3.32583200
H	2.78140600	-0.16483700	-3.96287000
C	2.94233800	-1.71063700	-1.65571500
H	3.27292100	-1.90682000	-0.63011200
H	2.11828300	-2.39473100	-1.88621700
H	3.77417300	-1.93696100	-2.33236800
C	3.62822900	0.69942400	-1.45188300
H	4.48297100	0.56192100	-2.12403200
H	3.29211100	1.73859400	-1.52996000
H	3.96734600	0.52958900	-0.42461700
C	-1.48152600	3.16642300	4.59258500
C	-2.88274100	2.55311100	4.56448200
C	-1.46844200	4.53066000	5.28094600
H	-0.82066900	2.49660400	5.16224300
H	-2.86098200	1.56786300	4.09078600
H	-3.27564300	2.44249300	5.58073900
H	-3.56748900	3.19539700	4.00059600
H	-0.45824300	4.94936900	5.29389900
H	-2.12009100	5.23291900	4.75099100
H	-1.82181400	4.44266300	6.31299800
C	-1.34154800	3.77413500	0.32389800
C	-1.79047900	3.39934700	-1.08496900
C	-0.27566000	4.86899200	0.30874500
H	-2.21110900	4.14287500	0.88751800
H	-2.57278100	2.63212700	-1.06406300
H	-2.19171400	4.26959200	-1.61326300
H	-0.94284700	3.02614700	-1.67579200
H	0.02868000	5.12053200	1.32823500
H	0.60833800	4.53419400	-0.24476800
H	-0.65896800	5.77699800	-0.16948700

Int-2A (^tBuOH)

H= -1114.907948 au

N	-0.48937600	2.23444900	1.12135500
C	-0.87901400	2.12397700	2.40842000
N	-1.60986300	2.91750900	3.08533900
O	-0.41699600	0.83239400	2.91963700
C	0.82966600	0.75707900	3.69571300
C	0.52360700	-0.14383100	4.88953000
H	1.42747300	-0.31453400	5.48278200
H	-0.23168300	0.30939000	5.53590000
H	0.14579600	-1.11554700	4.55523600
C	1.89405500	0.10439100	2.80748600
H	2.10843700	0.71546400	1.92266100
H	2.83733100	-0.01312000	3.34898600
H	1.59969300	-0.91314200	2.50533200
C	1.31401200	2.13298700	4.13976100
H	0.58707800	2.62363100	4.78834500
H	2.24836800	2.01771400	4.69784700
H	1.50436000	2.77980800	3.27929400
U	-0.29519300	-0.10090000	0.41169600
O	-2.22411600	-0.80949500	-0.35439400
O	1.34633300	-0.36730500	-1.03164200
C	-3.40515200	-1.22980300	-0.98597100
C	-3.20882800	-1.18863800	-2.50748800
H	-2.37750500	-1.83942700	-2.79857100
H	-4.10695500	-1.51811400	-3.04200000
H	-2.97317900	-0.16934000	-2.83120000
C	-3.71688200	-2.66500300	-0.53836700
H	-2.89359100	-3.33320900	-0.81344600
H	-3.84008700	-2.70137500	0.54929400
H	-4.63492700	-3.04519900	-1.00026100
C	-4.55049900	-0.29400300	-0.57668900

H	-4.67763200	-0.30764900	0.51064600	H	-4.31053600	-0.16425200	-0.78908600
H	-4.32506700	0.73397700	-0.87827300	C	-2.45996300	-2.12007000	-2.97620000
H	-5.49969000	-0.58771000	-1.03897000	H	-2.18233900	-1.31215100	-3.66177600
C	2.26646600	-0.54902100	-2.07488200	H	-1.59829000	-2.78804000	-2.87270700
C	1.60517100	-0.16342300	-3.40534500	H	-3.28100100	-2.68742900	-3.42930800
H	0.72265900	-0.78658900	-3.58335300	C	-3.21513600	-2.68481200	-0.64652400
H	1.28377700	0.88297900	-3.37737400	H	-2.36185100	-3.36026900	-0.52223300
H	2.29026800	-0.28864700	-4.25143200	H	-3.47562100	-2.27900600	0.33622000
C	2.69028800	-2.02440600	-2.11163200	H	-4.06500000	-3.27116100	-1.01396700
H	3.14687200	-2.30978500	-1.15756300	C	2.78886900	-0.80323800	-2.61747800
H	1.81642200	-2.66337500	-2.27830800	C	2.59718700	-2.30375100	-2.88608500
H	3.41523400	-2.22075500	-2.90959600	H	2.73596900	-2.87414400	-1.96129000
C	3.49201900	0.34055200	-1.82302500	H	1.58351500	-2.49411400	-3.25407400
H	4.24016300	0.23718900	-2.61710400	H	3.30936000	-2.68177900	-3.62862300
H	3.18979100	1.39156400	-1.77019300	C	4.21029400	-0.54792300	-2.09334200
H	3.96394700	0.07330500	-0.87145000	H	4.34627800	0.51716000	-1.87691200
C	-2.13294300	2.62682000	4.40186900	H	4.38147100	-1.10783200	-1.16806400
C	-3.58667600	2.15548700	4.27547500	H	4.97314200	-0.85080300	-2.81977000
C	-2.04903400	3.88747900	5.26555000	C	2.57828800	-0.01928700	-3.92191000
H	-1.56999800	1.82254900	4.90182400	H	3.28500800	-0.32459900	-4.70208700
H	-3.64567600	1.22917300	3.69561500	H	1.56256700	-0.18129800	-4.29851300
H	-4.02986300	1.97363300	5.26125800	H	2.71431400	1.05309500	-3.74271200
H	-4.18356400	2.91489800	3.76002800	C	-0.67773500	-1.74363800	4.27496300
H	-1.01426600	4.22962700	5.37069200	C	-1.98550600	-2.45735400	3.90979600
H	-2.61709100	4.69835900	4.79803000	C	-0.50365400	-1.69612900	5.79493200
H	-2.45614900	3.70867000	6.26687400	H	0.14523100	-2.33270300	3.84158200
C	-0.92384200	3.43584600	0.41134900	H	-2.10213400	-2.52306800	2.82369600
C	-0.87916100	3.16490900	-1.09094400	H	-2.00741100	-3.47409800	4.31916100
C	-0.05766000	4.64135100	0.78497600	H	-2.84296700	-1.90512000	4.30891000
H	-1.95916800	3.66536000	0.70504500	H	0.43396600	-1.20471000	6.07238500
H	-1.55551500	2.34600700	-1.37062500	H	-1.32249900	-1.12566800	6.24617000
H	-1.18941800	4.04559200	-1.66245300	H	-0.50525200	-2.70359600	6.22604900
H	0.13801800	2.90461900	-1.41034400	C	-1.05891700	2.18371400	2.51711200
H	-0.11509400	4.82058500	1.86163000	C	-0.61216700	2.72371000	3.88042600
H	0.98810000	4.46352100	0.50858200	C	-2.54433500	1.79998800	2.52067300
H	-0.39980500	5.54619000	0.26985400	H	-0.95740600	3.02897400	1.80945100
				H	0.43421900	3.04487600	3.84117000
				H	-1.22433300	3.58299900	4.17699700
				H	-0.70994700	1.94379900	4.63885000

Int-3A (^tBuOH)

H= -1348.386727 au

N	-0.17529800	1.13391100	2.00376800
C	-0.08308200	-0.01061800	2.70730800
N	-0.71285600	-0.39365800	3.75237900
O	0.82314400	-0.91206700	1.98929700
C	2.26538900	-0.87033700	2.31433500
C	2.80159500	-2.18468200	1.75784300
H	3.87698100	-2.26493700	1.94504500
H	2.30145100	-3.03403400	2.23186500
H	2.64438000	-2.24158500	0.67577600
C	2.92221300	0.32884400	1.62531900
H	2.44801900	1.25951500	1.94719000
H	3.98494700	0.36976100	1.88511200
H	2.87184700	0.24402200	0.53190700
C	2.48893300	-0.78479300	3.82096000
H	2.08771000	-1.65835800	4.33809400
H	3.56504200	-0.74103900	4.01600900
H	2.02969500	0.11231700	4.24336200
U	0.10853400	0.06006500	-0.32984200
O	-1.76415400	-0.83189600	-1.07787000
O	1.85244000	-0.37850600	-1.66604300
C	-2.84903600	-1.54425000	-1.60686100
C	-4.04372100	-0.59209700	-1.76083200
H	-3.78596000	0.23012800	-2.43740300
H	-4.92383800	-1.10469100	-2.16555000

TS_{3A-4A} (^tBuOH)

H= -1348.387023 au

N	-0.84821900	1.16312200	1.68147100
C	-0.28956600	0.22355500	2.48238700
N	-0.68945600	-0.16959800	3.62599200
O	-0.13653900	2.58370000	-0.75393700

O	0.78349600	-0.43266000	1.75233600	H	-0.27285100	1.98462200	0.67961300
C	2.21136400	-0.17103100	2.05784500	C	0.15110400	3.60632200	-0.80903600
C	2.88114300	-1.53716100	2.17442800	C	1.13977600	4.32874100	0.10993800
H	3.95932200	-1.41293600	2.31607500	H	1.24467600	5.37962600	-0.17893800
H	2.49019100	-2.10900900	3.01947300	H	0.79480000	4.29721400	1.14850500
H	2.72693900	-2.11860700	1.26028000	H	2.12850500	3.86258000	0.05944200
C	2.79297700	0.59317100	0.86882400	C	-1.21605500	4.29415400	-0.77056300
H	2.27829800	1.54775700	0.73124400	H	-1.15162700	5.31435900	-1.16319900
H	3.85450800	0.80089200	1.03698900	H	-1.94015100	3.73939600	-1.37550200
H	2.72174100	0.00982700	-0.05758800	H	-1.59636900	4.35195300	0.25399600
C	2.36646400	0.65274400	3.33038600	C	0.68399700	3.56128300	-2.24107700
H	1.99611700	0.12852500	4.21190900	H	1.63718500	3.02461800	-2.27795300
H	3.43005600	0.86251600	3.48018000	H	-0.02642300	3.05117600	-2.90096500
H	1.84167600	1.60871900	3.24834800	H	0.84183700	4.57054500	-2.63423700
U	-0.20110100	-0.18096400	-0.67465000	O	0.01592100	2.24819000	-0.37732300
O	-2.11447800	-0.99008400	-1.38847000				
O	1.41197700	-0.93254600	-1.99799800				
C	-3.26620800	-1.58717800	-1.92293000				
C	-4.37445800	-0.53047800	-2.03187000				
H	-4.04949300	0.29029300	-2.68016500				
H	-5.29670100	-0.95145500	-2.44806200				
H	-4.60118400	-0.11571800	-1.04451900				
C	-2.94384800	-2.14927900	-3.31446400				
H	-2.60272000	-1.34593600	-3.97614700				
H	-2.14501000	-2.89508000	-3.24520500				
H	-3.81809100	-2.62433200	-3.77384900				
C	-3.71653200	-2.72253100	-0.99257900				
H	-2.92472800	-3.47436700	-0.90448100				
H	-3.92827600	-2.32959100	0.00717700				
H	-4.61949700	-3.21921200	-1.36511800				
C	2.19607500	-1.54577800	-2.98696500				
C	1.98996500	-3.06612400	-2.92195700				
H	2.27647600	-3.44376500	-1.93428100				
H	0.93581200	-3.31121100	-3.08899000				
H	2.58768000	-3.59231000	-3.67492500				
C	3.67444900	-1.21065600	-2.74254000				
H	3.82259800	-0.12579300	-2.76024900				
H	3.99175000	-1.58292900	-1.76255500				
H	4.32379700	-1.65873200	-3.50312700				
C	1.76765600	-1.02182000	-4.36543800				
H	2.35772100	-1.46974600	-5.17307800				
H	0.71222600	-1.25165300	-4.54530100				
H	1.89486800	0.06499400	-4.41142800				
C	-0.23711400	-1.37450800	4.28738600				
C	-1.23612000	-2.50777400	4.02375000				
C	-0.11462100	-1.10538100	5.78866800				
H	0.74139300	-1.70958200	3.91338700				
H	-1.31091400	-2.72227200	2.95288000				
H	-0.93039100	-3.42700200	4.53600100				
H	-2.23208100	-2.22801300	4.38238600				
H	0.59996600	-0.30133300	5.99177900				
H	-1.08334900	-0.79445800	6.19331300				
H	0.21489000	-2.00220700	6.32440400				
C	-2.11608300	1.78686900	2.10146000				
C	-1.95088600	2.68241100	3.33412000				
C	-3.27112200	0.79597500	2.27099500				
H	-2.38187300	2.43792500	1.25678600				
H	-1.16381500	3.42741300	3.17244100				
H	-2.88327800	3.21700000	3.54768600				
H	-1.68394800	2.07950000	4.20484100				
H	-3.38939700	0.18272100	1.37123700				
H	-3.09604300	0.13972000	3.12509500				
H	-4.20830400	1.33983800	2.43327000				

