Supporting Information for the Paper Entitled "Understanding Competitive Dehydroalkoxylation and Dehydrogenation of Ethers with Ti−C Multiple Bonds."

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Experimental Section.

I. General considerations. Unless otherwise stated, all operations were performed either in double or single M. Braun Lab Master glove-boxes under purified nitrogen or argon atmospheres or using high vacuum standard Schlenk techniques in vacuum/gas double-manifold glass lines, under argon. All glassware used was flame- or oven-dried overnight at 145 °C and cooled under dynamic vacuum before use. Celite, alumina and molecular sieves used were first activated at 250 ºC under vacuum for at least 24 h.

II. Materials and methods. Anhydrous hydrocarbon solvents (benzene, toluene, *n*-hexane and *n*-pentane) were purchased from Aldrich in 20 L stainless-steel sure-sealed reservoirs and dispensed by passage through activated alumina and Q-5 drying agent columns installed in an M. Braun solvent purifier system (MB-SPS). Tetrahydrofuran (THF, J.T. Baker) and diethyl ether (Et_2O, Aldrich) were purchased anhydrous and further dried and distilled from sodium/benzophenone ketyl solutions.[1] Absolute, anhydrous methanol (MeOH, Mallinckrodt), ethanol (EtOH, Pharmco-Aaper), 1-propanol (^{n}PrOH, Mallinckrodt), 1-butanol (^{n}BuOH, Mallinckrodt) and 2-propanol (^{i}PrOH, Macron Chemicals) were stirred over CaH_2 for 1 day, distilled under argon and used immediately. Di-*n*-propyl ether ($^n Pr_2O$, Acros), di-*n*-butyl ether ($n Bu_2O$, Aldrich), methyl *tert*-butyl ether (^{t}BuOMe, J.T. Baker), ethyl *tert*-butyl ether (^{t}BuOEt, Aldrich) and di-*iso*-propyl ether ($^i Pr_2O$, Sigma-Aldrich) were purchased in high purity grade, degassed by three consecutive freeze-pump-thaw (FTP) cycles and then stored over sodium and 4 Å molecular sieves in a glovebox for at least 24 h before use. C_6D_6 (CIL), THF-d_8 (CIL) and diethyl ether-d_{10} (Et_2O-d_{10}, 99 %D, Acros) were also degassed by FTP and stored over sodium and molecular sieves, prior to use. [(PNP)Ti=CH^{t}Bu(OTf)] (PNP = N[2-P($CHMe_2$)$_2$-4-methylphenyl]$_2^-$, OTf = $[OSO_2CF_3]^-$) and [(PNP)Ti=CH^{t}Bu($CH_2{}^t$Bu)] were prepared according to the literature procedures.[2] Sodium methoxide (NaOMe), ethoxide (NaOEt), *n*-propoxide (NaO^{n}Pr), *n*-butoxide (NaO^{n}Bu) and *iso*-propoxide (NaO^{i}Pr) were prepared from their respective

freshly distilled alcohols (~40 mL; *vide supra*), slowly added to stirred pentane suspensions of sodium under argon. After reaction (~12 h), the remaining alkoxide solutions were taken to dryness under high dynamic vacuum (≤60 mTorr) and the remaining solids further dried *in vacuo* for 24 h under mild heating, to ensure complete evaporation of trace alcohol.[3] Sodium *tert*-butoxide (NaO^tBu) and phenyl silane ($PhSiH_3$) were purchased from Aldrich in reagent grade and used as received. $LiCH_2{}^tBu$ and KCH_2Ph were prepared following the reported procedures.[4] Ethylene (C_2H_4, 99.5+%) was purchased anhydrous from Aldrich and used as received. All other chemicals, chromatographic materials and filter aids were purchased in high purity grade and used without further purification.

III. Characterization. Unless otherwise stated, the NMR spectroscopic characterization of all air and moisture sensitive compounds was done in solution using sealed J-Young NMR tubes under argon. All 1D (^1H, $^{31}P\{^1H\}$, $^{13}C\{^1H\}$, DEPT-135, 1D-gHSQC) and 2D NMR spectra (gCOSY, dqCOSY, 2D-gHSQC and multiplicity edited gHSQC) were recorded on Varian 300, 400, 500 or 800 MHz NMR spectrometers operating at 25 °C. ^1H and $^{13}C\{^1H\}$ chemical shifts are reported referenced to the internal residual solvent resonances. $^{31}P\{^1H\}$ NMR chemical shifts are reported with respect to external H_3PO_4 in aqueous solution (δ 0.0 ppm). NMR data is listed including: 1) the chemical shift, 2) the multiplicity of the peak (*s* = singlet, *d* = doublet, *dd* = doublet of doublets, *ddd* = doublet of doublets of doublets, *t* = triplet, *dq* = doublet of quartets, *m* = multiplet), 3) the *J*-coupling constant values, 4) the integration value and, 5) the chemical assignment. The $^1J_{CH}$ values of alkylidene protons are all reported as measured from the carbon-satellites around the alkylidene peak in the respective ^1H NMR spectra, also confirmed for compounds **1** and **2** by high resolution 1D-gHSQC experiments calibrated for 100 MHz one-bond coupling constants in a 500 MHz spectrometer.

GC/MS analyses of organics were performed by manual injection into an Agilent Technologies

6890N Network GC system equipped with MS detector. Organics from ether activation reactions were first vacuum transferred into separate J-Young NMR tubes charged with C_6D_6 (*vide infra*) and checked by ^{1}H NMR. The Teflon valves in the receiving J-Young tubes were then capped with rubber septa, the valves opened and 10 μL of gas from the headspace removed for injection into the GC/MS using a gas-tight syringe (Hamilton).

CHN analyses of the independently prepared compounds **1**-**7** were performed by Midwest Microlab, LLC. However, with the exception of **2**, the results of these tests were not passing, presumably due to the extreme sensitivity of these compounds. We therefore provide high-resolution NMR spectra for compounds **1**-**7** as proofs of their syntheses, in lieu of these data.

IV. GC/MS method. As indicated above, the headspaces of the NMR tubes with the vacuum-transferred organics were manually injected into a GC/MS. A splitless injection (50 μL) was employed using Helium (1.0 mL/min) as the carrier gas. Separation was achieved using a non-polar Restek RTx-5Sil MS column (Capillary: 30.0 m x 250 μm x 0.25 μm nominal; 350 °C maximum temperature) equivalent to a DB5-MS column. The temperature program for the oven was typically set as follows: 31 °C hold for 5 minutes, ramp at 5 °C/min to 112 °C, and then ramp at 20 °C/min to 290 °C, hold of 9 min.

V. Summary of kinetics experiments. All kinetics measurements were performed using sealed J-Young NMR tubes. The experiments were performed a minimum of two times to ensure consistency of data. Flame-sealed capillaries charged with dilute C_6D_6 solutions of PMe_3 (Aldrich; $^{31}P\{^1H\}$ NMR (162 MHz): δ -61.9 ppm, *s*) were used as internal standards. The tubes were charged in an argon glovebox with neat solutions of [(PNP)Ti=CH^{t}Bu($CH_2{}^t$Bu)] (0.010 g, 0.016 mmol) in the corresponding ether (~0.7 mL) or mixture of ethers (^{t}BuOMe:Et_2O, *vide infra*). The tubes were sealed, taken out from the glovebox and immediately placed in a 400 MHz NMR spectrometer with the probe previously calibrated to

~29 °C. The temperature calibration was done using neat ethylene glycol (100%), prior to each experiment. The reactions were then monitored using arrays of $^{31}P\{^{1}H\}$ NMR spectra (162 MHz; 64 transients, 1.8 s per transient) acquired at fixed intervals of 280 s over a period of 12-14 h after which, ~90 % conversion of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)] to the respective product or mixture of products typically occurred. Reaction rates were determined monitoring the decay of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)] across the arrays, normalizing the integrated spectra relative to the internal reference. The resulting decay curves of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)] were then fit to first-order kinetics plots using the general equation, $\ln[C] = -kt + \ln[C]_0$. At longer times there were more scattered data points due to low resolution due to low concentration of precursor. Unless otherwise stated, the reported rate constants (k_{avg}) are averages of at least two independent runs. The kinetic isotopic effect (KIE = 1.1(0)) is calculated as k_H/k_D of two consecutive, individual runs for Et_2O and Et_2O-d_{10}, respectively. For comparison purposes, the respective measurements using pentane and cyclohexane are also included. **Table S1** summarizes the kinetic data from all runs, including standard deviations (σ) and $t_{1/2}$ values; $t_{1/2} = \ln(2)/k_{avg}$.