H	2.17403800	0.02680400	-4.24295900	H	-1.33206000	-1.10255600	5.40127800
C	-0.08094800	-1.64223900	4.29929200	H	-1.65904000	0.62661000	5.23784600
C	-1.10319600	-2.74037500	3.98788700	H	0.04607900	-2.30494700	3.62901600
C	0.10481300	-1.48938500	5.80956300	H	-1.14624900	-1.79369700	2.42523400
H	0.87673700	-1.93978200	3.85103200	H	0.58708000	-1.43723400	2.18655500
H	-1.22549800	-2.87136600	2.90824500	U	-0.93452300	0.50020000	0.26938000
H	-0.78250400	-3.69707500	4.41366500	O	-1.18932200	0.61566100	-1.87646900
H	-2.07959900	-2.48352600	4.41103000	O	-2.52395600	-0.92275800	0.57304000
H	0.83830000	-0.71320700	6.04908700	O	1.14267000	-0.07838900	0.17231300
H	-0.84298000	-1.20625300	6.27842000	O	-3.22750400	3.66433200	3.49827600
H	0.44561500	-2.42980100	6.25472300	O	0.31034500	4.65004500	2.87644700
C	-1.96689200	1.81125600	2.46363600	O	-0.74427300	3.00553700	5.39980000
C	-1.78597800	2.55751000	3.78716600	C	-3.57557800	-1.85567900	0.45920600
C	-3.14517800	0.84025000	2.49626900	C	-3.00662600	-3.19584100	-0.02222400
H	-2.16304700	2.54719900	1.67535200	C	-4.23462000	-2.02516000	1.83353700
H	-0.97366000	3.28888600	3.71861900	C	-4.60288300	-1.32309100	-0.54655000
H	-2.70334000	3.09847100	4.04096800	H	-2.52231100	-3.07499100	-0.99630100
H	-1.56078200	1.85540800	4.59305800	H	-2.26069900	-3.56994400	0.68664300
H	-3.25739700	0.33373300	1.53283300	H	-3.79281900	-3.95228400	-0.12119900
H	-3.01075500	0.08959000	3.27724800	H	-4.60242300	-1.06023000	2.19657000
H	-4.06789100	1.39306600	2.69901700	H	-5.07986600	-2.72047300	1.78628800
H	-0.13618300	1.76616200	1.43232400	H	-3.51531100	-2.41421200	2.56094300
C	0.22012400	3.40064500	-1.24063800	H	-5.43809600	-2.02052900	-0.67370500
C	1.50234200	4.16397400	-0.87767500	H	-5.00544900	-0.36416500	-0.20429500
H	1.54918200	5.14147000	-1.37092700	H	-4.13258400	-1.16716300	-1.52197100
H	1.55032400	4.32690300	0.20480000	C	2.46804300	-0.36679300	-0.21423400
H	2.38332300	3.58624900	-1.17629200	C	3.04369300	0.84878800	-0.95144500
C	-1.00795800	4.22119900	-0.81879900	C	3.30491200	-0.65139800	1.03859400
H	-1.04949100	5.18939100	-1.33074800	C	2.46438100	-1.59532900	-1.13095100
H	-1.92571000	3.67026600	-1.05048100	H	2.44722400	1.07630300	-1.83989300
H	-0.98498700	4.41077900	0.26026100	H	3.03020100	1.72637400	-0.29661800
C	0.17804500	3.15324600	-2.75601800	H	4.07798100	0.67378600	-1.26764000
H	1.03980400	2.54948300	-3.06158400	H	2.90663700	-1.51395000	1.58189300
H	-0.73626400	2.61101200	-3.02452000	H	4.34723300	-0.86572600	0.77827900
H	0.19597400	4.08755500	-3.32851000	H	3.29101200	0.21465800	1.70770000
O	0.20922400	2.16784600	-0.56799400	H	3.47703200	-1.85598200	-1.45764200
				H	2.04060000	-2.45789400	-0.60620800
				H	1.85546000	-1.40231500	-2.01946900
				C	-1.25205100	0.38278800	-3.26788800
O	-0.71582700	0.87222100	2.72844300	C	-2.48467100	1.08713700	-3.84774200
O	-1.42978000	2.73266900	0.81798000	C	0.01844100	0.92867200	-3.93077600
U	-1.15691800	3.12210100	3.27935500	C	-1.35493200	-1.12809500	-3.51032000
C	-1.90168400	3.73442300	-0.12065900	H	-3.39544500	0.72787200	-3.35821200
C	-3.20348600	3.22976600	-0.74748200	H	-2.41777300	2.16902100	-3.69764000
C	-2.16686300	5.04728900	0.61795700	H	-2.57696900	0.89851700	-4.92290900
C	-0.82236600	3.95798700	-1.18207800	H	0.90342300	0.43212900	-3.52197100
H	-3.03462100	2.30559200	-1.30886900	H	0.00360900	0.76376500	-5.01373100
H	-3.94857000	3.04211700	0.03161200	H	0.11529400	2.00421600	-3.75256700
H	-3.61618700	3.96738000	-1.44433600	H	-1.38984600	-1.36040900	-4.58040800
H	-1.25347400	5.41211700	1.09814100	H	-0.49124400	-1.64183700	-3.07588300
H	-2.51015400	5.81513600	-0.08307700	H	-2.26065300	-1.52699100	-3.04365000
H	-2.94187100	4.91521600	1.37922300	C	-4.51933600	4.06114900	3.90314100
H	-1.13306200	4.72696500	-1.89773700	C	-4.53898900	5.58305100	4.08971100
H	0.10752100	4.28734200	-0.70907600	C	-5.52257700	3.64685500	2.82011600
H	-0.63156200	3.03690200	-1.74048100	C	-4.86159800	3.36429500	5.22430400
C	-0.38488300	-0.18062200	3.67108900	H	-3.80522000	5.88103100	4.84558500
C	0.92964200	0.18333300	4.36291100	H	-4.28695800	6.08763300	3.15153100
C	-1.53094700	-0.30447700	4.67761800	H	-5.52537400	5.93417800	4.41186100
C	-0.21682800	-1.50701200	2.92676600	H	-5.47790700	2.56517000	2.65800100
H	1.73036500	0.27371300	3.62320000	H	-6.54708900	3.91038600	3.10472700
H	0.83260600	1.12948300	4.90262600	H	-5.29419400	4.14574800	1.87314600
H	1.21832300	-0.58781500	5.08550400	H	-5.86666600	3.63144300	5.56856700
H	-2.46459100	-0.54090700	4.15808600	H	-4.81673600	2.27726800	5.10263000

H	-4.14503500	3.65195200	5.99924100	H	2.88308800	2.27297900	4.65997800
C	1.29996200	5.65461100	2.88412700	H	3.59209100	2.00212900	3.05528600
C	2.38789800	5.27188600	3.89345100	H	2.56384300	3.41952500	3.34292800
C	1.90843400	5.76298900	1.48074500	O	2.55253600	0.90066600	-1.39725000
C	0.65609900	6.98803100	3.28344100	O	1.29537100	1.70945700	1.76389700
H	1.95765600	5.18333700	4.89522200	O	-0.89424400	1.20427900	-0.91160900
H	2.83211700	4.30790000	3.62481100	C	-2.13679200	0.65853800	-1.29082800
H	3.18605300	6.02150200	3.92620900	C	3.54616900	0.17615900	-2.08518800
H	1.14560900	6.05153500	0.75094700	C	1.47107800	1.55469900	3.15339700
H	2.70714200	6.51226000	1.45099500	O	1.13770500	4.05553000	-0.82732000
H	2.32924100	4.79964500	1.17565800	C	1.21211800	5.42526900	-1.14865800
H	1.39379100	7.79768500	3.30446800	C	0.40567500	6.21471400	-0.11127700
H	-0.13035800	7.26144000	2.57259400	C	2.68336800	5.85438700	-1.11872900
H	0.20556400	6.90921600	4.27802300	C	0.62485900	5.63162100	-2.54958000
C	-0.56197300	3.28244200	6.77336100	H	-0.64018500	5.89084300	-0.11842800
C	-1.49346600	2.38934000	7.60190200	H	0.81078200	6.04411000	0.89137600
C	0.89550600	3.00554000	7.16279800	H	0.43367200	7.29057600	-0.31542500
C	-0.89634600	4.75858300	7.02052300	H	3.26224500	5.26944900	-1.84071100
H	-2.53605700	2.54857400	7.31191000	H	2.79705300	6.91557400	-1.36556600
H	-1.25208100	1.33337700	7.44674700	H	3.10622900	5.68588900	-0.12297800
H	-1.39739800	2.60484900	8.67175400	H	0.65694800	6.68538900	-2.84698100
H	1.57669900	3.60210100	6.54927700	H	1.18867500	5.04979800	-3.28603700
H	1.07509400	3.25147700	8.21508800	H	-0.41787800	5.29905400	-2.57491400
H	1.14026700	1.94912600	7.01701600	U	1.02372100	1.97060300	-0.34562500
H	-0.77499200	5.02749900	8.07562200				
H	-0.23878000	5.40008100	6.42518300				
H	-1.93131500	4.96543000	6.72986500				

Cat_B (^tBuOH)

H= -969.20983 au

C	3.60420500	0.68016300	-3.53170100
H	3.84232000	1.74852700	-3.55049600
H	4.36556800	0.14761100	-4.11193600
H	2.63594900	0.53629200	-4.02221500
C	3.17652800	-1.31121600	-2.05318400
H	2.20383200	-1.46980400	-2.52993600
H	3.92012500	-1.92099900	-2.57771700
H	3.11225100	-1.66299700	-1.01829500
C	4.89085900	0.40600100	-1.38628100
H	5.14153200	1.47170000	-1.38906100
H	4.83887100	0.06864800	-0.34615200
H	5.70004400	-0.13866300	-1.88473800
C	-2.19891800	0.60300400	-2.82149900
H	-1.38353100	-0.01557400	-3.21034900
H	-3.14746700	0.17983200	-3.16942900
H	-2.09671600	1.60884800	-3.24155600
C	-3.25210700	1.55653500	-0.74397300
H	-4.24276100	1.17200000	-1.00974600
H	-3.18827300	1.61676200	0.34727500
H	-3.15614900	2.56886200	-1.14944500
C	-2.25107100	-0.75209300	-0.70166400
H	-2.18110300	-0.71261600	0.39014900
H	-3.20361600	-1.22248200	-0.96848200
H	-1.43914500	-1.38475400	-1.07494200
C	1.67591900	0.06620100	3.45711600
H	0.80534500	-0.51019000	3.12775700
H	2.55704000	-0.31015500	2.92750000
H	1.81835600	-0.10853400	4.52910000
C	0.21793300	2.07656100	3.86553600
H	0.05943700	3.13335400	3.62703100
H	-0.66374200	1.51537800	3.53957700
H	0.30460600	1.97954700	4.95317700
C	2.70231900	2.36042600	3.58315800

Int-1B (^tBuOH)

H= -1353.533451 au

N	-0.59046600	2.40825700	0.32120900
C	-1.07129400	2.59967500	1.45153600
N	-1.40416000	2.77804200	2.60188100
O	0.95680600	0.07791200	1.87901200
C	1.61709600	0.15238100	3.11831600
C	0.63271200	-0.24963000	4.22395200
H	1.09793400	-0.20634100	5.21510900
H	-0.22843400	0.42584500	4.21763100
H	0.27117200	-1.26934500	4.05626900
C	2.81491900	-0.80551600	3.10594600
H	3.51127200	-0.52938900	2.30708300
H	3.35827700	-0.78243100	4.05718800
H	2.47840100	-1.83129600	2.92678400
C	2.10192800	1.59050100	3.34251400
H	1.25234500	2.27951500	3.35426400
H	2.63809700	1.68670700	4.29351700
H	2.78009400	1.88904100	2.53619400
U	0.21769600	-0.24620700	-0.12812200
O	-1.93870300	-0.50582300	-0.36952700
O	1.33341600	0.53257800	-1.83944700
C	-2.67949100	2.59757000	3.29388000
C	-3.79555000	2.12839100	2.36718100
C	-3.02222800	3.89318900	4.02605600
H	-2.48789900	1.82030400	4.04489300
H	-3.51093800	1.21153300	1.84348500
H	-4.70619400	1.93137300	2.94116300
H	-4.02579400	2.89529500	1.61932300
H	-2.19954100	4.20251900	4.67580200
H	-3.21927800	4.69955800	3.31215700
H	-3.91697000	3.75185100	4.63950000
C	-0.56924000	3.53444400	-0.65820600
C	-1.12207900	3.05222400	-1.99274000
C	0.86038900	4.05315200	-0.77061000
H	-1.21242700	4.33746400	-0.27346500
H	-2.14187400	2.67417800	-1.88235900
H	-1.13463400	3.87843400	-2.71092900

H	-0.48934800	2.25522900	-2.39538100	H	1.31163700	3.18816800	2.92953800
H	1.22326600	4.42190700	0.19317500	U	-0.21268300	0.10298300	0.17309400
H	1.51977300	3.24998900	-1.11050100	O	-2.14017300	-0.28358200	-0.68508700
H	0.90814700	4.87363600	-1.49412800	O	1.26228600	0.45805800	-1.34396900
O	0.78159500	-2.30627400	-0.31978500	C	-2.39068400	2.73084400	3.93987400
C	1.16640000	-3.65684500	-0.21927700	C	-3.78037600	2.15673300	3.65047000
C	0.56441300	-4.43285900	-1.39687300	C	-2.46050500	3.89319400	4.92816100
C	2.69726500	-3.73895200	-0.26131400	H	-1.77198100	1.92859800	4.36686300
C	0.64449500	-4.22840400	1.10486200	H	-3.71496000	1.30503300	2.96727700
H	-0.52826400	-4.37409500	-1.37082700	H	-4.25564000	1.81780700	4.57718200
H	0.90712500	-4.01053800	-2.34659800	H	-4.42106300	2.91721000	3.19248600
H	0.85117700	-5.48989000	-1.36684900	H	-1.46459400	4.29538200	5.13531600
H	3.12906900	-3.16144900	0.56201700	H	-3.07201000	4.70425800	4.51954800
H	3.04544300	-4.77429700	-0.17617700	H	-2.90576200	3.56780200	5.87356100
H	3.07403600	-3.32732200	-1.20306800	C	-1.54782300	3.55861700	-0.28144600
H	0.91265400	-5.28463200	1.21805400	C	-1.44098900	3.13249600	-1.74013100
H	1.06491800	-3.67495300	1.95018900	C	-0.94431900	4.94425100	-0.05409900
H	-0.44604100	-4.14398500	1.15023900	H	-2.60964700	3.59053500	0.00519400
C	2.31660100	0.39851000	-2.84394100	H	-1.90181800	2.15259600	-1.89723300
C	2.00299700	-0.84289600	-3.68849800	H	-1.94607900	3.85527800	-2.38885200
C	2.29859000	1.64645600	-3.73488700	H	-0.39089000	3.07414200	-2.04577000
C	3.69114200	0.25195900	-2.17818100	H	-1.03012500	5.23850200	0.99559400
H	1.97382200	-1.73210100	-3.05151500	H	0.11499300	4.94776100	-0.33244100
H	1.02467300	-0.73522200	-4.16863400	H	-1.46251000	5.69364400	-0.66233600
H	2.75378800	-0.99980700	-4.47100100	O	0.30339200	-1.89460500	0.80355500
H	2.52682400	2.54290900	-3.15016900	C	0.53426600	-3.25798700	1.07225600
H	3.03768700	1.56811300	-4.53985000	C	0.36842000	-4.04757700	-0.23211600
H	1.31125400	1.77506000	-4.18970600	C	1.96104500	-3.42718700	1.60824900
H	4.49338500	0.16021000	-2.91884900	C	-0.48182400	-3.74063500	2.11418900
H	3.90184700	1.12478800	-1.55117800	H	-0.64144200	-3.90947600	-0.63131600
H	3.71089900	-0.63983400	-1.54266900	H	1.08339100	-3.69323000	-0.98155400
C	-3.04504800	-1.13675300	-0.97087900	H	0.53356300	-5.11962900	-0.07811000
C	-2.64393700	-1.65479800	-2.35919000	H	2.08657800	-2.87184500	2.54345200
C	-3.49381000	-2.30447600	-0.08289200	H	2.19154000	-4.47995700	1.80490400
C	-4.18424800	-0.11919100	-1.11098200	H	2.68562500	-3.04635700	0.88151700
H	-2.31890600	-0.82270200	-2.99373000	H	-0.34637800	-4.80350700	2.34282000
H	-1.81531000	-2.36519100	-2.27297400	H	-0.37290000	-3.17371400	3.04422800
H	-3.47577500	-2.16049900	-2.86216700	H	-1.50140800	-3.59491800	1.74442300
H	-3.75136100	-1.93924800	0.91656100	C	2.24496200	0.51780600	-2.35175100
H	-4.36825700	-2.81695300	-0.49948100	C	1.55834500	0.38338000	-3.71591400
H	-2.68372500	-3.03342900	0.01933000	C	2.96763700	1.86630100	-2.25146600
H	-5.06278200	-0.56514800	-1.59055500	C	3.23943000	-0.63013700	-2.14374200
H	-4.48569800	0.25617000	-0.12846300	H	1.02599100	-0.57114000	-3.77905100
H	-3.85794200	0.73201200	-1.71698100	H	0.83113300	1.18939400	-3.85537000
TS_{1B-2B} (^tBuOH)							
H= -1353.51314 au							
N	-0.85908300	2.55393100	0.56279300	H	3.44311000	1.96979800	-1.27076200
C	-1.16335600	2.59371900	1.81816200	H	3.74185500	1.96344700	-3.02041500
N	-1.76474100	3.17539400	2.71600700	H	2.25621300	2.68891300	-2.37354300
O	-0.21694900	1.01273300	2.35396700	H	4.02551200	-0.62082300	-2.90668700
C	0.93480800	1.06334300	3.21510900	H	3.71361700	-0.54703400	-1.16048900
C	0.69481000	0.08550200	4.36753700	H	2.72245100	-1.59356700	-2.19397000
H	1.55226200	0.05534600	5.04880600	C	-3.33052500	-0.83618600	-1.20224800
H	-0.18782900	0.38009900	4.94360600	C	-3.05768700	-1.36309400	-2.61571700
H	0.52520600	-0.92170200	3.97629700	C	-3.78313100	-1.97994200	-0.28728600
C	2.16741400	0.62912400	2.40663000	C	-4.40396800	0.25773000	-1.24114800
H	2.34330600	1.31657900	1.56858200	H	-2.70561900	-0.55204300	-3.26094500
H	3.07329100	0.63814600	3.02145600	H	-2.28482700	-2.13821500	-2.58897300
H	2.05119200	-0.39442600	2.02833900	H	-3.95983200	-1.79329000	-3.06428100
C	1.17616600	2.47715500	3.74987100	H	-3.95625200	-1.60679700	0.72748500
H	0.34529500	2.82215300	4.36783600	H	-4.71036100	-2.43840600	-0.64792700
H	2.08254900	2.48920300	4.36435300	H	-3.01206400	-2.75499100	-0.24037300
				H	-5.35620000	-0.13435300	-1.61476800
				H	-4.56850300	0.66258400	-0.23773000