Table S1. Summary of reaction kinetics in neat ethers and alkanes

Entry	Substrate	T (°C)	T avg. (°C)	Conv. (%)	Conv. avg. (%)	k x 10^{-5} (s^{-1})	k_{avg} x 10^{-5} (s^{-1})	σ x 10^{-5}	$t_{1/2}$ (h)
1	^{t}BuOMe	29.3		90		5.7			
2	^{t}BuOMe	29.5	29.4	90	90	6.0	5.8	0.2	3.3
3	Et_2O	29.6		97		7.3			
4	Et_2O	29.6	29.6	97	97	6.8	7.0	0.2	2.7
5	Et_2O-d_{10}	29.2		91		6.6			
6	Et_2O-d_{10}	29.2	29.2	90	91	6.2	6.4	0.2	3.0
7	$^{n}Pr_2O$	29.2		83		5.2			
8	$^{n}Pr_2O$	29.7		83		6.2			
9	$^{n}Pr_2O$	29.7	29.5	82	83	6.3	5.9	0.5	3.3
10	$^{n}Bu_2O$	29.2		85		5.0			
11	$^{n}Bu_2O$	29.9	29.6	85	85	5.0	5.0	0.0	3.9
12	^{t}BuOEt	29.5		98		7.6			
13	^{t}BuOEt	29.6	29.6	94	96	7.4	7.5	0.1	2.6
14	$^{i}Pr_2O$	29.5		94		5.5			

15	$^{i}Pr_2O$	29.6	29.6	95	95	6.5	6.0	0.5	3.2
16	^{t}BuOMe:Et_2O	29.4		91		5.3			
17	^{t}BuOMe:Et_2O	29.5	29.5	93	92	6.2	5.7	0.5	3.4
18	Pentane	29.7		89		6.4			
19	Pentane	29.7	29.7	90	90	5.5	6.0	0.5	3.2
20	Cyclohexane	29.6		88		5.0			
21	Cyclohexane	29.7	29.6	89	89	4.9	4.97	0.02	3.9

VI. Composition analyses from ether activation experiments. The composition of the mixtures resulting from the kinetics experiments was analyzed by $^{31}P\{^{1}H\}$ NMR spectroscopy after completion of each experiment. The volatile organics were vacuum-transferred in a Schlenk line to a separate J. Young tube charged with C_6D_6 and checked by ^{1}H NMR and GC/MS. The remaining organometallic residues in the initial NMR tubes recovered in the glovebox, re-dissolved in C_6D_6 and re-examined by NMR comparing the spectra of these residues with those of the independently prepared PNP-titanium(IV) alkoxides, [(PNP)Ti=CH^{t}Bu(OR)] (R = Me, Et, ^{n}Pr, ^{n}Bu, ^{i}Pr, ^{t}Bu), (*vide infra*). The findings for the activation of the neat ethers or their mixtures (e.g., ^{t}BuOMe:Et_2O) after vacuum transfer of the organics are indicated below.

1) Activation of ^{t}BuOMe.

Organometallic product: exclusively [(PNP)Ti=CH^{t}Bu(OMe)] (**2**). $^{31}P\{^{1}H\}$ NMR (25 °C, 162 MHz, MTBE): δ 36.8 (*d*, $^{2}J_{P\text{-}P}$ = 48.1 Hz), 25.3 (*d*, $^{2}J_{P\text{-}P}$ = 48.1 Hz). **Organic product after vacuum transfer:** Isobutene. ^{1}H NMR (25 °C, 400 MHz, C_6D_6): δ 4.70 (*pseudo t*, *J* = 1.2 Hz, 2H, H_2C=C(Me)$_2$), 1.59 (*pseudo t*, *J* = 1.2 Hz, 6H, H_2C=C(*Me*)$_2$). GC/MS: 56 Da ([M^+]); retention time: 3.880-3.921 min.

2) Activation of Et_2O.

Organometallic product: mixture of [(PNP)Ti=CH*t*Bu(OEt)] (**1**) and a minor by-product assigned as [(PNP)Ti(η^2-H_2C=CH_2)(CH_2*t*Bu)] in ~10:1 ratio. $^{31}P\{^{1}H\}$ NMR (25 °C, 162 MHz, Et_2O), for **1**: δ 35.7 (*d*, $^{2}J_{P\text{-}P}$ = 48.0 Hz), 25.8 (*d*, $^{2}J_{P\text{-}P}$ = 48.0 Hz). For [(PNP)Ti(η^2-

$H_2C{=}CH_2)(CH_2tBu)]$: δ 27.8 (*d*, $^2J_{P\text{-}P}$ = 20.9 Hz), 25.5 (*d*, $^2J_{P\text{-}P}$ = 20.9 Hz). **Organic product after vacuum transfer:** Ethylene. ^{1}H NMR (25 °C, 400 MHz, C_6D_6): δ 5.252 (*s*, 4H, $H_2C{=}CH_2$). GC-MS: 28 Da (M^+); retention time: 5.044-5.979 min.

3) Activation of Et_2O-d_{10}.

Organometallic residue: mixture of [(PNP)Ti=CD^{t}Bu(OCD_2CD_3)] and [(PNP)Ti(η^2-D_2C-CD_2)($CD_2{}^t$Bu)] in approximate ratio of 5:1. ^{31}P{^{1}H} NMR (25 °C, 162 MHz, Et_2O-d_{10}), for [(PNP)Ti=CD^{t}Bu(OCD_2CD_3)]: δ 36.52 (*d*, $^2J_{P\text{-}P}$ = 47.9 Hz), 26.65 (overlapping *d*, $^2J_{P\text{-}P}$ = 47.9 Hz). For [(PNP)Ti(η^2-D_2C-CD_2)($CD_2{}^t$Bu)]: δ 28.77 (*d*, $^2J_{P\text{-}P}$ = 20.7 Hz), 26.39 (overlapping *d*, $^2J_{P\text{-}P}$ = 20.7 Hz).

4) Activation of ^{n}Pr$_2$O.

Organometallic residue: complex mixture of [(PNP)Ti=CH^{t}Bu(O^{n}Pr)] (**4**) and two additional by-products assigned as the C-H activation diastereomers, [(PNP)Ti(η^2-$H_2C{=}CH$–CH_2O^nPr)($CH_2{}^t$Bu)] (**5a**, **5b**; 2:1 relative ratio of diastereomers). The total by-product-to-alkoxide ratio was systematically gauged to be ~1:1 by integration of the ^{31}P{^{1}H} NMR spectra of duplicate samples. ^{31}P{^{1}H} NMR (25 °C, 162 MHz, ^{n}Pr$_2$O), for **4**: δ 35.18 (*d*, $^2J_{P\text{-}P}$ = 48 Hz), 25.60 (*d*, $^2J_{P\text{-}P}$ = 48 Hz). For **5a** (major by-product): δ 37.82 (*d*, $^2J_{P\text{-}P}$ = 27 Hz), 28.24 (*d*, $^2J_{P\text{-}P}$ = 27 Hz). For **5b** (minor by-product): δ 37.10 (*d*, $^2J_{P\text{-}P}$ = 26 Hz), 33.56 (*d*, $^2J_{P\text{-}P}$ = 26 Hz). The free organic product from this reaction, propene could not be detected in sufficient concentration to be fully characterized (under these conditions given the large amount of ether used).

5) Activation of ^{n}Bu$_2$O.

Organometallic residue: complex mixture of [(PNP)Ti=CH^{t}Bu(O^{n}Bu)] (**6**) and two meta-stable by-products assigned to C-H activation diastereomers, [(PNP)Ti(η^2-$H_2C{=}CH$–$CH_2CH_2O^n$Bu)($CH_2{}^t$Bu)] (**7a**, **7b**; 3:1 relative ratio). The total by-product-to-alkoxide ratio was

systematically gauged as ~2:1, determined from the $^{31}P\{^{1}H\}$ NMR spectra of duplicate samples. Formation of additional intractable by-products in solution was observed on standing at room temperature. $^{31}P\{^{1}H\}$ NMR (25 °C, 162 MHz, $^{n}Bu_2O$), for **6**: δ 35.09 (*d*, $^{2}J_{P\text{-}P}$ = 48 Hz), 25.57 (*d*, $^{2}J_{P\text{-}P}$ = 48 Hz). For **7a** (major by-product): δ 26.65 (overlapping *d*, $^{2}J_{P\text{-}P}$ = 21.8 Hz), 20.02 (*d*, $^{2}J_{P\text{-}P}$ = 21.8 Hz). For **7b** (minor by-product): δ 26.54 (overlapping *d*, $^{2}J_{P\text{-}P}$ = 20.7 Hz), 20.67 (*d*, $^{2}J_{P\text{-}P}$ = 20.7 Hz). The free organic from this reaction, 1-butene could not be detected in sufficient concentration to be fully characterized, despite repetitive efforts (under these conditions given the large amount of ether used).

6) Activation of ^{t}BuOEt.

Organometallic residue: mixture of **1** and [(PNP)Ti=CH^{t}Bu(O^{t}Bu)] (**3**) in ~1:1 ratio. $^{31}P\{^{1}H\}$ NMR (25 °C, 162 MHz, ^{t}BuOEt). For **1**: δ 35.57 (*d*, $^{2}J_{P\text{-}P}$ = 47.8 Hz), 25.54 (overlapping *d*, $^{2}J_{P\text{-}P}$ = 48 Hz). For **3**: δ 31.56 (*d*, $^{2}J_{P\text{-}P}$ = 46.8 Hz), 25.54 (overlapping *d*, $^{2}J_{P\text{-}P}$ = 48 Hz). **Organic residue after vacuum transfer:** Ethylene and isobutene, confirmed by ^{1}H NMR spectroscopy.

7) Activation of $^{i}Pr_2O$.

Organometallic residue: exclusively [(PNP)Ti=CH^{t}Bu(O^{i}Pr)] (**8**). $^{31}P\{^{1}H\}$ NMR (25 °C, 162 MHz, $^{i}Pr_2O$): δ 34.05 (*d*, $^{2}J_{P\text{-}P}$ = 48.1 Hz), 25.76 (*d*, $^{2}J_{P\text{-}P}$ = 48.1 Hz). **Organic product after vacuum transfer:** Propene. ^{1}H NMR (25 °C, 400 MHz, C_6D_6): δ 5.70 (*m*, H_aH_bC=C*H*(Me)), 5.32 (*m*, *H*$_a$H$_b$C=CH(Me)), 5.11 (*m*, H$_a$*H*$_b$C=CH(Me)). The methyl peak of propene could not be observed due to overlap with the strong methyl peak of $^{i}Pr_2O$, also vacuum transferred mixture. GC-MS: 43 Da ($[M+1]^{+}$); retention time: 1.672-1.722 min.

8) Competing activation of a 1:1 mixture of ^{t}BuOMe:Et$_2$O. An NMR tube was charged with [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)] (0.010 g, 0.016 mmol) and dissolved in a 1:1 mixture of ^{t}BuOMe (0.35 mL, 2.9 mmol) and Et$_2$O (0.30 mL, 2.9 mmol) prior to the kinetics measurement. **Organometallic residue:** mixture of **1** and **2** in 1:1 ratio. $^{31}P\{^{1}H\}$ NMR (25 °C,

162 MHz, ^{t}BuOMe:Et$_2$O), for **1**: δ 36.67 (*d*, $^{2}J_{P\text{-}P}$ = 48 Hz), 25.25 (overlapping *d*, $^{2}J_{P\text{-}P}$ = 48 Hz). For **2**: δ 35.44 (*d*, $^{2}J_{P\text{-}P}$ = 48 Hz), 25.47 (overlapping *d*, $^{2}J_{P\text{-}P}$ = 48 Hz). **Organic residue after vacuum transfer:** Ethylene and isobutene, confirmed by ^{1}H NMR spectroscopy.

VII. Reactions with N_2O: oxidative release of olefins. A series of J. Young tubes charged with degassed, thawing C_6D_6 (~ 0.7 mL) solutions of isolated mixtures resulting from activation of: a) $^{n}Pr_2O$ and b) $^{n}Bu_2O$ were charged with N_2O (~1 atm) to induce oxidative release of vinylic ethers attributed to competing C-H activation of these long-chain ethers. Both mixtures immediately changed from dark brown to dark wine-red. The tubes were placed in a rotator at room temperature for 1h after which, the free organics were vacuum-transferred to empty NMR tubes and analyzed by ^{1}H NMR and GC/MS. The non-volatile organometallic residue was re-dissolved in C_6D_6 and analyzed by NMR separately; *showing no reaction between N_2O and either of the pre-existent alkoxides*, [(PNP)Ti=CH^{t}Bu(OR)] (R = ^{n}Pr, ^{n}Bu; **4**, **6**) in the respective mixtures. The diastereomeric by-products raising from competing C–H activation were completely consumed in presence of N_2O, with release of the respective ether substituted α-olefins.

a) Isolated mixture from $^{n}Pr_2O$-activation, after N_2O addition. Evidence of terminal vinylic proton peaks consistent with presence of terminal olefins. The presence of 3-propoxy-1-propene could not be unequivocally established presumably due to thermal instability of this compound. The latter was further supported by GC/MS, which showed presence of several olefinic products in trace amounts; among them: 4-methyl-1-pentene, 3-methyl-1,4-pentadiene, 1-hexene, 1,3-hexadiene and 5,5-dimethyl-1-hexene. ^{1}H NMR (25 °C, 400 MHz, C_6D_6): δ 5.79 (*ddt*, $J_1 = J_{trans}$ = 17.2 Hz, $J_2 = J_{cis}$ = 10.0 Hz, $J_3 = {}^{3}J_{HH}$ = 6.8 Hz, 1H, H_2C=C*H*–R), 5.02 (*ddd*, $J_1 = J_{trans}$ = 17.2 Hz, $J_2 = J_{gem}$ = 3.5 Hz, $J_3 = {}^{4}J_{HH}$ = 1.7 Hz, 1H, *H*$_2$C=CH–R), 4.95 (*ddt*, $J_1 = J_{cis}$ = 10.2 Hz, $J_2 = J_{gem}$ = 2.2 Hz, $J_3 = {}^{4}J_{HH}$ = 1.2 Hz, 1H, *H*$_2$C=CH–R).

b) Isolated mixture from $^{n}Bu_2O$-activation, after N_2O addition. Evidence of terminal vinylic proton peaks consistent with presence of terminal olefins. The presence of 4-butoxy-butene was definitely confirmed by GC-MS. ^1H NMR (25 °C, 400 MHz, C_6D_6): δ 5.89–5.74 (*m*, 1H, H_2C=C*H*–R), 5.07–4.92 (*m*, 2H, *H*$_2$C=CH–R). GC-MS: Butoxy-4-butene, among other olefins, was detected by single injection into the GC-MS, at a retention time of 7.718-7.728 min. The spectrum, which does not show the molecular ion of this molecule, was compared with the reported one and was found to be an exact match. Relevant fragments: 85 ($[H_2C=CH-(CH_2)_2-O-CH_2]^+$), 55 ($[H_2C=CH-(CH_2)_2]^+$), 41 ($[H_2C=CH-(CH_2)]^+$), 27 ($[H_2C=CH]^+$).

VIII. Thermolysis of $^{n}Pr_2O$ and $^{n}Bu_2O$ solutions. A series of NMR tubes were charged with neat solutions of **1** (0.030 g, 0.048 mmol) in a) $^{n}Pr_2O$ and b) $^{n}Bu_2O$, and placed in a rotator at room temperature for 24 h to ensure conversion to the respective mixtures of alkoxides and C-H activation by-products. The tubes were then placed in a thermostated oil bath at 65 °C and the evolution of the mixtures constantly monitored by $^{31}P\{^1H\}$ NMR spectroscopy over the following 48h. Only in the case of the mixture in *n*Bu_2O, were the initial peaks resulting from C-H activation of the ether observed to decay into a myriad of intractable by-products. The mixture in $^{n}Pr_2O$ remained stationary over the entire follow-up, indicative of a greater kinetic stability of the C-H activation products. In both cases, the peaks assigned to the respective titanium alkoxides **4** and **6** remained stationary, therefore ruling out interconversion of the C-H activation by-products to the latter.