H -4.09308000 1.07857900 -1.89458100

Int-2B (^tBuOH)

H= -1353.525228 au

N -0.42079800 2.03572900 0.27174900
C -0.71924100 1.85838000 1.57900000
N -1.56632000 2.48499200 2.29310500
O 0.01682300 0.69734900 2.03153600
C 1.32241000 0.90200600 2.70421100
C 1.35466700 -0.13493000 3.81981200
H 2.32157600 -0.11382400 4.33270200
H 0.56972000 0.06147900 4.55498800
H 1.20119000 -1.13513700 3.40777200
C 2.42518200 0.63073300 1.67906800
H 2.37508000 1.35207300 0.85426100
H 3.41371000 0.73804100 2.13597000
H 2.36537900 -0.39977400 1.30525300
C 1.46512100 2.31747900 3.25096000
H 0.70020500 2.54555700 3.99436000
H 2.44370000 2.40430100 3.73377200
H 1.41336000 3.06272200 2.45298300
U 0.12432800 -0.21137200 -0.48243700
O -1.68709700 -0.72152500 -1.47286600
O 1.59035200 0.07050700 -2.00612900
C -1.94829400 2.07890300 3.62988600
C -3.27736500 1.31740900 3.56378900
C -2.08277900 3.32166800 4.51243700
H -1.20654100 1.40273000 4.08432200
H -3.17013000 0.40001300 2.97649800
H -3.62481300 1.04378800 4.56652200
H -4.04321200 1.93795200 3.08710300
H -1.13798000 3.87165300 4.57159600
H -2.83186200 3.99976500 4.09054700
H -2.38886600 3.05341800 5.52953300
C -1.07578400 3.15950500 -0.40084800
C -0.99605700 2.96240600 -1.91240800
C -0.44533000 4.49028500 0.01717600
H -2.13302200 3.18153700 -0.09609500
H -1.49849700 2.03854400 -2.22129100
H -1.48034300 3.79109200 -2.43890300
H 0.04794400 2.92010200 -2.24561100
H -0.52893800 4.62175400 1.09888000
H 0.61319300 4.51868000 -0.26642400
H -0.95252300 5.33164000 -0.46850400
O 0.67328500 -2.09119000 0.43538800
C 0.83318700 -3.42392100 0.86660500
C 0.63910700 -4.35542800 -0.33665300
C 2.24758900 -3.59864600 1.43314400
C -0.21441500 -3.73283500 1.94283600
H -0.36169700 -4.22265000 -0.75994400
H 1.37442500 -4.12647700 -1.11469500
H 0.75414100 -5.40754800 -0.05358500
H 2.40288500 -2.94198600 2.29512800
H 2.42279800 -4.63032200 1.75705400
H 2.99254500 -3.34696300 0.67145900
H -0.12523000 -4.76300200 2.30471600
H -0.09848800 -3.05889300 2.79718300
H -1.22304300 -3.59735500 1.53942500
C 2.52816600 0.04101200 -3.06096700
C 1.77497500 0.17957800 -4.38824100
C 3.50024500 1.21118200 -2.87587600
C 3.28327300 -1.29158400 -3.01309800
H 1.06843300 -0.64732700 -4.51175100

H 1.21135000 1.11740800 -4.40808000
H 2.46405500 0.17292300 -5.23967100
H 4.02832900 1.11944200 -1.92127300
H 4.24509100 1.24003700 -3.67837800
H 2.95541000 2.16031700 -2.87664100
H 4.03328800 -1.35410100 -3.80897400
H 3.79257600 -1.40502300 -2.05073300
H 2.58640100 -2.12746100 -3.13206800
C -2.84072100 -1.28595000 -2.06291000
C -2.41277800 -2.11372700 -3.27877600
C -3.53274500 -2.17578300 -1.02493000
C -3.77369400 -0.14931500 -2.49241700
H -1.90070700 -1.47788000 -4.00777900
H -1.72514300 -2.90919400 -2.97396100
H -3.27618200 -2.57470000 -3.77057000
H -3.81742800 -1.58506500 -0.14816300
H -4.43705000 -2.63803500 -1.43498700
H -2.85782500 -2.97331400 -0.69808200
H -4.69391200 -0.54052800 -2.93946900
H -4.04414000 0.46627200 -1.62906500
H -3.28023300 0.49051800 -3.23051100

Int-3B (^tBuOH)

H= -1586.995027 au

N -0.55496900 0.73322500 1.82208900
C 0.23768200 -0.08405000 2.56641400
N 0.00711200 -0.54958400 3.72888100
O 1.36507600 -0.43757300 1.72990300
C 2.71815000 0.09447200 2.01070900
C 3.57997700 -1.01021700 2.62084500
H 4.63139900 -0.70500100 2.60393800
H 3.31403800 -1.22024100 3.65749900
H 3.48294700 -1.93087500 2.03842200
C 3.28950700 0.47803400 0.64889100
H 2.70931300 1.28470500 0.19294900
H 4.32062400 0.82797200 0.76101700
H 3.29868000 -0.37996800 -0.02908600
C 2.65246500 1.31946000 2.91705800
H 2.18673500 1.08791500 3.87685500
H 3.66856900 1.68023700 3.10456800
H 2.08725400 2.12595700 2.44397400
H -0.12844100 -0.09061300 -0.53307600
O -1.91900000 0.56104600 -1.50727800
O 1.34584900 -0.15907900 -2.10992900
C 0.70934800 -1.64845300 4.35606700
C -0.30056500 -2.76957400 4.63084100
C 1.34586100 -1.19283200 5.67265000
H 1.48833900 -2.06126500 3.70092900
H -0.76188200 -3.11363200 3.70077300
H 0.18622200 -3.62644100 5.11044600
H -1.09726600 -2.40931800 5.29018400
H 2.11391900 -0.42898700 5.51517000
H 0.57901700 -0.76127900 6.32449500
H 1.81003800 -2.03555600 6.19682300
C -1.87262600 1.12955600 2.35194100
C -1.75974000 2.01727700 3.59593800
C -2.82913900 -0.04487200 2.58514100
H -2.31201500 1.74286700 1.55175900
H -1.11390300 2.88146900 3.40202000
H -2.74629700 2.39197900 3.89072600
H -1.33439200 1.44957900 4.42629900
H -2.91915400 -0.65963000 1.68285100
H -2.47199900 -0.67694400 3.40010300

H	-3.82815800	0.32674700	2.83939600	C	2.44808000	0.17756800	1.91735000
H	0.13307200	2.18233200	0.93677200	C	3.28225100	-0.95835300	2.50598800
C	0.33116300	3.79681400	-0.33195500	H	4.34085900	-0.67962200	2.48421200
C	1.25653000	4.61906400	0.56547500	H	3.02024600	-1.17485400	3.54224000
H	1.20118600	5.68194400	0.30923700	H	3.15830600	-1.86828800	1.91194200
H	0.97404700	4.51446300	1.61866700	C	3.01710800	0.56493800	0.55556000
H	2.29374900	4.29086800	0.45111900	H	2.44034200	1.38118300	0.11340000
C	-1.12670500	4.21752800	-0.15159400	H	4.05326000	0.89921900	0.66774600
H	-1.27205300	5.25465600	-0.47037800	H	3.01565700	-0.28831400	-0.12955600
H	-1.78090500	3.57406300	-0.74596500	C	2.40943500	1.39006300	2.83988100
H	-1.43059700	4.14423100	0.89829600	H	1.94848200	1.15233500	3.80089100
C	0.75421300	3.90144800	-1.79242300	H	3.43249700	1.73135700	3.02578500
H	1.78072100	3.54704000	-1.92026400	H	1.85428700	2.20978000	2.37859400
H	0.09834800	3.29978200	-2.42820500	U	-0.38015300	-0.04665100	-0.67772100
H	0.70229600	4.94076000	-2.13030300	O	-2.16376700	0.55860000	-1.68062600
O	0.47185000	2.40238500	0.02410100	O	1.06777700	-0.17960700	-2.25641300
O	-0.57548900	-2.16552200	-0.33313600	C	0.42034500	-1.60689000	4.23587200
C	-0.80806800	-3.55529900	-0.29951400	C	-0.60680600	-2.71137600	4.51076500
C	0.35267000	-4.22553300	0.44403400	C	1.08038300	-1.17692900	5.54934900
C	-2.13034100	-3.81475500	0.43045400	H	1.18359200	-2.02241000	3.56435600
C	-0.88695400	-4.07782600	-1.73837000	H	-1.09054200	-3.03368300	3.58455100
H	1.29669900	-4.02647900	-0.07347600	H	-0.12741000	-3.58370200	4.96884400
H	0.42966900	-3.82828100	1.46031100	H	-1.38436400	-2.34626900	5.18984600
H	0.21497700	-5.31071100	0.50431500	H	1.85585100	-0.42057600	5.39298300
H	-2.95554300	-3.32261400	-0.09406900	H	0.32817600	-0.74644600	6.21852000
H	-2.35059200	-4.88632800	0.48793900	H	1.54065400	-2.03373300	6.05333900
H	-2.08681400	-3.41533800	1.44811100	C	-2.16847900	1.22398600	2.32102600
H	-1.06866700	-5.15798100	-1.76042700	C	-2.07524100	2.06309300	3.59899700
H	-1.69873400	-3.58093100	-2.27832500	C	-3.10680900	0.02729200	2.49223000
H	0.05026300	-3.87669600	-2.26704500	H	-2.60180900	1.86288700	1.53886500
C	2.18680400	-0.37264100	-3.21884500	H	-1.43889900	2.94106200	3.44311900
C	3.14138300	0.81866800	-3.36427700	H	-3.06940800	2.41438900	3.89641300
C	2.98573300	-1.66366500	-2.99938400	H	-1.65290200	1.46928500	4.41225900
C	1.31871900	-0.50342900	-4.47662700	H	-3.16598300	-0.55771500	1.56803900
H	2.57335700	1.74043600	-3.52281200	H	-2.76000900	-0.62636100	3.29453800
H	3.74343700	0.93747400	-2.45805600	H	-4.11692600	0.37482100	2.73470400
H	3.82141300	0.68499400	-4.21289000	H	-0.27835300	1.85146500	1.03906400
H	2.30526200	-2.50934300	-2.86008200	C	0.05307400	3.65133500	-0.30351900
H	3.63658800	-1.88189600	-3.85324800	C	1.02851700	4.45345000	0.56245600
H	3.61387100	-1.58025100	-2.10650900	H	1.00001900	5.51774300	0.30552400
H	1.92982400	-0.66203900	-5.37219400	H	0.77324100	4.35700800	1.62312600
H	0.63038400	-1.34864000	-4.37550000	H	2.05221400	4.09432200	0.41941300
H	0.72657100	0.40580000	-4.62144700	C	-1.38069800	4.14076100	-0.08153300
C	-3.09288800	0.66916200	-2.28296200	H	-1.49123600	5.18483700	-0.39335900
C	-3.46742300	-0.71620700	-2.82106100	H	-2.08212400	3.53153300	-0.65915700
C	-4.21926100	1.21079200	-1.39587200	H	-1.65562800	4.07639900	0.97645400
C	-2.82508900	1.62961600	-3.44769400	C	0.43124800	3.76830300	-1.77983900
H	-2.66253000	-1.11042800	-3.44965600	H	1.44146300	3.38251700	-1.94562500
H	-3.62780400	-1.41218500	-1.99204900	H	-0.26351700	3.19022800	-2.39736200
H	-4.38325200	-0.67652500	-3.42084700	H	0.40020800	4.81085000	-2.11294500
H	-3.94869300	2.19080200	-0.99039700	O	0.15170800	2.26870300	0.04924600
H	-5.15221400	1.31910400	-1.95967800	O	-0.83003700	-2.12280200	-0.39728600
H	-4.40058100	0.53240600	-0.55670500	C	-1.08757800	-3.50596500	-0.32761000
H	-3.70905600	1.73877900	-4.08546400	C	0.04660500	-4.17807200	0.45459900
H	-2.55168700	2.62076600	-3.07171900	C	-2.42873700	-3.72386000	0.38144400
H	-2.00091500	1.25625500	-4.06352000	C	-1.14747600	-4.06707000	-1.75331500
				H	1.00339100	-4.00824800	-0.04985300
TS_{3B-4B} ('BuOH)				H	0.11241100	-3.75802000	1.46244700
<i>H= -1586.996363 au</i>				H	-0.11096300	-5.25895600	0.53902300
N	-0.84414800	0.85960600	1.78428400	H	-3.23375000	-3.23046300	-0.17272100
C	-0.03101400	0.01407100	2.49187000	H	-2.67012800	-4.78937000	0.46244200
N	-0.27203300	-0.48691700	3.63343600	H	-2.39917600	-3.29864100	1.38917600
O	1.07444700	-0.31164600	1.63562600	H	-1.34722200	-5.14426500	-1.75058600

H	-1.93900500	-3.57118900	-2.32352200	C	-2.88371100	-0.04111400	2.74895400
H	-0.19672900	-3.89528500	-2.26804500	H	-2.35546800	1.84982000	1.91604200
C	1.88767300	-0.42095900	-3.37728200	H	-1.14090600	2.77132600	3.86744700
C	2.81792500	0.78049800	-3.58007700	H	-2.76470500	2.23716400	4.32579400
C	2.70996300	-1.69080700	-3.12670900	H	-1.35583900	1.23577500	4.73751300
C	0.99445300	-0.60843400	-4.60931200	H	-2.95869500	-0.56182800	1.78992800
H	2.23105200	1.68815300	-3.75074100	H	-2.54092600	-0.75018900	3.50427000
H	3.43909300	0.93527800	-2.69222200	H	-3.88303000	0.30966800	3.02557000
H	3.47949000	0.63182100	-4.44056500	H	-0.16005100	1.59203600	1.61650300
H	2.04555100	-2.54175500	-2.94756300	C	0.33879800	3.62126200	-0.38035700
H	3.35042700	-1.92768100	-3.98332100	C	1.36621000	4.41589200	0.43710600
H	3.35044800	-1.56610700	-2.24749200	H	1.36800600	5.47641500	0.16124000
H	1.58942300	-0.78865100	-5.51147600	H	1.13940400	4.34728200	1.50691500
H	0.32296500	-1.46065900	-4.46413000	H	2.37379600	4.02019300	0.27325300
H	0.38501300	0.28596400	-4.77273900	C	-1.06893600	4.17168400	-0.11183000
C	-3.33634700	0.66854800	-2.45873800	H	-1.16067400	5.22118600	-0.41406200
C	-3.57222700	-0.65454800	-3.19527600	H	-1.81033500	3.58642000	-0.66469400
C	-4.51519300	0.97258300	-1.52772300	H	-1.30651700	4.10672300	0.95608100
C	-3.14952400	1.80676900	-3.46825800	C	0.66567800	3.73997500	-1.87479000
H	-2.72216600	-0.88322100	-3.84592600	H	1.66174800	3.33287600	-2.07516000
H	-3.68525000	-1.47243500	-2.47703600	H	-0.06132800	3.17069500	-2.46376000
H	-4.47604200	-0.61113800	-3.81279100	H	0.64285100	4.78090000	-2.21661000
H	-4.33927300	1.90503900	-0.98214900	O	0.38810800	2.26387600	0.00355000
H	-5.44991300	1.07515800	-2.08972500	O	-0.56304700	-1.95664700	-0.28452600
H	-4.64015700	0.16723400	-0.79726600	C	-0.80631600	-3.33481900	-0.16582900
H	-4.03543700	1.92553000	-4.10147900	C	0.38274300	-3.99026600	0.54834800
H	-2.97107100	2.75355500	-2.94903700	C	-2.09558900	-3.54836900	0.63654600
H	-2.29002700	1.60209200	-4.11432200	C	-0.96116100	-3.93499100	-1.56960700
				H	1.29907800	-3.83271600	-0.02996500
				H	0.52364500	-3.54205500	1.53612800
				H	0.23567300	-5.06891000	0.67384400
				H	-2.93937600	-3.07476400	0.12403500
				H	-2.32359100	-4.61281200	0.76182900
				H	-2.00417100	-3.09451000	1.62791600
				H	-1.14424600	-5.01465900	-1.52762300
				H	-1.79814300	-3.46413100	-2.09414000
				H	-0.05227500	-3.76246000	-2.15481000
				C	2.16686600	-0.47349100	-3.34050900
				C	3.11010500	0.69815400	-3.63714700
				C	2.97591400	-1.73195500	-3.00376900
				C	1.26015000	-0.73866600	-4.54808800
				H	2.53321400	1.59804100	-3.87097800
				H	3.73670400	0.91058700	-2.76506000
				H	3.76559100	0.47750300	-4.48685000
				H	2.30284200	-2.55773300	-2.75335700
				H	3.60381300	-2.04121200	-3.84653400
				H	3.62734100	-1.54827600	-2.14300300
				H	1.84477800	-0.99216400	-5.43934400
				H	0.57941500	-1.56924000	-4.33584700
				H	0.66064900	0.14940500	-4.77144900
				C	-3.03179600	0.72681100	-2.53433900
				C	-3.24699100	-0.61722800	-3.23851400
				C	-4.22080000	1.03874200	-1.61788800
				C	-2.85476800	1.84308500	-3.56992200
				H	-2.38715200	-0.85389100	-3.87306100
				H	-3.35827000	-1.41685700	-2.49978500
				H	-4.14456800	-0.59991400	-3.86651100
				H	-4.05672600	1.98456700	-1.09180500
				H	-5.15310100	1.11990000	-2.18747800
				H	-4.34281600	0.24689000	-0.87185600
				H	-3.73884700	1.93545300	-4.21022000
				H	-2.68951200	2.80338200	-3.07174500
				H	-1.98931900	1.63394200	-4.20650500