IX. Reactions with ethene. NMR tubes charged with neat solutions of [(PNP)Ti=CH^{t}Bu($CH_2{}^t$Bu)] (0.030 g, 0.048 mmol) in a) $^{n}Pr_2O$ and b) $^{n}Bu_2O$, and then pressurized with ethene (1 atm) in the Schlenk line. The mixtures were followed up by $^{31}P\{^1H\}$ NMR, at r.t. In both cases, formation of the ethene adduct, [(PNP)Ti($CH_2{}^t$Bu)(η^2-$H_2C=CH_2$)] at

δ = 27.8 (*d*, $^2J_{P\text{-}P}$ = 21.5 Hz), 25.6 (*d*, $^2J_{P\text{-}P}$ = 21.5 Hz) was confirmed. The mixtures are complicated as at least one more by-product with asymmetric doublets at δ = 38.19 (*d*, $^2J_{P\text{-}P}$ = 25.6 Hz), 31.79 (*d*, $^2J_{P\text{-}P}$ = 24.6 Hz), presumably due to a separate reaction involving the titanium alkoxides was formed in both mixtures. Both this new, unidentified product and the ethene-adduct react when exposed to N_2O, releasing free ethene (^{1}H NMR: δ 5.26) and their respective oxo-derivatives.

X. Independent preparations of [(PNP)Ti=CH^{t}Bu(OR)] (R = Me, Et, ^{n}Pr, ^{n}Bu, ^{i}Pr, ^{t}Bu).

1) [(PNP)Ti=CH^{t}Bu(OEt)] (1).

a) Direct synthesis in Et_2O. [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)] (0.045 g, 0.073 mmol; 1 equiv.) was dissolved in Et_2O (1 mL) and heated to 45 °C in a thermostated oil bath for 24 h. Formation of small amounts of [(PNP)Ti(η^2-H_2C=CH_2)(CH$_2$^{t}Bu)] cannot be avoided. The mixture was worked-up in the box, evaporating the ether and extracting the product in cold pentane. The latter solution was filtered through a plug of Celite and then evaporated to dryness. Yield of **1** after work-up: 98.6 % (0.042 g, 0.072 mmol) of a light-brown solid. No X-ray quality single-crystals could be grown either from cold (-35 °C) concentrated solutions, solvent pairs layers or slow evaporation, despite extensive efforts. ^{1}H NMR of **1** (25 °C, 500 MHz, C_6D_6): δ 10.76 (*s*, 1H, Ti=C*H*C(CH$_3$)$_3$), 7.36 (*dd*, J_1 = 8.7 Hz, J_2 = 4.3 Hz, 1H, Ar-C*H*), 7.09 (*dd*, J_1 = 8.8 Hz, J_2 = 4.3 Hz, 1H, Ar-C*H*), 6.98 (*dd*, J_1 = 5.5 Hz, J_2 = 1.5 Hz, 1H, Ar-C*H*), 6.91 (*dd*, J_1 = 8.8 Hz, J_2 = 1.7 Hz, 1H, Ar-C*H*), 6.88 (*dd*, J_1 = 5.5 Hz, J_2 = 2 Hz, 1H, Ar-C*H*), 6.79 (*dd*, J_1 = 8.8 Hz, J_2 = 1.8 Hz, 1H, Ar-C*H*), 4.70 (*dq*, $J_1 = J_{gem}$ = 11 Hz, $J_2 = {}^3J_{HH}$ = 6.9 Hz, 1H, Ti–OCH_aH$_b$-CH$_3$), 4.48 (*dq*, $J_1 = J_{gem}$ = 11 Hz, $J_2 = {}^3J_{HH}$ = 6.9 Hz, 1H, Ti–OCH$_a$$H_b$-CH$_3$), 2.37–2.21 (*m*, 2H, P–C*H*(CH$_3$)$_2$), 2.19 (*s*, 3H, *p*-CH$_3$), 2.13 (*s*, 3H, *p*-CH$_3$), 2.06–1.97 (*septet*, *J* = 7 Hz, 1H, P–C*H*(CH$_3$)$_2$), 1.94–1.83 (*septet*, *J* = 7 Hz, 1H, P–C*H*(CH$_3$)$_2$), 1.49 (*dd*, J_1 = 16 Hz, J_2 = 6.5 Hz, 3H, P–CH(C*H*$_3$)$_2$), 1.415 (*t*, *J* = 7.2 Hz, 3H, Ti–OCH$_a$H$_b$-C*H*$_3$), 1.39–1.31 (*m*, 6H, P–

$CH(CH_3)_2$), 1.30 (*s*, 9H, Ti=CHC(CH_3)$_3$), 1.26 (*dd*, J_1 = 16.5 Hz, J_2 = 7 Hz, 3H, P–CH(CH_3)$_2$), 1.15–1.04 (*m*, 6H, P–CH(CH_3)$_2$), 1.03–0.91 (*m*, 6H, P–CH(CH_3)$_2$). 1D-HSQC NMR of **1** (25 °C, 500 MHz, C_6D_6): δ 10.76 (*d*, $^1J_{C–H}$ = 97.5 Hz, Ti=*C*HC(CH_3)$_3$). $^{13}C\{^1H\}$ NMR of **1** (25 °C, 100 MHz, C_6D_6): δ 299.13 (*m*, 1C, Ti=*C*HC(CH_3)$_3$), 162.44 (*dd*, J_1 = 22.8 Hz, J_2 = 2.8 Hz, 1C, Ar-*C*), 160.42 (*dd*, J_1 = 23.4 Hz, J_2 = 4.5 Hz, 1C, Ar-*C*), 133.28 (*br s*, 1C, Ar-*C*H), 132.96 (*br s*, 2C, Ar-*C*H), 132.88 (*br s*, 1C, Ar-*C*H), 127.82 (*d*, *J* = 3.3 Hz, 1C, Ar-*C*), 125.01 (*d*, *J* = 4.5 Hz, 1C, Ar-*C*), 120.20 (*d*, *J* = 6.7 Hz, 1C, Ar-*C*), 120.11 (*d*, *J* = 25.6 Hz, 1C, Ar-*C*H), 119.58 (*d*, *J* = 25.7 Hz, 1C, Ar-*C*H), 116.79 (*d*, *J* = 7.8 Hz, 1C, Ar-*C*), 69.25 (*s*, 1C, Ti–O*C*$H_2$$CH_3$), 46.60 (*s*, 1C, Ti=CH*C*(CH_3)$_3$), 34.79 (*br s*, 3C, Ti=CHC(*C*H_3)$_3$), 25.19 (*d*, *J* = 10.0 Hz, 1C, P–*C*H(CH_3)$_2$), 24.36 (*d*, *J* = 4 Hz, 1C, P–*C*H(CH_3)$_2$), 22.37 (*s*, 1C, Ti–OCH$_2$*C*H_3), 21.27 (*br s*, 1C, *p*-CH_3), 20.99 (*br s*, 1C, *p*-CH_3), 20.69 (*d*, *J* = 12.2 Hz, 1C, P–*C*H(CH_3)$_2$), 20.51 (*d*, *J* = 7.8 Hz, 1C, P–CH(*C*H_3)$_2$), 20.16 (*d*, *J* = 6.7 Hz, 1C, P–CH(*C*H_3)$_2$), 19.57 (*d*, *J* = 2.7 Hz, 1C, P–CH(*C*H_3)$_2$), 19.48 (*d*, *J* = 3.4 Hz, 1C, P–CH(*C*H_3)$_2$), 19.23 (*d*, *J* = 6.7 Hz, 1C, P–CH(*C*H_3)$_2$), 19.09 (*d*, *J* = 10.1 Hz, 1C, P–*C*H(CH_3)$_2$), 18.68 (*d*, *J* = 7.8 Hz, 1C, P–CH(*C*H_3)$_2$), 17.21 (*d*, *J* = 5.6 Hz, 1C, P–CH(*C*H_3)$_2$), 16.37 (*d*, *J* = 6.7 Hz, 1C, P–CH(*C*H_3)$_2$). $^{31}P\{^1H\}$ NMR of **1** (25 °C, 162 MHz, C_6D_6): δ 35.54 (*d*, $^2J_{P-P}$ = 48.1 Hz, 1P), 25.73 (*d*, $^2J_{P-P}$ = 48.1 Hz, 1P).

b) One pot synthesis using [(PNP)Ti=CH^{t}Bu(OTf)] and LiCH$_2$^{t}Bu in Et$_2$O. [(PNP)Ti=CH^{t}Bu(OTf)] (0.099 g, 0.143 mmol; 1 equiv.) and LiCH$_2$^{t}Bu (0.014 g, 0.179 mmol; 1.2 equiv.) were mixed in Et_2O (5 mL) in a vial and stirred at room temperature for 24 h. The mixture was worked-up as indicated above, without difference in outcome. Yield of **1** after work-up: 91.0 % (0.076 g, 0.132 mmol) of light-brown solid.

c) Independent synthesis using [(PNP)Ti=CH^{t}Bu(OTf)] and NaOEt in THF. The reaction was performed in THF (1 mL) using [(PNP)Ti=CH^{t}Bu(OTf)] (0.040 g, 0.058 mmol; 1 equiv.) and NaOEt (0.006 g, 0.089 mmol; 1.5 equiv.), in a sealed NMR tube. The solution was heated in a

thermostated oil bath at 40 °C overnight, after which time complete conversion ensued. Formation of Na(PNP) and (PNP)H (~4–6 % by $^{31}P\{^{1}H\}$ NMR) took place in the crude mixture. (PNP)H could not be removed upon work-up and thus, no isolated yield is reported for this reaction.