dimer-C ('BuOH)			
<i>H= -1935.263130 au</i>			
O	-0.72218500	0.86013500	2.70972000
O	-1.42961000	2.72129200	0.78421100
Th	-1.13808000	3.15712300	3.23661900
C	-1.91063800	3.70725100	-0.16179700
C	-3.20805600	3.18586200	-0.78477000
C	-2.18682200	5.02430300	0.56658800
C	-0.83479400	3.92718500	-1.22750700
H	-3.02970200	2.25923200	-1.34004200
H	-3.95210900	2.99581200	-0.00506800
H	-3.62798800	3.91400300	-1.48731100
H	-1.27470700	5.40265400	1.04024700
H	-2.53988500	5.78579300	-0.13643700
H	-2.95919300	4.89060900	1.33131500
H	-1.15172000	4.68342000	-1.95398300
H	0.09348500	4.26942700	-0.76049900
H	-0.63740900	2.99984600	-1.77379900
C	-0.40733700	-0.18448300	3.66007500
C	0.92763200	0.14943200	4.32858800
C	-1.53797900	-0.26199200	4.68891700
C	-0.29125600	-1.52472800	2.92995800
H	1.72008600	0.20833400	3.57626300
H	0.86630400	1.10615100	4.85568100
H	1.20587500	-0.61902400	5.05814200
H	-2.48807900	-0.47595600	4.18973300
H	-1.35093700	-1.05554800	5.42076100
H	-1.62788200	0.68035700	5.23801900
H	-0.04032200	-2.32631600	3.63232200
H	-1.23765900	-1.78749500	2.44675600
H	0.50536300	-1.48910400	2.17808800
Th	-0.94248000	0.44957000	0.24892000
O	-1.20163000	0.53551100	-1.89692800
O	-2.58269700	-0.92706100	0.54417000
O	1.15399400	-0.08115000	0.13528100
O	-3.21667400	3.66753200	3.50103100
O	0.32156000	4.70368400	2.83884300
O	-0.69628700	3.06475400	5.35284700
C	-3.64386500	-1.85577500	0.48852700
C	-3.08148900	-3.24202700	0.15145900
C	-4.34479800	-1.88841000	1.85200700
C	-4.63339300	-1.41055000	-0.59397400
H	-2.57047200	-3.21990800	-0.81648600
H	-2.36010200	-3.55780100	0.91227200
H	-3.87550100	-3.99520900	0.10211100
H	-4.70520300	-0.88874500	2.11460100
H	-5.20076200	-2.57213700	1.84413600
H	-3.65373000	-2.22009000	2.63340200
H	-5.48208100	-2.09918500	-0.67005700
H	-5.01979900	-0.41204700	-0.36556300
H	-4.13542400	-1.36960400	-1.56725100
C	2.52220300	-0.34550300	-0.08702500
C	3.35248100	0.73229100	0.62078800
C	2.86975900	-1.73094000	0.47096700
C	2.80178600	-0.30855700	-1.59318000
H	3.09739000	1.72258700	0.22956300
H	3.14865900	0.72674300	1.69598000
H	4.42643800	0.57223900	0.47512900
H	2.24165200	-2.49650100	0.00364900
H	3.91812000	-1.98479400	0.27949400
H	2.70717000	-1.76570500	1.55287100
H	3.85459200	-0.52082900	-1.80929200
H	2.18780700	-1.05179900	-2.11121200
H	2.56093900	0.67896200	-1.99841800
C	-1.29186800	0.26405200	-3.28183400
C	-2.64254700	0.76087800	-3.81019100
C	-0.15266300	0.98052000	-4.01595500
C	-1.17351900	-1.25071500	-3.48900200
H	-3.46490500	0.28607300	-3.26639800
H	-2.72879500	1.84462100	-3.68476000
H	-2.75809500	0.53323600	-4.87553300
H	0.81494800	0.64740200	-3.63159000
H	-0.18550500	0.77637800	-5.09192000
H	-0.22454200	2.06351600	-3.87536100
H	-1.23826300	-1.51835300	-4.54943000
H	-0.21463800	-1.61168900	-3.10285700
H	-1.97602700	-1.76907400	-2.95483800
C	-4.51328700	4.04550000	3.91135300
C	-4.56121600	5.56967200	4.07110400
C	-5.51860800	3.59195400	2.84645000
C	-4.82681600	3.36581200	5.24838100
H	-3.82428500	5.89513900	4.81251800
H	-4.33031900	6.06215700	3.12100700
H	-5.55029300	5.90762000	4.39904700
H	-5.45494900	2.50837400	2.70451000
H	-6.54547000	3.84170700	3.13513700
H	-5.30790900	4.07640700	1.88785700
H	-5.83154500	3.62178900	5.60200500
H	-4.76485800	2.27776400	5.14452500
H	-4.10432800	3.67818500	6.00821800
C	1.29303300	5.72648600	2.79774000
C	2.40896000	5.39245600	3.79378500
C	1.87174000	5.80880500	1.38018500
C	0.63242600	7.05824200	3.17425900
H	2.00396300	5.33019700	4.80804900
H	2.86238100	4.42728900	3.54563400
H	3.19548400	6.15491500	3.78404400
H	1.08975900	6.06458900	0.65838700
H	2.65584400	6.57111500	1.31442600
H	2.30432800	4.84547800	1.09206200
H	1.35452000	7.88197700	3.15808500
H	-0.17340500	7.29732500	2.47269400
H	0.20356300	6.99863900	4.17970700
C	-0.47790000	3.35804000	6.71909600
C	-1.37934900	2.46731100	7.58192200
C	0.99202400	3.09540000	7.06807400
C	-0.81668700	4.83411000	6.95875500
H	-2.43087500	2.61873500	7.32115200
H	-1.13672500	1.41140100	7.42806600
H	-1.25327300	2.69182200	8.64684000
H	1.64979700	3.68901400	6.42680800
H	1.20243100	3.35426700	8.11155700
H	1.23925800	2.03879700	6.92682700
H	-0.66584200	5.11732300	8.00628900
H	-0.18281300	5.47311400	6.33565800
H	-1.86185000	5.02898600	6.69734100

Cat_c ('BuOH)

<i>H= -967.61671 au</i>			
Th	1.02950700	1.96780000	-0.34433200
C	3.60602100	0.66477600	-3.53347200
H	3.83801600	1.73450800	-3.55579700
H	4.36700700	0.13576300	-4.11749000
H	2.63588000	0.51456800	-4.01848100
C	3.19891800	-1.32618200	-2.04931100

H	2.22477400	-1.49187800	-2.52080000	H	1.56296800	-2.24836000	2.97695000
H	3.94344200	-1.93267200	-2.57640600	C	2.82540600	0.20297600	2.92594800
H	3.14195200	-1.67655800	-1.01347600	H	2.94957600	1.21260200	2.52030100
C	4.90603500	0.40244600	-1.39513800	H	3.39793300	0.13529000	3.85777200
H	5.15031800	1.46968800	-1.40079800	H	3.25279500	-0.50949000	2.21205400
H	4.86217800	0.06635000	-0.35416300	C	0.74383300	0.90929000	4.14111300
H	5.71607700	-0.13774000	-1.89712600	H	-0.31821200	0.69307800	4.29913200
C	-2.22167100	0.64054300	-2.82362300	H	1.25053800	0.86135400	5.11151900
H	-1.40916300	0.03376300	-3.23648600	H	0.83610300	1.92642000	3.74858800
H	-3.17289900	0.22365800	-3.17185200	Th	0.20756100	-0.28874800	-0.18784200
H	-2.12651100	1.65673200	-3.21989200	O	-1.90385100	-0.64991500	-0.61981500
C	-3.25384400	1.54090800	-0.71296800	O	1.60780100	0.44345100	-1.70623000
H	-4.24677000	1.16175100	-0.97814800	C	-2.10774400	3.31701700	3.23678600
H	-3.17945700	1.57456800	0.37881300	C	-3.31431200	2.49376800	2.79781500
H	-3.16350100	2.56312500	-1.09444800	C	-2.47260100	4.76051500	3.57951100
C	-2.24837600	-0.76578200	-0.73721200	H	-1.66326400	2.85471300	4.12650400
H	-2.16674900	-0.75279100	0.35451200	H	-3.02506500	1.46605000	2.56041900
H	-3.20281400	-1.23189600	-1.00489100	H	-4.06089400	2.46239000	3.59721000
H	-1.43936500	-1.38766500	-1.13433200	H	-3.78509500	2.93522900	1.91245300
C	1.65963800	0.06901800	3.46851900	H	-1.58700500	5.32357600	3.88496300
H	0.78379100	-0.49864000	3.13771400	H	-2.91924000	5.26262200	2.71511900
H	2.53745200	-0.31463600	2.93848700	H	-3.19701600	4.77890600	4.39904000
H	1.80008500	-0.10991000	4.54010500	C	-1.01744400	3.26725800	-1.17366400
C	0.22069400	2.09160900	3.88108500	C	-1.18363400	2.38750800	-2.40300700
H	0.07165400	3.15031600	3.64480100	C	0.06519600	4.32676200	-1.35386700
H	-0.66620000	1.53921900	3.55404700	H	-1.97368200	3.76494500	-0.96336300
H	0.30606000	1.99168100	4.96859600	H	-1.94407300	1.62081900	-2.23259300
C	2.70729300	2.35289500	3.59989800	H	-1.48586200	2.99501800	-3.26167500
H	2.88686600	2.26217500	4.67667500	H	-0.23636100	1.89360700	-2.64470000
H	3.59420000	1.98717500	3.07213600	H	0.14681500	4.96567600	-0.46896300
H	2.57923700	3.41374900	3.36137300	H	1.03455400	3.85242000	-1.52915700
O	2.56353600	0.88340300	-1.39282100	H	-0.16973600	4.96322800	-2.21333500
O	1.29474200	1.71985800	1.77724300	O	0.82216800	-2.34328400	-0.29727400
O	-0.89573200	1.19784200	-0.91365200	C	1.18561900	-3.70153400	-0.36994300
C	-2.14256900	0.65896200	-1.29293500	C	1.14161800	-4.14666000	-1.83671000
C	3.55869500	0.16342200	-2.08566700	C	2.60485100	-3.86989700	0.18649500
C	1.46879800	1.55991200	3.16751900	C	0.19598000	-4.52708400	0.46112100
O	1.14006800	4.05837500	-0.84175800	H	0.13617600	-4.00458600	-2.24544700
C	1.20974500	5.43032200	-1.15997500	H	1.84057000	-3.55170700	-2.43314700
C	0.39535200	6.21429300	-0.12471800	H	1.41130300	-5.20325000	-1.94422700
C	2.67867500	5.86651500	-1.12274400	H	2.64517600	-3.54806700	1.23183100
C	0.62780000	5.63745400	-2.56289700	H	2.93261900	-4.91423400	0.13732100
H	-0.64908800	5.88579300	-0.13689900	H	3.31198400	-3.26064800	-0.38483200
H	0.79683400	6.04359900	0.87945800	H	0.44771700	-5.59336700	0.44158800
H	0.41896500	7.29079600	-0.32616100	H	0.20334100	-4.19039800	1.50258100
H	3.26355700	5.28607300	-1.84359900	H	-0.81924400	-4.40781200	0.06973100
H	2.78901000	6.92880500	-1.36646200	C	2.64423400	0.48386200	-2.65893600
H	3.09817300	5.69768100	-0.12554300	C	2.15542200	-0.16599600	-3.96014000
H	0.65685100	6.69183500	-2.85855100	C	3.03091800	1.94533300	-2.91945600
H	1.19693800	5.05919300	-3.29812900	C	3.85666600	-0.28065900	-2.11200800
H	-0.41355400	5.30084300	-2.59349100	H	1.86531000	-1.20569500	-3.77843100
Int-1C ('BuOH)							
<i>H= -1351.941282 au</i>							
N	-0.68041800	2.40501300	0.00442000	H	1.28165000	0.36916200	-4.34677900
C	-0.92754300	2.85635400	1.13835500	H	2.93157700	-0.15577500	-4.73362100
N	-1.03750900	3.33387100	2.24340700	H	3.33815400	2.42618700	-1.98500000
O	0.65629700	0.01154500	1.92153600	H	3.85983200	2.01960400	-3.63230700
C	1.33752700	-0.09836800	3.14993200	H	2.18104300	2.50001500	-3.33022300
C	1.16203000	-1.52249100	3.69057700	H	4.68912300	-0.28408200	-2.82460700
H	1.67719300	-1.65725300	4.64831400	H	4.20457700	0.17901800	-1.18083500
H	0.09927800	-1.74138500	3.83683600	H	3.58125500	-1.31797200	-1.89870300
C				C	-3.16635700	-1.25608500	-0.74458900
				C	-3.11994900	-2.27724400	-1.88855100
				C	-3.51612400	-1.95928000	0.57401300
				C	-4.21175400	-0.17571100	-1.05050000

H	-2.85173300	-1.78041000	-2.82675900	H	2.72561000	-3.03819900	0.79441800				
H	-2.36381600	-3.04047800	-1.67972600	H	-0.25086400	-4.86207500	2.29127200				
H	-4.08563600	-2.77644300	-2.02696100	H	-0.28192800	-3.24422000	3.01977200				
H	-3.55509200	-1.23243100	1.39257700	H	-1.43330800	-3.65849500	1.73767600				
H	-4.48640100	-2.46576200	0.52014300	C	2.24713500	0.50496800	-2.35611500				
H	-2.75193800	-2.70455100	0.81687600	C	1.56756900	0.40646900	-3.72677700				
H	-5.21989500	-0.59956400	-1.11986000	C	2.97446800	1.84767700	-2.21927100				
H	-4.20989400	0.58295800	-0.26129500	C	3.23666300	-0.65115300	-2.17171200				
H	-3.98489000	0.31740500	-2.00137200	H	1.02983000	-0.54308900	-3.81428800				
TS_{1C-2C} (^tBuOH)											
<i>H= -1351.920751 au</i>											
N	-0.84533900	2.56928700	0.56815100	H	0.84562200	1.21965600	-3.85155500				
C	-1.17435800	2.60912700	1.81692200	H	2.29736900	0.46543900	-4.54170300				
N	-1.78972100	3.19626200	2.70263300	H	3.44528900	1.92557100	-1.23382400				
O	-0.25936900	1.01886000	2.37906700	H	3.75344400	1.96108800	-2.98119900				
C	0.89073400	1.07686700	3.24008900	H	2.26708600	2.67612400	-2.32498600				
C	0.64708700	0.11403300	4.40453200	H	4.02623300	-0.62687000	-2.93073600				
H	1.50397700	0.08909000	5.08676800	H	3.70680400	-0.59355900	-1.18460100				
H	-0.23478400	0.41953300	4.97589000	H	2.71618800	-1.61106000	-2.24686100				
H	0.47365200	-0.89797800	4.02714500	C	-3.35493600	-0.85459900	-1.15279200				
C	2.12172800	0.62516800	2.43670800	C	-3.10722300	-1.38244100	-2.57034800				
H	2.30291100	1.30037400	1.58900000	C	-3.81904900	-1.99212600	-0.23590500				
H	3.02883600	0.63903100	3.04937000	C	-4.40636200	0.26046400	-1.17691900				
H	2.00343200	-0.40469700	2.07437300	H	-2.74744400	-0.57610400	-3.21735900				
C	1.14172000	2.49500600	3.75852600	H	-2.34797000	-2.17116900	-2.55359200				
H	0.31169700	2.85290200	4.37026700	H	-4.02155600	-1.79516700	-3.01065200				
H	2.04693500	2.50812000	4.37474900	H	-3.97645900	-1.61807000	0.78112700				
H	1.28362800	3.19528800	2.93005900	H	-4.75708000	-2.43466100	-0.58845700				
Th	-0.20865600	0.08429000	0.18597000	H	-3.06017900	-2.77974700	-0.19719000				
O	-2.14674300	-0.32958000	-0.64582400	H	-5.37078200	-0.11065800	-1.54062500				
O	1.25743900	0.42164600	-1.35547500	H	-4.55105200	0.66627700	-0.17082300				
C	-2.42692800	2.75602400	3.92208000	H	-4.08611000	1.07658300	-1.83187200				
C	-3.81452200	2.18215000	3.62234800	Int-2C (^tBuOH)							
C	-2.50513800	3.92189900	4.90570600	<i>H= -1351.932062 au</i>							
H	-1.81287100	1.95489200	4.35757400	N	-0.41168200	2.05311200	0.27243100				
H	-3.74357100	1.32733200	2.94364000	C	-0.72976300	1.88558900	1.57456800				
H	-4.29896600	1.84786700	4.54600800	N	-1.57562500	2.52575100	2.27918000				
H	-4.45001800	2.94124500	3.15488200	O	-0.01589200	0.71390200	2.04648000				
H	-1.51090200	4.32430100	5.12048700	C	1.28823300	0.90518200	2.72074400				
H	-3.11232000	4.73198700	4.48877000	C	1.30869900	-0.13283000	3.83592100				
H	-2.95915000	3.60017300	5.84822800	H	2.27348000	-0.11958500	4.35306500				
C	-1.50341100	3.58474900	-0.28576800	H	0.52189300	0.07011700	4.56727300				
C	-1.41169600	3.13884700	-1.73973700	H	1.14931800	-1.13279300	3.42463600				
C	-0.85719800	4.95333300	-0.07288800	C	2.39186000	0.62444300	1.69797700				
H	-2.56337400	3.65309200	0.00120600	H	2.34317400	1.34179600	0.86906700				
H	-1.90523700	2.17290000	-1.88616100	H	3.38090900	0.73259500	2.15321500				
H	-1.89316600	3.86936500	-2.39767200	H	2.33391700	-0.40991700	1.33224500				
H	-0.36440600	3.04204800	-2.04567500	C	1.44444200	2.31848000	3.26962200				
H	-0.93497800	5.26004400	0.97393800	H	0.67741600	2.55339200	4.00875700				
H	0.20212600	4.92097300	-0.34921900	H	2.42119100	2.39482500	3.75790800				
H	-1.35083200	5.71297700	-0.68885900	H	1.40401000	3.06480500	2.47205300				
O	0.32773500	-1.91791900	0.79009000	Th	0.12903200	-0.23237700	-0.47750800				
C	0.58283600	-3.28468000	1.02816700	O	-1.69641000	-0.74957200	-1.44729700				
C	0.39782000	-4.05247700	-0.28610900	O	1.58791100	0.03482900	-2.01902100				
C	2.02291300	-3.44275100	1.52979400	C	-1.97886300	2.12611200	3.61126800				
C	-0.40419500	-3.79744200	2.08308600	C	-3.31723900	1.38223500	3.53128400				
H	-0.62206000	-3.91890200	-0.66072000	C	-2.10701900	3.37140900	4.49130100				
H	1.09233000	-3.67702700	-1.04446400	H	-1.25155700	1.44046500	4.07509500				
H	0.57816000	-5.12510500	-0.15498200	H	-3.21582000	0.46302900	2.94572100				
H	2.16085200	-2.90244900	2.47216900	H	-3.67972300	1.11394300	4.53018500				
H	2.27288000	-4.49529200	1.70246500	H	-4.06937300	2.01247300	3.04552400				
				H	-1.15544800	3.90832700	4.56115900				
				H	-2.84138300	4.05936900	4.05958500				
				H	-2.42916200	3.10870000	5.50490800				

C	-1.04135400	3.18523300	-0.40828000	H	2.68436500	1.31983700	0.20323000
C	-0.96338200	2.97173300	-1.91795000	H	4.30046100	0.84621500	0.73889400
C	-0.38351500	4.50580300	-0.00051800	H	3.25813300	-0.35033300	-0.03865400
H	-2.09857700	3.23317700	-0.10668900	C	2.65763700	1.34395800	2.92171500
H	-1.49100500	2.05888700	-2.21884700	H	2.20632900	1.11042300	3.88783300
H	-1.42292100	3.80731600	-2.45567100	H	3.67574700	1.70656300	3.09421000
H	0.07997200	2.89674000	-2.24815800	H	2.08318600	2.14966800	2.45843000
H	-0.46754200	4.64730500	1.08000200	Th	-0.10710600	-0.09327900	-0.54606100
H	0.67643200	4.50838400	-0.28041400	O	-1.89392900	0.53299500	-1.55135700
H	-0.87023500	5.35472500	-0.49407400	O	1.33871800	-0.20615700	-2.14831200
O	0.68510100	-2.13516200	0.39033200	C	0.70635900	-1.60841800	4.37446300
C	0.88278800	-3.46464600	0.82305800	C	-0.30717400	-2.72531400	4.65364700
C	0.71132600	-4.39834200	-0.38124600	C	1.35323500	-1.15788600	5.68776600
C	2.30108500	-3.60018100	1.38914500	H	1.47973400	-2.02384600	3.71411400
C	-0.15569200	-3.79984900	1.89971800	H	-0.77798700	-3.06371800	3.72618700
H	-0.29328100	-4.29066500	-0.80261600	H	0.17858600	-3.58639600	5.12674000
H	1.43883500	-4.14869200	-1.16013200	H	-1.09673500	-2.36289300	5.32040100
H	0.85443400	-5.44743100	-0.09995400	H	2.12551900	-0.39911800	5.52624000
H	2.43746600	-2.93946000	2.25145300	H	0.59304200	-0.72147700	6.34414500
H	2.50488000	-4.62641500	1.71363300	H	1.81486900	-2.00386200	6.20898300
H	3.03918800	-3.32835100	0.62771200	C	-1.87595700	1.16804600	2.37286400
H	-0.04102500	-4.82764200	2.26116900	C	-1.76235600	2.05835100	3.61504000
H	-0.05503700	-3.12402400	2.75469700	C	-2.83166300	-0.00647400	2.60947800
H	-1.16768800	-3.68896500	1.49734100	H	-2.31823400	1.78000600	1.57286700
C	2.52600000	0.04013900	-3.07560100	H	-1.11701200	2.92235600	3.41852500
C	1.77068500	0.21334700	-4.39745400	H	-2.74857700	2.43330400	3.91080700
C	3.49451800	1.20767800	-2.85913200	H	-1.33516900	1.49233200	4.44562900
C	3.28534500	-1.29073700	-3.06614300	H	-2.91940300	-0.62439300	1.70897200
H	1.06528300	-0.61118600	-4.54178200	H	-2.47445500	-0.63529600	3.42695000
H	1.20529400	1.15038400	-4.39136500	H	-3.83174600	0.36409000	2.86090400
H	2.45806300	0.23090300	-5.25010500	H	0.11825800	2.18541800	0.93591800
H	4.02348700	1.09166000	-1.90755800	C	0.31624700	3.82032300	-0.31464100
H	4.23937400	1.26147100	-3.66040400	C	1.27863300	4.62348300	0.56102500
H	2.94689900	2.15495300	-2.83382800	H	1.22780800	5.68944000	0.31684500
H	4.03484200	-1.32852000	-3.86407800	H	1.02791000	4.51119600	1.62136500
H	3.79586400	-1.42952200	-2.10770100	H	2.30796100	4.28493400	0.41104200
H	2.59104900	-2.12518700	-3.20778200	C	-1.13011100	4.25576900	-0.08221500
C	-2.86342200	-1.28558300	-2.04044600	H	-1.27255500	5.29898800	-0.38175000
C	-2.45351700	-2.12101900	-3.25708700	H	-1.81222200	3.62993500	-0.66416000
C	-3.57563200	-2.16142400	-1.00425300	H	-1.40109800	4.17125300	0.97573600
C	-3.77033700	-0.12798500	-2.46881700	C	0.69301100	3.93630300	-1.78720200
H	-1.92800400	-1.49561700	-3.98566900	H	1.71162000	3.57380300	-1.95206200
H	-1.78301300	-2.93130800	-2.95312300	H	0.01045400	3.34771300	-2.40707300
H	-3.32641800	-2.56302300	-3.74958400	H	0.64080900	4.97934000	-2.11329300
H	-3.84630900	-1.56626500	-0.12600600	O	0.45168900	2.42108200	0.02098500
H	-4.49060200	-2.60199400	-1.41458200	O	-0.56665700	-2.16873100	-0.33762000
H	-2.91917100	-2.97505800	-0.67923700	C	-0.83628700	-3.55349500	-0.30608000
H	-4.69927000	-0.49737500	-2.91651500	C	0.28642200	-4.25017000	0.47031600
H	-4.02675500	0.49287600	-1.60491800	C	-2.18368200	-3.77528200	0.38897100
H	-3.26254100	0.50123700	-3.20642000	C	-0.88896700	-4.07872000	-1.74485100
				H	1.24882800	-4.07673500	-0.02208400
				H	0.34635500	-3.85190500	1.48740000
				H	0.12002400	-5.33136900	0.52993900
				H	-2.98012500	-3.25858900	-0.15620000
				H	-2.43672700	-4.83995400	0.43980900
				H	-2.15485500	-3.37790600	1.40805800
				H	-1.09926500	-5.15361100	-1.76988100
				H	-1.67079000	-3.56139800	-2.30932100
				H	0.06790800	-3.90435600	-2.24726100
				C	2.17006800	-0.42297200	-3.26622400
				C	3.08839300	0.79090400	-3.44959200
				C	3.00615300	-1.68629100	-3.02763400
				C	1.28785100	-0.60584800	-4.50700000

H	2.49195200	1.69369000	-3.61397200	H	-2.76062300	-0.59203200	3.31637600
H	3.70213700	0.94264300	-2.55595400	H	-4.11540700	0.41103400	2.75454000
H	3.75757200	0.66104600	-4.30736100	H	-0.27954600	1.87077500	1.02872200
H	2.35029300	-2.54623300	-2.86008400	C	0.05134400	3.66774300	-0.29753900
H	3.65235900	-1.90730700	-3.88429300	C	1.03367500	4.44623900	0.58219000
H	3.64251200	-1.56497000	-2.14483900	H	1.01815700	5.51412600	0.33951900
H	1.88995800	-0.76972900	-5.40766600	H	0.77409200	4.33886100	1.64073000
H	0.62416200	-1.46631100	-4.37535100	H	2.05387200	4.07793600	0.43721900
H	0.66948500	0.28362300	-4.66426300	C	-1.37673700	4.17219900	-0.07310200
C	-3.06396900	0.66448800	-2.33109500	H	-1.47293600	5.22216100	-0.36949300
C	-3.32326300	-0.65460900	-3.06715700	H	-2.08436900	3.58106400	-0.66183100
C	-4.23895200	0.99115400	-1.40305500	H	-1.65640800	4.09511000	0.98269400
C	-2.85723800	1.79651900	-3.34379600	C	0.43638500	3.80011000	-1.77088700
H	-2.47831300	-0.89746100	-3.71943100	H	1.44309400	3.40577500	-1.93864300
H	-3.44824200	-1.47030300	-2.34848700	H	-0.26209300	3.23828900	-2.39913800
H	-4.22742700	-0.59702800	-3.68309400	H	0.41824100	4.84726700	-2.09006800
H	-4.04761300	1.92156000	-0.85893500	O	0.12974200	2.27859600	0.03322300
H	-5.17141000	1.10871400	-1.96603100	O	-0.79223000	-2.15986700	-0.40569000
H	-4.37826800	0.19039100	-0.67026400	C	-1.07411000	-3.54136400	-0.36143700
H	-3.73810600	1.92584900	-3.98206700	C	0.04021800	-4.24334300	0.42248500
H	-2.66964100	2.74329000	-2.82743400	C	-2.42567000	-3.74669000	0.33089600
H	-1.99733400	1.57803100	-3.98485800	C	-1.12824800	-4.07797500	-1.79626700
				H	1.00562600	-4.07957800	-0.06741800
				H	0.09961400	-3.84152500	1.43831000
				H	-0.13432600	-5.32300700	0.48679300
N	-0.84019800	0.88671200	1.80971000	H	-3.21605700	-3.22904400	-0.22217300
C	-0.03457500	0.04215500	2.52197100	H	-2.68742200	-4.80876700	0.39146000
N	-0.27526400	-0.45581800	3.66584600	H	-2.39800900	-3.33968000	1.34629900
O	1.07196700	-0.29949000	1.66868400	H	-1.34882400	-5.15095800	-1.81414400
C	2.44594600	0.18928300	1.93955700	H	-1.90349500	-3.55698800	-2.36653900
C	3.28467000	-0.94769400	2.51957000	H	-0.16851000	-3.91631900	-2.29749000
H	4.34299300	-0.66813100	2.49435800	C	1.87873700	-0.44310800	-3.40737300
H	3.02641300	-1.16792300	3.55612500	C	2.78416600	0.77526800	-3.61971000
H	3.15863500	-1.85595300	1.92332800	C	2.72656400	-1.69610600	-3.15877700
C	3.00157300	0.57974200	0.57256500	C	0.97948000	-0.65056900	-4.63134100
H	2.42258800	1.40092000	0.14162100	H	2.17852900	1.67160400	-3.78492700
H	4.04038800	0.90977300	0.67103000	H	3.41065800	0.94237500	-2.73768800
H	2.99000300	-0.27092300	-0.11666500	H	3.44056500	0.63914300	-4.48624500
C	2.41565400	1.39942100	2.86524400	H	2.07962100	-2.55890800	-2.97238300
H	1.96690900	1.15718600	3.83083500	H	3.36608400	-1.92393900	-4.01856800
H	3.43975900	1.74378000	3.03926800	H	3.37014300	-1.55600400	-2.28400900
H	1.85139800	2.21871300	2.41434200	H	1.57022800	-0.82481000	-5.53744100
Th	-0.35952600	-0.07637100	-0.67283300	H	0.32334600	-1.51305200	-4.47730100
O	-2.15859600	0.48974100	-1.67917200	H	0.35394600	0.23282300	-4.79388200
O	1.06287900	-0.21384500	-2.27906300	C	-3.33051900	0.63641900	-2.45395200
C	0.41329700	-1.58195300	4.26109800	C	-3.58892800	-0.66832700	-3.21511500
C	-0.61589100	-2.68763200	4.52377300	C	-4.50342300	0.94267000	-1.51662200
C	1.07184800	-1.16360100	5.57899200	C	-3.12520200	1.78970500	-3.44228800
H	1.17755600	-1.99346400	3.58819800	H	-2.74341400	-0.89871400	-3.87105000
H	-1.09628800	-3.00187200	3.59291200	H	-3.71462300	-1.49761700	-2.51219200
H	-0.13937800	-3.56419900	4.97681200	H	-4.49262500	-0.59890900	-3.83048100
H	-1.39577800	-2.32708300	5.20263800	H	-4.31130600	1.86158000	-0.95372300
H	1.84979900	-0.40833500	5.42904900	H	-5.43696000	1.07145500	-2.07524800
H	0.31977000	-0.73541900	6.24980000	H	-4.64126900	0.12594500	-0.80125000
H	1.52897700	-2.02506600	6.07794700	H	-4.00833800	1.93479400	-4.07400000
C	-2.16402800	1.25629300	2.34153000	H	-2.93223900	2.72396600	-2.90574900
C	-2.07423900	2.09883100	3.61751500	H	-2.26841600	1.58329100	-4.09146900
C	-3.10557800	0.06174400	2.51334900				
H	-2.59440000	1.89327900	1.55594600				
H	-1.43606400	2.97538200	3.46095800				
H	-3.06864700	2.45236700	3.91160900				
H	-1.65455800	1.50650100	4.43330600				
H	-3.16593500	-0.52390500	1.58931900				