2) [(PNP)Ti=CH^{t}Bu(OMe)] (2).

a) Direct synthesis in ^{t}BuOMe. [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)] (0.050 g, 0.082 mmol; 1 equiv.) was dissolved in ^{t}BuOMe (2 mL) and vigorously stirred in a vial for 24 h, at room temperature. The mixture changed from the distinctive olive green color of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)] to yellow-brown. The solvent was then evaporated *in vacuo*, the remaining solid residue re-dissolved in pentane and filtered through a plug of Celite. The filtrate was taken to dryness and dried *in vacuo* for 6 h, to leave a spectroscopically pure solid. Yield of **2** after work-up: 92.7 % (0.044 g, 0.076 mmol) of brown solid. No X-ray quality single-crystals could be grown either from cold (-35 °C) concentrated solutions, solvent pairs layers or slow evaporation, despite extensive efforts. Anal. Calcd. for $C_{32}H_{53}NOP_2Ti$ (**2**): C, 66.54; H, 9.25; N, 2.43. Found: C, 66.34; H, 9.05; N, 2.89. ^{1}H NMR of **2** (25 °C, 400 MHz, C_6D_6): δ 11.15 (*s*, 1H, Ti=C*H*C(CH$_3$)$_3$), 7.37 (*dd*, J_1 = 8.2 Hz, J_2 = 4.2 Hz, 1H, Ar-C*H*), 7.09 (*dd*, J_1 = 8.2 Hz, J_2 = 4.6 Hz, 1H, Ar-C*H*), 6.99 (*dd*, J_1 = 5.5 Hz, J_2 = 1.6 Hz, 1H, Ar-C*H*), 6.92 (*d*, J = 8.4 Hz, 1H, Ar-C*H*), 6.89 (*dd*, J_1 = 5.2 Hz, J_2 = 1.6 Hz, 1H, Ar-C*H*), 6.79 (*dd*, J_1 = 8.8 Hz, J_2 = 1.5 Hz, 1H, Ar-C*H*), 4.39 (*s*, 3H, Ti–OC*H*$_3$), 2.35–2.22 (*m*, 3H, P–C*H*(CH$_3$)$_2$), 2.19 (*s*, 3H, *p*-CH$_3$), 2.13 (*s*, 3H, *p*-CH$_3$), 1.86 (*septet*, J = 7.7 Hz, 1H, P–C*H*(CH$_3$)$_2$), 1.49 (*dd*, J_1 = 16.4 Hz, J_2 = 6.8 Hz, 3H, P–CH(C*H*$_3$)$_2$), 1.38–1.32 (*m*, 6H, P–CH(C*H*$_3$)$_2$), 1.31 (*s*, 9H, Ti=CHC(C*H*$_3$)$_3$), 1.27 (*dd*, J_1 = 16.2 Hz, J_2 = 6.6 Hz, 3H, P–CH(C*H*$_3$)$_2$), 1.1–1.03 (*m*, 6H, P–CH(C*H*$_3$)$_2$), 0.96–0.9 (*m*, 6H, P–CH(C*H*$_3$)$_2$). 1D-HSQC NMR of **2** (25 °C, 500 MHz, C_6D_6): δ 11.14 (*d*, $^{1}J_{C–H}$ = 98.8 Hz, Ti=*C*HC(CH$_3$)$_3$). $^{13}C\{^{1}H\}$ NMR of **2** (25 °C, 100 MHz, C_6D_6): δ 302.08 (*m*, 1C, Ti=*C*HC(CH$_3$)$_3$), 162.35 (*d*, J = 25.6 Hz, 1C, Ar-*C*), 160.06 (*dd*, J_1 = 23.4 Hz, J_2 = 4.4 Hz, 1C,

Ar-*C*), 133.26 (*br s*, 1C, Ar-*C*H), 133.01 (overlapping *s*, 2C, Ar-*C*H), 132.77 (*br s*, 1C, Ar-*C*H), 127.9 (*d*, *J* = 4.2 Hz, 1C, Ar-*C*), 124.94 (*d*, *J* = 3.3 Hz, 1C, Ar-*C*), 120.36 (*d*, *J* = 7.8 Hz, 1C, Ar-*C*H), 120.15 (*d*, *J* = 26.8 Hz, 1C, Ar-*C*H), 119.89 (*d*, *J* = 25.6 Hz, 1C, Ar-*C*H), 116.47 (*d*, *J* = 6.7 Hz, 1C, Ar-*C*H), 61.71 (*s*, 1C, Ti–O*C*H_3), 46.72 (*s*, 1C, Ti=CH*C*$(CH_3)_3$), 34.66 (*s*, 3C, Ti=CHC($C$$H_3$)$_3$), 25.12 (*d*, *J* = 11.2 Hz, 1C, P–*C*H$(CH_3)_2$), 24.47 (*d*, *J* = 3.3 Hz, 1C, P–*C*H$(CH_3)_2$), 21.24 (*br s*, 1C, *p*-CH_3), 20.97 (overlapping *s*, 1C, *p*-CH_3), 20.85 (overlapping *d*, *J* = 13.3 Hz, 1C, P–CH($C$$H_3$)$_2$), 20.41 (*d*, *J* = 7.8 Hz, 1C, P–CH($C$$H_3$)$_2$), 20.21 (*d*, *J* = 6.7 Hz, 1C, P–CH($C$$H_3$)$_2$), 19.59–19.26 (overlapping *m*, 3C, P–*C*H$(CH_3)_2$, P–CH($C$$H_3$)$_2$), 19.10 (*d*, *J* = 12.3 Hz, 1C, P–CH($C$$H_3$)$_2$), 18.55 (*d*, *J* = 7.8 Hz, 1C, P–CH($C$$H_3$)$_2$), 17.63 (*d*, *J* = 3.3 Hz, 1C, P–CH($C$$H_3$)$_2$), 16.33 (*d*, *J* = 6.7 Hz, 1C, P–CH($C$$H_3$)$_2$). $^{31}P\{^1H\}$ NMR of **2** (25 °C, 162 MHz, C_6D_6): δ 36.83 (*d*, $^2J_{P\text{-}P}$ = 47.0 Hz, 1P), 25.6 (*d*, $^2J_{P\text{-}P}$ = 47 Hz, 1P).

b) One pot synthesis using [(PNP)Ti=CH^{t}Bu(OTf)] and LiCH$_2$^{t}Bu in ^{t}BuOMe. [(PNP)Ti=CH^{t}Bu(OTf)] (0.100 g, 0.144 mmol; 1 equiv.) was dissolved in ^{t}BuOMe (5 mL) and to it was added LiCH$_2$^{t}Bu (0.0135 g, 0.173 mmol; 1.2 equiv.). As in the above procedure, the mixture was stirred at room temperature for 24 h and the product isolated using the same procedure. Yield of **2**, after work-up: 91 % (0.076 g, 0.132 mmol).

c) Independent synthesis using [(PNP)Ti=CH^{t}Bu(OTf)] and NaOMe in THF. [(PNP)Ti=CH^{t}Bu(OTf)] (0.040 g, 0.058 mmol; 1 equiv.) was dissolved in THF (1 mL) in a vial and mixed with NaOMe (0.005 g, 0.098 mmol; 1.6 equiv.). The mixture was transferred to a J. Young NMR tube and placed in a thermostated oil bath at 45 °C, overnight. Complete conversion was gauged by $^{31}P\{^1H\}$ NMR after this time. Formation of (PNP)H (~50 % by $^{31}P\{^1H\}$ NMR) as a by-product of this reaction also took place. (PNP)H could not be removed completely despite repeated work-up attempts and thus, no isolated yield is reported for this procedure.