Int-4C (*t*BuOH)

$H = -1585.414477 \text{ au}$

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N      -0.63513500  0.83781800  2.07858700
C      0.24335500 -0.04971600  2.69545300
N     -0.02651800 -0.64926800  3.77369000

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O	1.32620500	-0.24520600	1.82405900	H	-1.10624500	-5.00271700	-1.64544400
C	2.68725200	0.28306400	2.11725900	H	-1.69027100	-3.41722400	-2.19309900
C	3.55123900	-0.83384200	2.69403600	H	0.04736200	-3.76566000	-2.18571200
H	4.59885600	-0.51603300	2.69279000	C	2.16229600	-0.47586000	-3.37202700
H	3.28272600	-1.08114100	3.72193800	C	3.05855600	0.72891000	-3.68158700
H	3.46861500	-1.73420800	2.07900300	C	3.02157400	-1.70111600	-3.03703800
C	3.22421800	0.69984900	0.75237700	C	1.25687900	-0.78034100	-4.57125600
H	2.59472900	1.48123700	0.31547900	H	2.44569600	1.60624300	-3.90957400
H	4.24078600	1.09176500	0.85440300	H	3.68648700	0.96612200	-2.81670600
H	3.26720500	-0.15537600	0.06998100	H	3.71274300	0.53209700	-4.53824600
C	2.60159400	1.48166300	3.05391200	H	2.38257100	-2.55037100	-2.77603400
H	2.13713200	1.21849700	4.00787900	H	3.65415600	-1.99125500	-3.88318200
H	3.61146500	1.84838800	3.26055500	H	3.67283000	-1.48787600	-2.18274900
H	2.03626100	2.29704800	2.59530700	H	1.84290200	-1.02017300	-5.46545700
Th	-0.07218400	0.10057500	-0.67592400	H	0.60586600	-1.63156000	-4.34790200
O	-1.88845500	0.56554800	-1.71017900	H	0.62560800	0.08514500	-4.79605300
O	1.35646700	-0.16724700	-2.25832700	C	-3.05672900	0.68823200	-2.48937800
C	0.69558300	-1.78291200	4.31846100	C	-3.31832000	-0.63899200	-3.21004100
C	-0.30252000	-2.92411200	4.53674000	C	-4.23071400	1.02481300	-1.56237900
C	1.33635300	-1.38975700	5.65245600	C	-2.85332400	1.81125100	-3.51292900
H	1.47338600	-2.13779600	3.62899200	H	-2.46959000	-0.89377700	-3.85256300
H	-0.77559100	-3.21867100	3.59657600	H	-3.45048100	-1.44458100	-2.48118700
H	0.20281400	-3.80140800	4.95445300	H	-4.21837800	-0.58611800	-3.83264900
H	-1.08905700	-2.61305800	5.23188300	H	-4.03457600	1.95882000	-1.02603100
H	2.06817300	-0.58428500	5.53699100	H	-5.16392200	1.14109600	-2.12450000
H	0.56611900	-1.04069400	6.34785400	H	-4.37196000	0.22810400	-0.82491700
H	1.84460600	-2.24827000	6.10364700	H	-3.73747600	1.93821500	-4.14735900
C	-1.93569100	1.21870100	2.66725700	H	-2.65711400	2.76023500	-3.00431600
C	-1.79018700	1.96465300	3.99525600	H	-1.99770400	1.58470000	-4.15691600
C	-2.88958000	0.03108600	2.76483800				
H	-2.34870700	1.91711100	1.92882000				
H	-1.14237400	2.84080500	3.88523100				
H	-2.77016000	2.31346000	4.33708100				
H	-1.36675100	1.30813900	4.75810300				
H	-2.95961300	-0.49282200	1.80683100				
H	-2.55531800	-0.67626100	3.52555100				
H	-3.88980500	0.38631500	3.03206500				
H	-0.15910700	1.63292100	1.62341600				
C	0.33671800	3.64226500	-0.42790100				
C	1.36786200	4.39605000	0.42314200				
H	1.38342100	5.46520800	0.18336100				
H	1.13279100	4.29568200	1.48885500				
H	2.37240300	3.99551100	0.25242600				
C	-1.06519500	4.20199100	-0.14905600				
H	-1.14229400	5.26086600	-0.42102800				
H	-1.81172300	3.64226400	-0.72073300				
H	-1.30924500	4.10992600	0.91548500				
C	0.67676800	3.80915700	-1.91487200				
H	1.66870800	3.39536500	-2.12148000				
H	-0.05175900	3.27036100	-2.52957100				
H	0.67097400	4.86186200	-2.21933400				
O	0.36446300	2.27095300	-0.09841300				
O	-0.51081400	-1.99449800	-0.28794400				
C	-0.78472800	-3.37204900	-0.22093400				
C	0.36058000	-4.06937000	0.52392200				
C	-2.10988200	-3.58179200	0.52173200				
C	-0.89155600	-3.92807400	-1.64669500				
H	1.30452900	-3.90883600	-0.00727600				
H	0.46301000	-3.65535900	1.53143200				
H	0.19172500	-5.14886300	0.60805200				
H	-2.92297900	-3.07773400	-0.01083300				
H	-2.36244000	-4.64457900	0.60822500				
H	-2.05071300	-3.15726100	1.52877000				

EtOH

H= -154.88845 au	C 3.13311100 1.42451700 -0.28394200 C 3.92112000 2.43419700 -1.09406200 H 4.43962800 1.93793600 -1.92100500 H 3.25094500 3.19034000 -1.51603800 H 4.66506000 2.93738900 -0.46678600 O 2.19156500 0.81043900 -1.14817300 H 1.68856000 0.16698400 -0.63063100 H 3.81864300 0.67754200 0.15192800 H 2.62919000 1.93098100 0.55716300
<i>t</i>BuOH	
H= -233.438507 au	C 3.14643200 1.42482900 -0.24479100 C 4.08387800 0.34876600 0.31269000 H 4.84617900 0.78044200 0.97186200 H 3.52242800 -0.39270700 0.89687500 H 4.58805800 -0.17450500 -0.50671000 C 2.39341700 2.12997000 0.88793200 H 3.08082700 2.64486800 1.56937200 H 1.69435300 2.86601800 0.47692000 H 1.81779900 1.40750000 1.48213900 C 3.92145300 2.43289900 -1.08895000 H 4.42578600 1.92438800 -1.91735300 H 3.23832700 3.17705900 -1.51188400 H 4.67450200 2.95164200 -0.48613800 O 2.21128700 0.82903100 -1.14860500 H 1.69839200 0.17983900 -0.64464900
<i>i</i>Pr-N=C=N-<i>i</i>Pr	
H= -384.317346 au	C 1.12914400 1.19179700 -0.46540600 N 2.23801700 1.09261300 -0.97495800 N 0.00570900 1.44919400 -0.04777500 C 3.48828900 0.66075800 -0.35561100 C 4.07962100 -0.47484800 -1.18991600 C 3.34336600 0.27959600 1.11571900 H 4.16881000 1.52070700 -0.42783700 H 4.16643400 -0.17685700 -2.23808400 H 5.07356400 -0.74630400 -0.82008500 H 3.43905800 -1.36177000 -1.13975100 H 2.92379800 1.10528800 1.69869900 H 2.68388900 -0.58871200 1.22689000 H 4.31728300 0.02099200 1.54330900 C -1.14029500 0.53821600 -0.00861200 C -2.23379300 1.08681700 -0.92321400 C -1.62035900 0.41117500 1.43545100 H -0.84513900 -0.45736200 -0.37185600 H -1.87987300 1.15900100 -1.95552900 H -3.11291000 0.43428300 -0.90337800 H -2.53518100 2.08683300 -0.59580000 H -0.83260000 0.00431000 2.07614800 H -1.90418900 1.39280200 1.82788500 H -2.48979900 -0.25173200 1.49410300
isourea (EtOH)	
H= -539.240420 au	C 1.24808900 1.07189500 -0.63951100 N 2.42254800 1.51264200 -0.84125800 N 0.16935400 1.57929400 -1.35985200 C 3.60863300 0.90149300 -0.24784100 C 3.78613600 -0.58084700 -0.59541300
C 3.68637600 1.14945000 1.26254700 H 4.45427400 1.43503000 -0.70328900 H 3.68880800 -0.73698800 -1.67469500 H 4.78145800 -0.92549000 -0.29337900 H 3.04519300 -1.20129000 -0.08426800 H 3.57167400 2.21604800 1.47977100 H 2.89732700 0.60397400 1.78755800 H 4.65577500 0.82450300 1.65698500 C -1.01297300 2.08087200 -0.64351000 C -2.15707200 2.25293700 -1.63877300 C -0.72278400 3.37393200 0.12392400 H -1.29197300 1.30890400 0.08203700 H -2.36399800 1.31542300 -2.16270800 H -3.06971400 2.57933600 -1.13070700 H -1.90776000 3.01163400 -2.39040200 H 0.10390500 3.23533300 0.82678800 H -0.44780800 4.18091700 -0.56551300 H -1.60200000 3.70066600 0.68969200 H 0.52858200 2.25535600 -2.02568700 O 0.91752500 0.09955000 0.27040200 C 0.14097400 -1.01195700 -0.20334300 C -0.23902200 -1.85277900 0.99643400 H 0.65180900 -2.20423000 1.52463000 H -0.84659400 -1.27495200 1.69914700 H -0.81667500 -2.72543300 0.67620200 H -0.74545200 -0.65784500 -0.73945300 H 0.74797200 -1.59006900 -0.91297200	

H -2.11408700 -1.90244500 -0.15918000
C 0.32231700 -1.71256400 -1.52046600
H 1.39546500 -1.90848500 -1.58419200
H -0.20705900 -2.64562700 -1.73856200
H 0.04957000 -0.97712800 -2.28115000

ad-A (^tBuOH)

H= -1175.904537 au

U 0.13564600 1.22449000 0.02814600
Si 0.73961700 3.47611500 2.13931100
Si 1.63620300 0.79468300 3.46377500
Si -3.22202100 1.03283300 1.52007900
Si -2.94969300 0.26645100 -1.38840000
Si 1.17647200 -2.18473000 -0.79873300
Si 3.30444000 -0.00420900 -0.97598900
N 0.85576100 1.68663800 2.14790200
N -2.14342100 0.72306600 0.12817600
N 1.62877700 -0.47388600 -0.64656900
C 3.84583800 -0.37257200 -2.75983500
H 3.12497900 -0.00000900 -3.49287100
H 4.81705700 0.09117900 -2.96806200
H 3.95851800 -1.44969400 -2.92230100
C 4.60273300 -0.81247000 0.15370900
H 4.87721900 -1.81455700 -0.18541700
H 5.51374500 -0.20254300 0.15074200
H 4.25720000 -0.89266700 1.18761700
C 3.43950600 1.86977800 -0.67403000
H 2.78610000 2.45982500 -1.32415000
H 3.22023500 2.12143800 0.37015300
H 4.46777300 2.19467500 -0.86893100
C -1.65505000 0.23194300 -2.77831700
H -0.77700500 -0.38560100 -2.55983000
H -2.12148200 -0.19896400 -3.67172700
H -1.30911100 1.23453000 -3.03385100
C -4.25901800 1.53460300 -1.92564000
H -4.65401700 1.27011700 -2.91337500
H -5.10633400 1.57910700 -1.23536000
H -3.82724000 2.53852000 -1.99157200
C -3.75688500 -1.45230800 -1.40608000
H -4.59807300 -1.53681100 -0.71583000
H -4.13532400 -1.64601500 -2.41695400
H -3.03918900 -2.24115400 -1.16457200
C -2.35882000 0.59102800 3.14224500
H -2.17551400 -0.48745600 3.19487000
H -1.40184600 1.10747200 3.24298400
H -2.99495800 0.86531300 3.99126200
C -4.82032400 0.00065200 1.51773600
H -5.38202900 0.26463900 2.42196200
H -5.47670800 0.18792000 0.66329900
H -4.60983800 -1.07198600 1.56401600
C -3.75544000 2.85547100 1.55687700
H -4.34611100 3.06938600 2.45498100
H -2.89627600 3.53253900 1.55273000
H -4.37215300 3.09812200 0.68570300
C 0.18587200 3.75957900 0.35695400
H 0.85240400 4.52507500 -0.06412800
H 0.34945400 3.40058300 -1.52413100
H -0.83894800 4.15700800 0.31894200
C -0.47887000 4.14962000 3.43093300
H -0.10857700 4.00488700 4.45042200
H -0.61491800 5.22599900 3.27456300
H -1.45999900 3.67290400 3.36184800

C 2.40007100 4.34117100 2.46366200
H 3.18657000 4.00660700 1.78109000
H 2.27051100 5.42093200 2.32457600
H 2.74896100 4.18207600 3.48886000
C 1.33062800 -1.06202300 3.25364900
H 0.26486300 -1.30094800 3.32288300
H 1.70226700 -1.40885100 2.28498600
H 1.85123800 -1.62466600 4.03628700
C 0.98490200 1.30647600 5.17394000
H 1.26898200 2.33327100 5.42517100
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H 3.76677500 2.09728700 3.79406700
C 0.88212100 -2.73052500 -2.59831200
H 0.04286900 -2.22221200 -3.07996300
H 1.77098500 -2.55887400 -3.21294300
H 0.67043600 -3.80623200 -2.61683000
C 2.47764300 -3.40214600 -0.13299500
H 3.36672100 -3.45844900 -0.76822900
H 2.79841700 -3.16263100 0.88449800
H 2.02782000 -4.40210000 -0.11391400
C -0.39984100 -2.52572100 0.20677600
H -0.83914900 -3.47521800 -0.12052900
H -0.15925600 -2.62465700 1.26955300
H -1.17373200 -1.75715900 0.11411000
O 0.43797600 2.71341800 -2.23426800
C 0.61350500 3.34513700 -3.53296900
C 1.69016200 4.42519500 -3.41037200
C 1.05418900 2.25663300 -4.50268000
C -0.71792000 3.96748100 -3.95866000
H 1.39550000 5.19544100 -2.68921400
H 2.64210000 3.99477500 -3.08756600
H 1.84757400 4.91697100 -4.37545700
H 0.31232000 1.45677600 -4.56483100
H 1.18921200 2.67775600 -5.50361200
H 2.00440300 1.82244000 -4.18217400
H -0.61766700 4.46008600 -4.93132600
H -1.49962300 3.20765100 -4.04132000
H -1.04565900 4.71913100 -3.23286500

TS_{ad-IA} (^tBuOH)