3) [(PNP)Ti=CH^{t}Bu(O^{t}Bu)] (3).

a) Independent synthesis using [(PNP)Ti=CH^{t}Bu(OTf)] and NaO^{t}Bu in THF. The reaction was set up using [(PNP)Ti=CH^{t}Bu(OTf)] (0.100 g, 0.144 mmol; 1 equiv.) and NaO^{t}Bu (0.021g, 0.216 mmol; 1.5 equiv.) in THF (1 mL) heating the mixture at 40 °C for 2 d. No by-products were produced. Yield of **3** after work-up: 98.6 % (0.088 g, 0.142 mmol) of golden-brown solid. X-ray quality single-crystals of **3** were successfully grown slowly from a concentrated, pentane:Et_2O mixture, at -35 °C. ^{1}H NMR of **3** (25 °C, 800 MHz, C_6D_6): δ 9.34 (*s*, 1H, Ti=C*H*C(CH$_3$)$_3$), 7.26 (*dd*, J_1 = 8.4 Hz, J_2 = 4.4 Hz, 1H, Ar-C*H*), 7.02 (*dd*, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H, Ar-C*H*), 6.92 (*br d*, J = 4.8 Hz, 1H, Ar-C*H*), 6.84 (*d*, J = 8.8 Hz, 1H, Ar-C*H*), 6.81 (*br d*, J = 4.8 Hz, 1H, Ar-C*H*), 6.72 (*d*, J = 8.0 Hz, 1H, Ar-C*H*), 2.29 (*septet*, J = 6.9 Hz, 2H, P–C*H*(CH$_3$)$_2$), 2.25 (*septet*, J = 6 Hz, 1H, P–C*H*(CH$_3$)$_2$), 2.14 (*s*, 3H, *p*-CH$_3$), 2.08 (*s*, 3H, *p*-CH$_3$), 1.94 (*septet*, J = 7.1 Hz, 1H, P–C*H*(CH$_3$)$_2$), 1.479 (*s*, 9H, Ti–OC(C*H*$_3$)$_3$), 1.44 (*dd*, J_1 = 15.6 Hz, J_2 = 6.8 Hz, 3H, P–CH(C*H*$_3$)$_2$), 1.31 (*dd*, J_1 = 15.2 Hz, J_2 = 7.2 Hz, 3H, P–CH(C*H*$_3$)$_2$), 1.27 (*dd*, J_1 = 15.2 Hz, J_2 = 7.2 Hz, 3H, P–CH(C*H*$_3$)$_2$), 1.25 (*s*, 9H, Ti=CHC(C*H*$_3$)$_3$), 1.23–1.14 (*m*, 6H, P–CH(C*H*$_3$)$_2$), 1.01–0.95 (*m*, 6H, P–CH(C*H*$_3$)$_2$), 0.82 (*t*, J = 7.2 Hz, 3H, P–CH(C*H*$_3$)$_2$). ^{13}C{^{1}H} NMR of **3** (25 °C, 100 MHz, C_6D_6): δ 290.80 (*m*, $^1J_{C\text{-}H}$ = 94.8 Hz (measured from the doublet described by the carbon satellites on the ^{1}H NMR spectrum), $^2J_{C\text{-}P}$ = 8.5 Hz, 1C, Ti=*C*HC(CH$_3$)$_3$), 162.66 (*dd*, J_1 = 23 Hz, J_2 = 3.4 Hz, 1C, Ar-*C*), 161.39 (*dd*, J_1 = 22.4 Hz, J_2 = 4.0 Hz, 1C, Ar-*C*), 133.19 (*d*, J_1 = 2.1 Hz, 1C, Ar-*C*H), 132.78 (*d*, J_1 = 1.4 Hz, 1C, Ar-*C*H), 132.69 (*d*, J_1 = 1.4 Hz, 1C, Ar-*C*H), 132.57 (*d*, J_1 = 2.7 Hz, 1C, Ar-*C*H), 127.19 (*d*, J = 4.1 Hz, 1C, Ar-*C*), 125.39 (*d*, J = 4.0 Hz, 1C, Ar-*C*), 120.85 (*d*, J = 24.4 Hz, 1C, Ar-*C*), 119.51 (*d*, J = 7.5 Hz, 1C, Ar-*C*H), 118.56 (*d*, J = 26.4 Hz, 1C, Ar-*C*), 118.15 (*d*, J = 6.8 Hz, 1C, Ar-*C*H), 79.51 (*s*, 1C, Ti–O*C*(CH$_3$)$_3$), 46.53 (*s*, 1C, Ti=CH*C*(CH$_3$)$_3$), 35.53 (*s*, 3C, Ti-OC(*C*H$_3$)$_3$), 35.13 (*t*, J = 2.4 Hz, 1C, Ti=CHC(*C*H$_3$)$_3$), 25.57 (*d*, J = 9.5 Hz, 1C, P–*C*H(CH$_3$)$_2$), 24.34 (*br s*, 1C, P–*C*H(CH$_3$)$_2$), 21.27 (*br s*, 1C, *p*-CH$_3$), 21.05 (*br s*, 1C, *p*-CH$_3$), 20.67 (*d*, J = 8.2 Hz, 1C, P–CH(*C*H$_3$)$_2$), 20.29 (*d*, J = 6.1 Hz, 1C, P–CH(*C*H$_3$)$_2$), 19.97 (*d*, J = 11.6 Hz, 1C, P–*C*H(CH$_3$)$_2$),

19.82 (*d*, J = 4.8 Hz, 1C, P–CH(CH$_3$)$_2$), 19.54 (*d*, J = 8.1 Hz, 1C, P–CH(CH$_3$)$_2$), 19.43 (*d*, J = 10.8 Hz, 1C, P–CH(CH$_3$)$_2$), 19.23 (*d*, J = 6.1 Hz, 1C, P–CH(CH$_3$)$_2$), 19.09 (*d*, J = 2.7 Hz, 1C, P–CH(CH$_3$)$_2$), 16.53 (*d*, J = 7.5 Hz, 1C, P–CH(CH$_3$)$_2$), 16.37 (*d*, J = 6.8 Hz, 1C, P–CH(CH$_3$)$_2$). ^{31}P{^{1}H} NMR of **3** (25 °C, 162 MHz, C$_6$D$_6$): δ 31.62 (*d*, $^2J_{P\text{-}P}$ = 47 Hz, 1P), 25.69 (*d*, $^2J_{P\text{-}P}$ = 47 Hz, 1P).

4) [(PNP)Ti=CH*t*Bu(O^{n}Pr)] (4).

a) Independent synthesis using [(PNP)Ti=CH^{t}Bu(OTf)] and NaO^{n}Pr in THF. The synthesis was performed in a sealed NMR tube using [(PNP)Ti=CH^{t}Bu(OTf)] (0.050 g, 0.073 mmol; 1 equiv.) and NaO^{n}Pr (0.0067 g, 0.082 mmol; 1.0 equiv.), in THF (1 mL). The tube was placed in a rotator at room temperature for 24 h, after which time complete conversion ensued. A small amount of Na(PNP) was produced in the crude mixture, which was removed during work-up. A golden-brown solid residue remained, which was washed two times with pentane (2 x 5 mL) and then extracted into pentane and filtered through a plug of Celite. The filtrates were combined and taken to dryness leaving a light yellow-brown solid, spectroscopically pure. Yield of **4** after work-up: 97.2 % (0.043 g, 0.07 mmol) of light yellow-brown solid. No X-ray quality single-crystals could be grown either from cold (-35 °C) concentrated solutions, solvent pairs layers or slow evaporation, despite extensive efforts. ^{1}H NMR of **4** (25 °C, 800 MHz, C$_6$D$_6$): δ 10.63 (*s*, 1H, Ti=CHC(CH$_3$)$_3$), 7.36 (*dd*, J_1 = 8.0 Hz, J_2 = 4.8 Hz, 1H, Ar-CH), 7.10 (*dd*, J_1 = 8.4 Hz, J_2 = 4.4 Hz, 1H, Ar-CH), 6.98 (*dd*, J_1 = 5.6 Hz, J_2 = 1.6 Hz, 1H, Ar-CH), 6.92 (*dd*, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H, Ar-CH), 6.89 (*dd*, J_1 = 5.6 Hz, J_2 = 2.4 Hz, 1H, Ar-CH), 6.79 (*dd*, J_1 = 8.4 Hz, J_2 = 2.0 Hz, 1H, Ar-CH), 4.67 (*ddd*, $J_1 = J_{gem}$ = 10.8 Hz, $J_2 = {}^3J_{HH}$ = 8 Hz, $J_3 = {}^4J_{HH}$ = 6 Hz, 1H, Ti–OCH_aH$_b$-CH$_2$-CH$_3$), 4.44 (*ddd*, $J_1 = J_{gem}$ = 10.8 Hz, $J_2 = {}^3J_{HH}$ = 8 Hz, $J_3 = {}^4J_{HH}$ = 6 Hz, 1H, Ti–OCH$_a$$H_b$-CH$_2$-CH$_3$), 2.37–2.22 (overlapping *m*, 3H, P–CH(CH$_3$)$_2$), 2.19 (*s*, 3H, *p*-CH$_3$), 2.13 (*s*, 3H, *p*-CH$_3$), 2.03 (*septet*, J = 6.5 Hz, 1H, P–CH(CH$_3$)$_2$), 1.94–1.79 (*m*, 2H, Ti–OCH$_a$H$_b$-CH_2-