H= -1170.833493 au

U 0.37125700 1.22162700 0.09512400
Si 0.15487800 4.32560400 1.44960000
Si 1.95162200 2.76018200 3.29224200
Si -2.34488000 -0.33339000 1.34909700
Si -3.28050500 1.32714200 -1.04345200
Si 1.16273500 -1.98954000 -1.83223000
Si 3.47742600 -0.96828900 -0.09607300
N 0.94009400 2.81047300 1.85018600
N -2.00628800 0.75692100 0.02648400
N 1.93424100 -0.67734700 -0.91470800
C 4.80529800 -1.82063600 -1.15655500
H 4.92662300 -1.34594400 -2.13493700
H 5.76851400 -1.76693600 -0.63569700
C 3.29993800 -2.03891600 1.46555200
H 3.07165700 -3.07748400 1.20760800
H 4.24163300 -2.03872700 2.02649600

H	2.51434300	-1.68859100	2.14162900	H	-1.15784900	-0.96034400	-1.76962800
C	4.19854200	0.72016500	0.39911900	H	-0.31384500	-0.58157200	-3.28284800
H	4.61028000	1.23546400	-0.47447900	O	1.66856500	1.56837200	-1.97499800
H	3.47410800	1.39822400	0.86404800	H	1.99364600	0.51065500	-1.72073500
H	5.01381700	0.58429300	1.11806200	C	2.32062200	2.30000800	-3.02579100
C	-2.53991800	1.92707900	-2.69103600	C	3.30561600	1.37688800	-3.74515700
H	-2.05754100	1.10492600	-3.22837900	H	2.78413000	0.52485500	-4.19045500
H	-3.33994100	2.31600000	-3.33125200	H	3.82001600	1.91564700	-4.54718800
H	-1.80727000	2.73132700	-2.57080100	H	4.06404500	0.99592800	-3.05458200
C	-4.26975200	2.77092300	-0.29366900	C	1.25072200	2.78740500	-4.00448600
H	-5.04393600	3.10724700	-0.99318300	H	0.52761300	3.43588000	-3.50036500
H	-4.76804000	2.46693800	0.63271300	H	1.70123900	3.35849200	-4.82329400
H	-3.63738500	3.63243900	-0.05804600	H	0.70713100	1.94051800	-4.43312800
C	-4.55753700	-0.00694700	-1.50153400	C	3.06573500	3.48885600	-2.41301100
H	-4.08222500	-0.90148700	-1.91549300	H	2.37449200	4.15678000	-1.88983300
H	-5.16622100	-0.31099600	-0.64382000	H	3.81552800	3.14788600	-1.69361500
H	-5.24110200	0.39114400	-2.26040100	H	3.57343100	4.07326000	-3.18754200
C	-0.66240200	-0.65388300	2.23332200				
H	0.08854600	-1.17481100	1.61743200				
H	-0.22062400	0.23777000	2.69990600				
H	-0.85589200	-1.34119400	3.06387200				
C	-2.96428400	-2.06033600	0.86016300				
H	-2.95541600	-2.72175400	1.73437500				
H	-3.98690100	-2.03372100	0.47496100				
H	-2.32920300	-2.50934200	0.09045400				
C	-3.51888200	0.35635700	2.67017500				
H	-3.60952000	-0.33300700	3.51723100				
H	-3.16595700	1.32016200	3.04963100				
H	-4.52271600	0.50644700	2.25878800				
C	-0.51262400	4.15983300	-0.34402700				
H	-0.92579900	5.13012100	-0.64060800				
H	0.24981100	3.92435200	-1.09922500				
H	-1.35342700	3.45900300	-0.42539600				
C	-1.37268600	4.74263000	2.49693800				
H	-2.08876600	3.91463600	2.48748000				
H	-1.10946700	4.94537900	3.53875700				
H	-1.88024600	5.63083300	2.10271300				
C	1.29151100	5.84773900	1.43391900				
H	2.17531800	5.68050600	0.81039000				
H	0.75215500	6.71499500	1.03566400				
H	1.63436900	6.10951500	2.43990800				
C	2.29736300	0.97350100	3.84496800				
H	1.40181300	0.47083900	4.22335600				
H	2.72964900	0.35505700	3.05295900				
H	3.02589100	0.99440400	4.66376600				
C	1.15832100	3.61765200	4.79659900				
H	1.05014700	4.69780600	4.65337800				
H	0.16892000	3.20583800	5.02027300				
H	1.79027100	3.46925900	5.68005300				
C	3.65158300	3.58038600	3.04079000				
H	4.21530400	3.11281300	2.22783600				
H	3.55776400	4.64555100	2.81043800				
H	4.24880500	3.49007700	3.95590400				
C	2.16695900	-2.57781500	-3.33590900				
H	3.08385000	-3.10282500	-3.05678400				
H	1.55480300	-3.26954200	-3.92647200				
H	2.44304100	-1.74360200	-3.98786500				
C	0.81516100	-3.52673100	-0.77033400				
H	1.73852800	-4.04814600	-0.49839000				
H	0.28362300	-3.28389700	0.15493400				
H	0.19580100	-4.23376300	-1.33410400				
C	-0.48335200	-1.36258300	-2.53391000				
H	-1.00382300	-2.18796800	-3.03299000				

C	2.16463100	-0.34274100	3.39759600	H	3.65767400	-2.63914600	1.12663600
H	1.16831200	-0.68979800	3.69529600	H	3.01147800	-4.27110100	0.87610600
H	2.39607500	-0.75748000	2.40888900	C	0.38286900	-2.46561900	1.55181900
H	2.88357500	-0.77265500	4.10381100	H	0.28009000	-3.45956600	2.00089300
C	1.83658000	2.14404100	5.16651400	H	0.83967400	-1.83018400	2.32332100
H	1.95586300	3.22763700	5.27468800	H	-0.63883600	-2.11326900	1.35383300
H	0.80458300	1.88992900	5.42879800	C	-3.20523600	0.50803400	0.63663500
H	2.49779700	1.66783900	5.89944900	O	-1.81528800	0.66965000	0.52325700
C	4.06415400	2.04698700	3.05836600	O	1.27453500	1.29041200	2.59300800
H	4.74383700	1.60065100	3.79327200	C	1.80214600	1.48056400	3.87984900
H	4.37779100	1.70964000	2.06477800	C	0.95231200	0.70658600	4.89677900
H	4.19768700	3.13293000	3.09752500	C	3.24908500	0.96873700	3.90718400
C	0.06259800	-3.24796900	-1.84273700	C	1.77073600	2.97983500	4.20835700
H	-0.85475800	-2.66293200	-1.97039600	H	-0.08450500	1.05741100	4.86840700
H	0.63372100	-3.18037900	-2.77403500	H	0.95770000	-0.36263400	4.65988500
H	-0.22617300	-4.29605500	-1.70316800	H	1.32935400	0.83093800	5.91810800
C	2.59496300	-3.73028100	-0.16914900	H	3.85475500	1.51175400	3.17383000
H	3.22456200	-3.71307400	-1.06567900	H	3.70888500	1.09581800	4.89381500
H	3.21058900	-3.41773100	0.68044500	H	3.27759000	-0.09514700	3.64947100
H	2.29350200	-4.77052200	-0.00129300	H	2.17933700	3.18669100	5.20387600
C	-0.01632200	-2.82679400	1.18906300	H	2.36033800	3.53892700	3.47378200
H	-0.38226400	-3.85671000	1.26576300	H	0.74106700	3.35142400	4.17607000
H	0.54002100	-2.60478300	2.10549400				
H	-0.89633500	-2.17331100	1.15170600				
C	-3.25833000	0.23230100	1.07209400				
O	-1.91628400	0.45162200	0.71182000				

Int-IIA ('BuOH)

H= -799.510442 au

U	0.38051200	0.80409000	0.63809400
Si	1.43924700	-2.54185000	-0.04042800
Si	2.30162700	-0.17792900	-1.96965400
N	1.52777900	-0.90305600	-0.61065500
C	1.64059700	-0.72450200	-3.66119600
H	0.55563900	-0.59236400	-3.72347700
H	2.10335900	-0.15668900	-4.47620400
H	1.85378400	-1.78482100	-3.83199400
C	4.19392000	-0.30872300	-1.98739600
H	4.50615900	-1.35253300	-2.09717600
H	4.62784800	0.25710500	-2.81951400
H	4.62573000	0.06754800	-1.05452500
C	1.91565600	1.72635000	-1.85826500
H	0.85083300	1.98959500	-1.97307700
H	2.33916900	2.23173300	-0.97465000
H	2.40525700	2.21330800	-2.70859500
C	-3.56564800	0.23715700	2.10372200
H	-3.06821000	-0.67382300	2.45344600
H	-3.23410400	1.06925600	2.73393900
H	-4.64544800	0.11099800	2.24124200
C	-3.64648700	-0.67225500	-0.23974200
H	-4.72939600	-0.83283700	-0.19065500
H	-3.37204400	-0.48975200	-1.28386600
H	-3.14936600	-1.59189600	0.08610800
C	-3.88905100	1.79695800	0.15923300
H	-4.98078600	1.72443400	0.21849800
H	-3.56815100	2.64463200	0.77420900
H	-3.61560300	2.00476900	-0.88074500
C	0.58017700	-3.72699500	-1.24933200
H	-0.41220000	-3.35579000	-1.52441700
H	1.16047100	-3.84218000	-2.17107300
H	0.46024800	-4.72265800	-0.80735400
C	3.12646700	-3.28231100	0.41771500
H	3.76233000	-3.39987100	-0.46627900

ad-B ('BuOH)

H= -1170.831886 au

U	0.00605700	0.14314200	-0.00578000
Si	-0.22657000	3.16381100	1.53102800
Si	1.37655400	1.42177600	3.40118600
Si	-2.85179200	-1.31430400	1.22180700
Si	-3.56032600	0.32437000	-1.25292400
Si	0.79332900	-3.19964900	-1.45950800
Si	3.19109700	-1.72597600	-0.26782900
N	0.50764100	1.61275300	1.87890900
N	-2.37335300	-0.29209800	-0.11572400
N	1.50584700	-1.73034400	-0.78193900
C	4.45254000	-2.04232100	-1.66167300
H	4.25394500	-1.43047600	-2.54803900
H	5.45644900	-1.78480600	-1.30362800
H	4.47369100	-3.08758400	-1.97968700
C	3.58227300	-2.99256700	1.09435400
H	3.53215600	-4.01412100	0.70244300
H	4.59564200	-2.83998600	1.48267300
H	2.88513900	-2.92528900	1.93504300
C	3.61802100	0.01818300	0.36757000
H	3.67335200	0.73748600	-0.45643600
H	2.91814200	0.41916100	1.10751900
H	4.60299300	0.00040100	0.84757200
C	-2.69135300	0.85930000	-2.85919900
H	-2.16870400	0.01798800	-3.32573800
H	-3.43211400	1.23173100	-3.57573500
H	-1.97029500	1.66719600	-2.69830500
C	-4.49756500	1.84414800	-0.59399900
H	-5.20942100	2.21062000	-1.34286600
H	-5.06264800	1.60070000	0.31131900
H	-3.82095500	2.66801300	-0.34578100
C	-4.88199500	-0.94434600	-1.76664000
H	-4.43373800	-1.86597200	-2.15046400
H	-5.54766300	-1.20971900	-0.93885400
H	-5.50575300	-0.51800000	-2.56096700
C	-1.26492700	-1.60902300	2.25350000
H	-0.46123000	-2.14636700	1.72698600
H	-0.87096700	-0.67865700	2.68232300
H	-1.51344900	-2.24983200	3.10647500

C	-3.50479400	-3.03191800	0.74021100	U	0.13495900	1.25874300	-0.07351300
H	-3.56807300	-3.66991300	1.62954100	Si	0.63222000	3.62797100	1.99381700
H	-4.50482000	-2.97611400	0.30175300	Si	1.73053300	1.02699000	3.32209400
H	-2.85037100	-3.52604700	0.01614200	Si	-3.16563100	0.83057900	1.47696800
C	-4.11807700	-0.54146500	2.40781200	Si	-2.91068000	0.28129300	-1.49314600
H	-4.29122000	-1.19978000	3.26694200	Si	0.97083800	-2.26010000	-0.72493300
H	-3.77478700	0.42636800	2.78615000	Si	3.22197200	-0.22365900	-0.94263400
H	-5.08343300	-0.38650800	1.91458100	N	0.87544700	1.85350100	2.00577800
C	-0.59615200	3.20832700	-0.35708800	N	-2.10408200	0.67133800	0.04516500
H	-0.93105400	4.22041200	-0.61049600	N	1.51328700	-0.56568100	-0.60277100
H	0.29264000	3.02525000	-0.97550400	C	3.72059100	-0.71347000	-2.70946000
H	-1.41879000	2.55673300	-0.68198300	H	3.05008700	-0.27594200	-3.45532600
C	-1.89354500	3.46166500	2.38659400	H	4.73959000	-0.37252800	-2.92598300
H	-2.59683400	2.65753400	2.14834400	H	3.70448800	-1.80023400	-2.84382900
H	-1.78261900	3.49906900	3.47419100	C	4.46509200	-1.04761000	0.23658100
H	-2.34075900	4.40866900	2.06284900	H	4.67153200	-2.08643500	-0.03099100
C	0.86937500	4.68442500	1.84547100	H	5.41366200	-0.49975500	0.18908800
H	1.84109300	4.59408600	1.35017800	H	4.12228100	-1.02954300	1.27469000
H	0.37306500	5.58359000	1.46216800	C	3.50395500	1.64776900	-0.74864500
H	1.04931100	4.84197800	2.91353000	H	2.88519500	2.24815800	-1.42109500
C	1.76706400	-0.40611200	3.76558500	H	3.33404600	1.98542900	0.27982600
H	0.88209800	-0.97267100	4.06760400	H	4.55052800	1.86969100	-0.98690600
H	2.22957300	-0.92291900	2.91925400	C	-1.64827700	0.44690400	-2.90514000
H	2.48249700	-0.45112300	4.59482200	H	-0.72995600	-0.13598300	-2.77080700
C	0.38926200	2.05343400	4.90310100	H	-2.11807400	0.07036100	-3.82115300
H	0.25062200	3.13958600	4.88495500	H	-1.37198900	1.48796000	-3.07921100
H	-0.60076600	1.58892500	4.95598700	C	-4.31616300	1.48875500	-1.91034300
H	0.92374800	1.80955600	5.82864600	H	-4.70129100	1.27497600	-2.91406500
C	3.05066200	2.32998300	3.43807900	H	-5.15670700	1.41283300	-1.21429600
H	3.71721500	1.99086400	2.63965800	H	-3.96160200	2.52437400	-1.89855100
H	2.93296300	3.41229800	3.33691000	C	-3.59276500	-1.48563300	-1.61885300
H	3.55114600	2.13828600	4.39462100	H	-4.40299000	-1.68343300	-0.91399900
C	1.90404300	-4.12211000	-2.70156300	H	-3.98892800	-1.63461800	-2.63051300
H	2.75377500	-4.60990500	-2.21387500	H	-2.81178900	-2.23328700	-1.45545400
H	1.31170400	-4.90707900	-3.18618400	C	-2.22478100	0.39931300	3.05900000
H	2.29375000	-3.46738300	-3.48702400	H	-1.93915000	-0.65763500	3.06221600
C	0.32266900	-4.48920800	-0.14217600	H	-1.32092800	1.00190100	3.17589500
H	1.19318800	-4.80407000	0.44181800	H	-2.87008800	0.57393900	3.92742100
H	-0.42958100	-4.11415600	0.55795000	C	-4.66319100	-0.34039700	1.45048200
H	-0.09441500	-5.38154500	-0.62356600	H	-5.22820200	-0.17997400	2.37648100
C	-0.78732100	-2.73392600	-2.40638600	H	-5.34901600	-0.16294500	0.61755900
H	-1.29151600	-3.64062100	-2.75976500	H	-4.35795100	-1.39091300	1.42945700
H	-1.50216800	-2.17980100	-1.78708000	C	-3.84866800	2.59513100	1.62436200
H	-0.55328100	-2.12330400	-3.28520000	H	-4.48232400	2.68384400	2.51428400
O	1.14151300	0.53695400	-2.32856400	H	-3.04912700	3.33659600	1.71089700
H	1.52574300	-0.36433600	-2.13401600	H	-4.45603100	2.86009600	0.75362400
C	1.68712100	1.11357500	-3.54698800	C	-0.11972900	3.89944800	0.28584900
C	1.77196700	0.01439400	-4.60519400	H	0.24476300	4.88007800	-0.05026000
H	0.78267500	-0.40665200	-4.80555200	H	0.26750700	3.42684300	-1.16313800
H	2.16931200	0.41680900	-5.54206700	H	-1.21474900	3.98903900	0.34858200
H	2.43474100	-0.79515100	-4.28212200	C	-0.49826800	4.23907900	3.39308500
C	0.72846500	2.21029300	-3.99432000	H	-0.01061900	4.19948500	4.37142200
H	0.63294400	2.98847100	-3.23166900	H	-0.77474300	5.28191200	3.19918100
H	1.10340800	2.68168300	-4.90779900	H	-1.42024400	3.65381800	3.45438600
H	-0.26307200	1.80043500	-4.20008100	C	2.26007800	4.59874200	2.12355600
C	3.06789600	1.69561200	-3.24513500	H	2.98291300	4.28810800	1.36299600
H	3.00162500	2.45899900	-2.46386900	H	2.05872600	5.66685200	1.98009900
H	3.76063500	0.91819900	-2.90986000	H	2.72985700	4.48419500	3.10557100
H	3.49214100	2.16120800	-4.14054200	C	1.47628300	-0.84667400	3.20161000
				H	0.44277300	-1.12412400	3.42984500
				H	1.72102800	-1.21614700	2.20172400
				H	2.12483900	-1.35882500	3.92114700
				C	1.12656000	1.57399400	5.03865000

TS_{ad-IB} ('BuOH)
H= -1175.905633 au

H	1.42425600	2.60159300	5.26889600	H	-4.52821700	1.33485600	-3.21785800
H	0.03987900	1.50241800	5.13824800	H	-5.00364800	1.50633700	-1.52631800
H	1.57677100	0.92510300	5.79899500	H	-3.76755000	2.57603000	-2.20682600
C	3.60132300	1.35917400	3.29374500	C	-3.55312800	-1.43561800	-1.84589400
H	4.08257500	0.80456600	4.10799900	H	-4.50160300	-1.52284800	-1.31115500
H	4.06679500	1.04134400	2.35718800	H	-3.74677900	-1.66949500	-2.89955200
H	3.82792500	2.41945000	3.43774900	H	-2.87583900	-2.20065500	-1.45574800
C	0.47271100	-2.74058700	-2.49742100	C	-2.08828600	0.40015300	2.82267700
H	-0.46441400	-2.27781300	-2.81826800	H	-1.78473100	-0.65121800	2.84973800
H	1.24787300	-2.46489600	-3.21919800	H	-1.19316900	1.02184700	2.91410500
H	0.33571700	-3.82681900	-2.55454700	H	-2.71773100	0.58504500	3.70077500
C	2.28334300	-3.53659100	-0.21327100	C	-4.50512100	-0.48588900	1.24038800
H	3.12974300	-3.57931100	-0.90517900	H	-5.01731000	-0.41784900	2.20752400
H	2.66981000	-3.36274600	0.79463200	H	-5.24858900	-0.28288400	0.46424100
H	1.80646200	-4.52405800	-0.22083700	H	-4.15304000	-1.51456500	1.12251300
C	-0.50837500	-2.57028000	0.42364000	C	-3.90701400	2.47429700	1.44813900
H	-0.96315000	-3.53590500	0.17394000	H	-4.60974500	2.44574100	2.28918400
H	-0.18065500	-2.61867400	1.46651700	H	-3.18811900	3.27297300	1.64771700
H	-1.28579900	-1.80441200	0.34745700	H	-4.47219000	2.74887300	0.55224600
O	0.51332400	2.76148000	-2.01099100	C	-0.62762300	4.42129700	0.60374600
C	0.80306600	3.45289200	-3.24727300	H	-1.07477800	5.38630400	0.86862700
C	1.88841300	4.50269800	-2.98759900	H	-0.00622700	4.57239700	-0.27935900
C	1.29068000	2.42122600	-4.25971700	H	-1.45911100	3.76171600	0.32835400
C	-0.47528300	4.14163500	-3.73489400	C	-0.75177500	4.05078900	3.59779600
H	1.55678300	5.23356100	-2.24358500	H	-0.22915800	3.95143700	4.55115700
H	2.80933700	4.03813400	-2.62544700	H	-1.17711800	5.06066100	3.55732400
H	2.12148600	5.04394200	-3.91035600	H	-1.58361300	3.34090900	3.59247200
H	0.53340500	1.65230300	-4.43363100	C	1.85244700	5.00910800	2.28693500
H	1.51379200	2.90411300	-5.21674200	H	2.53584000	4.93689100	1.43491900
H	2.20316900	1.93475400	-3.90424600	H	1.49430600	6.04328500	2.34693700
H	-0.28093200	4.70329400	-4.65458800	H	2.42611700	4.80834100	3.19759400
H	-1.26391600	3.41418200	-3.94553800	C	1.74318500	-0.49897000	3.00923500
H	-0.84773900	4.84297500	-2.98163300	H	0.74625000	-0.78066800	3.36264200
				H	1.89074900	-0.92510500	2.01290100
				H	2.47599300	-0.95714600	3.68321400
Int-IB (^tBuOH)				C	1.57175100	1.91355100	4.81959200
<i>H= -1175.959252 au</i>				H	1.79875400	2.96526100	5.01839700
U	0.26198300	1.15830600	-0.21257400	H	0.52933200	1.72608000	5.09206900
Si	0.38656100	3.81726500	2.09399600	H	2.20257400	1.31434500	5.48708100
Si	1.95788700	1.38432400	3.03475700	C	3.79627300	1.78558500	2.76693200
Si	-3.08195700	0.77367500	1.25159400	H	4.38436900	1.38339200	3.60017300
Si	-2.79750000	0.30620700	-1.74145000	H	4.19465200	1.35283800	1.84559600
Si	0.81511400	-2.45268300	-0.56171200	H	3.96689300	2.86581800	2.73099500
Si	3.18833900	-0.60495300	-1.05494800	C	0.19576800	-3.03009000	-2.26271500
N	0.90718300	2.14049400	1.80616000	H	-0.66671200	-2.45991000	-2.61691200
N	-2.02581600	0.68880400	-0.18442500	H	0.98196200	-2.95449400	-3.01996400
N	1.48000100	-0.79724500	-0.59813000	H	-0.10799400	-4.08180900	-2.20228200
C	3.55774300	-1.29099700	-2.78598400	C	2.05795000	-3.77589800	0.00159600
H	2.88720600	-0.85808300	-3.53499000	H	2.86940300	-3.93754400	-0.71439600
H	4.58802600	-1.05564300	-3.07634900	H	2.49697700	-3.54931300	0.97714000
H	3.44794500	-2.37950500	-2.82404800	H	1.51429900	-4.72381700	0.09397600
C	4.43408400	-1.38320000	0.15170100	C	-0.62595300	-2.54743800	0.66583800
H	4.46181100	-2.47334800	0.09553900	H	-1.11804900	-3.52275900	0.57744600
H	5.43552800	-1.01418900	-0.10029200	H	-0.26782900	-2.44874300	1.69532300
H	4.23030000	-1.10313400	1.18917300	H	-1.37797900	-1.77444800	0.48275600
C	3.61766900	1.24785900	-1.08460000	O	0.65726400	2.54849800	-1.79674100
H	3.15389900	1.76539500	-1.92490100	C	0.92215900	3.46324900	-2.85152600
H	3.35423000	1.78521600	-0.16569900	C	1.98734600	4.46975700	-2.39670300
H	4.70435700	1.34137500	-1.19298500	C	1.43165600	2.69347500	-4.07750800
C	-1.49023800	0.37193300	-3.12138500	C	-0.36987200	4.20849200	-3.21322300
H	-0.61300100	-0.26131600	-2.94495100	H	1.63761500	5.05244000	-1.53963300
H	-1.95611000	0.00226200	-4.04219500	H	2.90799500	3.95735600	-2.10508400
H	-1.14334600	1.38848800	-3.31123600	H	2.22678200	5.16983300	-3.20427100
C	-4.15132900	1.55093300	-2.21160800				

H 0.70285800 1.94378200 -4.39687900
H 1.60896500 3.37610500 -4.91549600
H 2.37253200 2.18066200 -3.85789400
H -0.18664800 4.93378100 -4.01318600
H -1.14009900 3.51323600 -3.55944000
H -0.76396300 4.74734600 -2.34748100

Int-IIIB (^tBuOH)

H= -1107.056407 au

U 0.52308800 1.15579800 0.01442500
Si 1.30494200 4.18272300 1.90292200
Si 1.37662600 1.46308200 3.33460700
Si 1.12050900 -2.30105600 -1.01708600
Si 3.46416600 -0.30993700 -1.00010000
N 1.22630300 2.41289000 1.85788200
N 1.78721800 -0.70586200 -0.63216300
C 3.93212300 -0.63181000 -2.81140300
H 3.26329700 -0.08677900 -3.48540000
H 4.95686900 -0.29810600 -3.01029600
H 3.87557000 -1.69343400 -3.07062700
C 4.72372400 -1.17325100 0.12651500
H 4.75312900 -2.25360300 -0.03876700
H 5.72949100 -0.77975000 -0.06101900
H 4.48803900 -1.00044100 1.18176500
C 3.68450800 1.56417200 -0.70390700
H 3.09736800 2.18753700 -1.38951500
H 3.47479700 1.87801700 0.32695300
H 4.73552200 1.81311300 -0.88962100
C 2.07025100 4.84934300 0.30052600
H 2.01468700 5.94380100 0.28848400
H 3.12402700 4.56543000 0.21568600
H 1.54572500 4.47518400 -0.58355000
C -0.43582400 4.92569700 2.07120300
H -0.92238100 4.59148800 2.99331000
H -0.39554200 6.02079200 2.09029600
H -1.07480200 4.63301500 1.23076500
C 2.37003800 4.86229300 3.32263700
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H 2.35962800 5.95758300 3.27841900
H 2.00883700 4.57243800 4.31370300
C 0.93220300 -0.34093100 2.89468000
H -0.11301200 -0.46595100 2.58596600
H 1.58224900 -0.78556400 2.13011500
H 1.05912000 -0.95207500 3.79546400
C 0.17187400 1.99830100 4.70119900
H 0.37583000 3.01202700 5.05931500
H -0.86057500 1.97289200 4.33771500
H 0.24362100 1.32365700 5.56185400
C 3.13533700 1.42568100 4.04611600
H 3.19510600 0.70527200 4.87003900
H 3.86124600 1.12449600 3.28382400
H 3.44130400 2.40097600 4.43426600
C 0.30712500 -2.28043700 -2.73380800
H -0.49894900 -1.53966800 -2.77735700
H 1.03398700 -2.02858900 -3.51282300
H -0.12550700 -3.25684900 -2.97966800
C 2.41251700 -3.69493800 -0.99549900
H 3.21228800 -3.55756400 -1.72931500
H 2.86998000 -3.80022200 -0.00687200
H 1.91326800 -4.64220700 -1.23050400
C -0.20433300 -2.78429000 0.25137500
H -0.70536200 -3.70616700 -0.06500200
H 0.23628100 -2.96295000 1.23730400

H -0.96518600 -2.00506600 0.35562500
O 0.32597000 2.44800000 -1.67463200
C -0.00896300 3.00099200 -2.93565900
C 1.27640400 3.48141000 -3.61735500
C -0.68357400 1.92047100 -3.78693100
C -0.96499000 4.17704300 -2.71237600
H 1.78028400 4.23291300 -3.00205500
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H -0.01106300 1.06714300 -3.92101300
H -1.25030200 4.64101500 -3.66257100
H -1.87636300 3.83593800 -2.21112500
H -0.49417100 4.94008200 -2.08535300
O -1.49238900 0.54661300 0.37085200
C -2.89491700 0.50580300 0.56811600
C -3.18412800 -0.23411000 1.87829500
C -3.42573100 1.94078800 0.64443200
C -3.53177300 -0.23481600 -0.61222000
H -2.78542800 -1.25244300 1.84013000
H -2.72002500 0.28676000 2.72172100
H -4.26137500 -0.29518900 2.06644400
H -3.21674200 2.47606200 -0.28754600
H -4.50844900 1.95532000 0.80919700
H -2.94714100 2.48060600 1.46776000
H -4.62051800 -0.28731400 -0.50475200
H -3.30508900 0.28006800 -1.55121900
H -3.14420600 -1.25576000 -0.67860400

Int-IIIIB (^tBuOH)

H= -1038.134948 au

U 0.48389400 1.02585300 -0.16328200
Si 0.74415200 -2.51188800 -0.83868100
Si 3.30822800 -0.76372800 -0.96222600
N 1.58568700 -0.96667200 -0.67461900
C 3.82080300 -1.15895700 -2.74598900
H 3.24956600 -0.55007600 -3.45418100
H 4.88540100 -0.95056900 -2.90183300
H 3.64957000 -2.21054100 -2.99621700
C 4.41033000 -1.73623200 0.23679900
H 4.35722600 -2.81424500 0.06323200
H 5.45692000 -1.43174900 0.12148400
H 4.11547800 -1.54512100 1.27373300
C 3.70554700 1.08298500 -0.66674000
H 3.17235000 1.76060800 -1.34544000
H 3.52289700 1.39975700 0.36796000
H 4.77361700 1.24169600 -0.85317500
C -0.29676600 -2.52123800 -2.42781500
H -1.02960600 -1.70672700 -2.42953100
H 0.34002500 -2.40086700 -3.31057800
H -0.84891100 -3.46171900 -2.53590700
C 1.88852500 -4.02771400 -0.89123700
H 2.62962800 -3.97945000 -1.69478600
H 2.41768200 -4.16827300 0.05593600
H 1.27783200 -4.92165000 -1.06355100
C -0.41314300 -2.74384800 0.64788800
H -0.99970900 -3.66417500 0.54917800
H 0.15997700 -2.80883500 1.57913700
H -1.11653600 -1.90927100 0.73548600
O 0.66873000 2.46949100 -1.73932700
C 0.69502800 3.46558200 -2.73903400
C 1.62936300 4.59384700 -2.28829000

C	1.20652500	2.83713000	-4.04031600
C	-0.72674000	4.00348500	-2.93495300
H	1.27798400	5.02258700	-1.34430900
H	2.64381800	4.21280600	-2.13416300
H	1.67438300	5.39523100	-3.03367800
H	0.54855900	2.01942500	-4.35146000
H	1.24593000	3.57375000	-4.85007300
H	2.21293300	2.43111000	-3.89736200
H	-0.75845400	4.77303200	-3.71385400
H	-1.40168800	3.19232400	-3.22629000
H	-1.09828200	4.44360200	-2.00385000
O	-1.60769500	0.62515400	0.02370800
C	-3.00663300	0.74947700	0.19655900
C	-3.38406100	0.17711900	1.56696100
C	-3.38489500	2.23270700	0.12083500
C	-3.70206200	-0.03407200	-0.92115400
H	-3.11209900	-0.88086500	1.63011600
H	-2.85594600	0.71506900	2.36060600
H	-4.46050600	0.26499500	1.74959700
H	-3.09514900	2.65054500	-0.84845200
H	-4.46346400	2.37550200	0.24681700
H	-2.87308300	2.79675500	0.90806600
H	-4.79191000	0.02312300	-0.82768300
H	-3.42003800	0.36876400	-1.89924600
H	-3.40825800	-1.08740400	-0.88584600
O	1.12185100	1.82647200	1.71956200
C	1.44278300	2.39658200	2.96985000
C	0.15262000	2.55285700	3.78264000
C	2.41652800	1.46245600	3.69702500
C	2.09144200	3.76500200	2.73463300
H	-0.55260100	3.20225700	3.25368100
H	-0.32265900	1.57795300	3.93118000
H	0.35070600	2.99163200	4.76649000
H	3.33585300	1.34149600	3.11525600
H	2.68517500	1.85545600	4.68356600
H	1.96414700	0.47479500	3.83152500
H	2.35826600	4.24793100	3.68094500
H	3.00129400	3.65692000	2.13581500
H	1.40281400	4.42347400	2.19532500

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