CH_3), 1.50 (*dd*, J_1 = 16.0 Hz, J_2 = 7.2 Hz, 3H, P–CH(CH_3)$_2$), 1.37 (overlapping *dd*, J_1 = 16.0 Hz, J_2 = 7.2 Hz, 3H, P–CH(CH_3)$_2$), 1.34 (overlapping *dd*, J_1 = 15.6 Hz, J_2 = 6.8 Hz, 3H, P–CH(CH_3)$_2$), 1.30 (overlapping *s*, 9H, Ti=CHC(CH_3)$_3$), 1.26 (overlapping *dd*, J_1 = 16.4 Hz, J_2 = 6.8 Hz, 3H, P–CH(CH_3)$_2$), 1.12–1.06 (*m*, 6H, P–CH(CH_3)$_2$), 0.98–0.93 (*m*, 9H, Ti–OCH$_a$H$_b$-CH$_2$-CH_3, P–CH(CH_3)$_2$). ^{13}C{^{1}H} NMR of **4** (25 °C, 125 MHz, C_6D_6): δ 298.16 (*m*, $^1J_{C\text{-}H}$ = 96.5 Hz (measured from the doublet described by the carbon satellites on the ^{1}H NMR spectrum), 1C, Ti=*C*HC(CH$_3$)$_3$), 162.4 (*dd*, J_1 = 23 Hz, J_2 = 2.9 Hz, 1C, Ar-*C*), 160.42 (*dd*, J_1 = 23 Hz, J_2 = 4.1 Hz, 1C, Ar-*C*), 133.30 (*s*, 1C, Ar-*C*H), 132.93–132.90 (*m*, 3C, Ar-*C*H), 127.82 (*d*, *J* = 4.1 Hz, 1C, Ar-*C*), 125.06 (*d*, *J* = 4.1 Hz, 1C, Ar-*C*), 120.18 (*d*, *J* = 24.5 Hz, 1C, Ar-*C*H), 120.13 (*d*, *J* = 7.8 Hz, 1C, Ar-*C*), 119.49 (*d*, *J* = 26.4 Hz, 1C, Ar-*C*H), 116.87 (*d*, *J* = 7.6 Hz, 1C, Ar-*C*), 76.16 (*s*, 1C, Ti–O*C*H$_2$CH$_2$CH$_3$), 46.77 (*s*, 1C, Ti=CH*C*(CH$_3$)$_3$), 34.77 (*s*, 3C, Ti=CHC(*C*H$_3$)$_3$), 29.76 (s, Ti–OCH$_2$*C*H$_2$CH$_3$), 25.20 (*d*, *J* = 10.5 Hz, 1C, P–*C*H(CH$_3$)$_2$), 24.26 (*d*, *J* = 3.5 Hz, 1C, P–*C*H(CH$_3$)$_2$), 21.26 (*br s*, 1C, *p*-CH$_3$), 21.00 (*br s*, 1C, *p*-CH$_3$), 20.73 (*d*, *J* = 13.1 Hz, 1C, P–CH(*C*H$_3$)$_2$), 20.56 (*d*, *J* = 8.2 Hz, 1C, P–CH(*C*H$_3$)$_2$), 20.18 (*d*, *J* = 6.3 Hz, 1C, P–CH(*C*H$_3$)$_2$), 19.57–19.41 (overlapping *m*, 2C, P–*C*H(CH$_3$)$_2$, P–CH(*C*H$_3$)$_2$), 19.23 (overlapping *d*, *J* = 12.5 Hz, 1C, P–CH(*C*H$_3$)$_2$), 19.11 (overlapping *d*, *J* = 16 Hz, 1C, P–CH(*C*H$_3$)$_2$), 18.73 (*d*, *J* = 7.6 Hz, 1C, P–CH(*C*H$_3$)$_2$), 17.09 (*d*, *J* = 5.6 Hz, 1C, P–CH(*C*H$_3$)$_2$), 16.36 (*d*, *J* = 7.6 Hz, 1C, P–CH(*C*H$_3$)$_2$), 11.08 (*s*, 1C, Ti–OCH$_2$CH$_2$*C*H$_3$). ^{31}P{^{1}H} NMR of **4** (25 °C, 162 MHz, C_6D_6): δ 35.18 (*d*, $^2J_{P\text{-}P}$ = 48.1 Hz, 1P), 25.73 (*d*, $^2J_{P\text{-}P}$ = 48.1 Hz, 1P).

5) [(PNP)Ti=CH^{t}Bu(O^{n}Bu)] (6).

a) Independent synthesis using [(PNP)Ti=CH^{t}Bu(OTf)] and NaO^{n}Bu in THF. The reaction and its work-up were set-up and performed as described for **4**, using [(PNP)Ti=CH^{t}Bu(OTf)] (0.050 g, 0.073 mmol; 1 equiv.) and NaO^{n}Bu (0.008 g, 0.088 mmol; 1.2 equiv.), in THF (1 mL). A small amount of Na(PNP) was formed in the crude mixture, which was removed during work-up.

Yield of **6** after work-up: 95.8 % (0.043 g, 0.069 mmol) of golden-brown solid. No X-ray quality single-crystals could be grown either from cold (-35 °C) concentrated solutions, solvent pairs layers or slow evaporation, despite extensive efforts. ^{1}H NMR of **6** (25 °C, 500 MHz, C_6D_6): δ 10.61 (*s*, 1H, Ti=C*H*C$(CH_3)_3$), 7.36 (*dd*, J_1 = 8.5 Hz, J_2 = 4.5 Hz, 1H, Ar-C*H*), 7.09 (*dd*, J_1 = 8.2 Hz, J_2 = 4.3 Hz, 1H, Ar-C*H*), 6.98 (*d*, *J* = 5.0 Hz, 1H, Ar-C*H*), 6.92 (*d*, *J* = 8.5 Hz, 1H, Ar-C*H*), 6.88 (*d*, *J* = 5.0 Hz, 1H, Ar-C*H*), 6.79 (*d*, *J* = 8.5 Hz, 1H, Ar-C*H*), 4.74 (*dt*, J_1 = 11.0 Hz, J_2 = 6.9 Hz, 1H, Ti–OCH_aH$_b$-CH_2-CH_2-CH_3), 4.51 (*dt*, J_1 = 10.5 Hz, J_2 = 7.0 Hz, 1H, Ti–OCH$_a$$H_b$-$CH_2$-$CH_2$-$CH_3$), 2.37–2.24 (*m*, 3H, P–C*H*$(CH_3)_2$), 2.19 (*s*, 3H, *p*-CH_3), 2.13 (*s*, 3H, *p*-CH_3), 1.95 (*septet*, *J* = 7.1 Hz, 1H, P–C*H*$(CH_3)_2$), 1.89–1.76 (*m*, 2H, Ti–OCH$_a$H$_b$-CH_2-CH_2-CH_3), 1.50 (overlapping *dd*, J_1 = 16 Hz, J_2 = 7.0 Hz, 3H, P–CH(CH_3)$_2$), 1.46 (overlapping *dd*, J_1 = 15 Hz, J_2 = 7.5 Hz, 3H, P–CH(CH_3)$_2$), 1.38 (overlapping *dd*, J_1 = 16.5 Hz, J_2 = 7.0 Hz, 3H, P–CH(CH_3)$_2$), 1.34 (overlapping *dd*, J_1 = 15.3 Hz, J_2 = 7.3 Hz, 3H, P–CH(CH_3)$_2$), 1.30 (overlapping *br s*, 10H, Ti=CHC(CH_3)$_3$ and P–CH(CH_3)$_2$), 1.29 (overlapping *dd*, J_1 = 16.0 Hz, J_2 = 6.5 Hz, 2H, P–CH(CH_3)$_2$), 1.12–1.06 (*m*, 6H, P–CH(CH_3)$_2$), 0.98–0.93 (*m*, 8H, Ti–OCH$_a$H$_b$-CH_2-CH_2-CH_3, P–CH(CH_3)$_2$). ^{13}C{^{1}H} NMR of **6** (25 °C, 125 MHz, C_6D_6): δ 298.02 (*m*, $^{1}J_{C\text{-}H}$ = 97.5 Hz (measured from the doublet described by the carbon satellites on the ^{1}H NMR spectrum), 1C, Ti=*C*HC$(CH_3)_3$), 162.4 (*dd*, J_1 = 22.6 Hz, J_2 = 2.5 Hz, 1C, Ar-*C*), 160.44 (*dd*, J_1 = 22.8 Hz, J_2 = 3.9 Hz, 1C, Ar-*C*), 133.30 (*s*, 1C, Ar-*C*H), 132.91 (*br s*, 3C, Ar-*C*H), 127.81 (*d*, *J* = 4.4 Hz, 1C, Ar-*C*), 125.07 (*d*, *J* = 3.4 Hz, 1C, Ar-*C*), 120.19 (overlapping *d*, *J* = 23.4 Hz, 1C, Ar-*C*H), 120.12 (overlapping *d*, *J* = 7.8 Hz, 1C, Ar-*C*), 119.46 (*d*, *J* = 25.6 Hz, 1C, Ar-*C*H), 116.89 (*d*, *J* = 6.6 Hz, 1C, Ar-*C*), 74.03 (*s*, 1C, Ti–O*C*$H_2$$CH_2$$CH_2$$CH_3$), 46.78 (*s*, 1C, Ti=CH*C*$(CH_3)_3$), 38.95 (*s*, 1C, Ti–OCH$_2$*C*H$_2$CH$_2$CH$_3$), 34.77 (*s*, 3C, Ti=CHC(*C*H_3)$_3$), 25.21 (*d*, *J* = 10.1 Hz, 1C, P–*C*H$(CH_3)_2$), 24.28 (*d*, *J* = 3.4 Hz, 1C, P–*C*H$(CH_3)_2$), 21.26 (*s*, 1C, *p*-CH_3), 20.99 (*s*, 1C, *p*-CH_3), 20.72 (*d*, *J* = 13.4 Hz, 1C, P–CH(*C*H_3)$_2$), 20.57 (*d*, *J* = 8.9 Hz, 1C, P–CH(*C*H_3)$_2$), 20.18 (*d*, *J* = 5.6 Hz, 1C, P–CH(*C*H_3)$_2$), 19.94 (*s*, 1C, Ti–

$OCH_2CH_2CH_2CH_3$), 19.56–19.44 (overlapping *m*, 2C, P–$CH(CH_3)_2$), 19.25 (overlapping *d*, *J* = 12.3 Hz, 1C, P–$CH(CH_3)_2$), 19.11 (overlapping *d*, *J* = 14.5 Hz, 1C, P–$CH(CH_3)_2$), 18.75 (*d*, *J* = 7.8 Hz, 1C, P–$CH(CH_3)_2$), 17.07 (*d*, *J* = 5.6 Hz, 1C, P–$CH(CH_3)_2$), 16.37 (*d*, *J* = 6.7 Hz, 1C, P–$CH(CH_3)_2$), 14.68 (*s*, 1C, Ti–$OCH_2CH_2CH_2CH_3$). $^{31}P\{^1H\}$ NMR of **6** (25 °C, 162 MHz, C_6D_6): δ 35.33 (*d*, $^2J_{P\text{-}P}$ = 48.1 Hz, 1P), 25.93 (*d*, $^2J_{P\text{-}P}$ = 48.1 Hz, 1P).

5) [(PNP)Ti=CH*t*Bu(O^{i}Pr)] (8).

a) One pot synthesis using [(PNP)Ti=CH^{t}Bu(OTf)] and LiCH$_2$^{t}Bu in ^{i}Pr$_2$O. Compound [(PNP)Ti=CH^{t}Bu(OTf)] (0.100 g, 0.144 mmol; 1 equiv.) and LiCH$_2$^{t}Bu (0.013 g, 0.169 mmol; 1.2 equiv.) were mixed in ^{i}Pr$_2$O (1 mL) and heated to 40 °C for 24 h. Yield of **8** after work-up: 89.6 % (0.078 g, 0.129 mmol) of olive-green solid. No X-ray quality single-crystals could be grown either from cold (-35 °C) concentrated solutions, solvent pairs layers or slow evaporation, despite extensive efforts. ^1H NMR of **8** (25 °C, 500 MHz, C_6D_6): δ 9.95 (*s*, 1H, Ti=C*H*C$(CH_3)_3$), 7.35 (*dd*, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H, Ar-C*H*), 7.09 (*dd*, J_1 = 8.3 Hz, J_2 = 4.3 Hz, 1H, Ar-C*H*), 6.98 (*br d*, *J* = 5.0 Hz, 1H, Ar-C*H*), 6.91 (*br d*, *J* = 8.5 Hz, 1H, Ar-C*H*), 6.87 (*dd*, J_1 = 5.5 Hz, J_2 = 1.5 Hz, 1H, Ar-C*H*), 6.79 (*dd*, J_1 = 8.5 Hz, J_2 = 2.0 Hz, 1H, Ar-C*H*), 4.86 (*septet*, *J* = 6.0 Hz, 1H, Ti–OC*H*$(CH_3)_2$), 2.37–2.23 (*m*, 3H, P–C*H*$(CH_3)_2$), 2.19 (*s*, 3H, *p*-CH_3), 2.13 (*s*, 3H, *p*-CH_3), 1.94 (*septet*, *J* = 7.1 Hz, 1H, P–C*H*$(CH_3)_2$), 1.53 (*d*, *J* = 6.0 Hz, 3H, Ti–OCH(C*H*$_3$)$_2$), 1.50 (*dd*, J_1 = 16.0 Hz, J_2 = 7.0 Hz, 3H, P–CH(C*H*$_3$)$_2$), 1.39–1.32 (*m*, 6H, P–CH(C*H*$_3$)$_2$), 1.31 (*d*, *J* = 6.0 Hz, 3H, Ti–OCH(C*H*$_3$)$_2$), 1.29 (*s*, 9H, Ti=CHC(C*H*$_3$)$_3$), 1.26 (*dd*, J_1 = 16.0 Hz, J_2 = 7.0 Hz, 3H, P–CH(C*H*$_3$)$_2$), 1.14–1.05 (*m*, 6H, P–CH(C*H*$_3$)$_2$), 0.99–0.93 (*m*, 6H, P–CH(C*H*$_3$)$_2$). $^{13}C\{^1H\}$ NMR of **8** (25 °C, 125 MHz, C_6D_6): δ 293.11 (*m*, $^1J_{C\text{-}H}$ = 96.0 Hz (measured from the doublet described by the carbon satellites on the ^1H NMR spectrum), 1C, Ti=*C*HC$(CH_3)_3$), 162.42 (*dd*, J_1 = 23 Hz, J_2 = 2.7 Hz, 1C, Ar-*C*), 160.72 (*dd*, J_1 = 22.2 Hz, J_2 = 4.1 Hz, 1C, Ar-*C*), 133.28 (*br s*, 1C, Ar-*C*H), 132.89 (*br s*, 2C, Ar-*C*H), 132.77 (*d*, J_1 = 2.0 Hz,

1C, Ar-*C*H), 127.60 (*d*, *J* = 3.4 Hz, 1C, Ar-*C*), 125.09 (*d*, *J* = 3.5 Hz, 1C, Ar-*C*), 120.36 (*d*, *J* = 24.4 Hz, 1C, Ar-*C*), 119.85 (*d*, *J* = 7.0 Hz, 1C, Ar-*C*H), 119.11 (*d*, *J* = 26.5 Hz, 1C, Ar-*C*), 117.21 (*d*, *J* = 7.6 Hz, 1C, Ar-*C*H), 74.85 (*s*, 1C, Ti–O*C*H(CH_3)$_2$), 46.45 (*s*, 1C, Ti=CH*C*(CH_3)$_3$), 34.93 (*s*, 3C, Ti=CHC(*C*H_3)$_3$), 29.78 (*s*, 1C, Ti–OCH(*C*H_3)$_2$), 29.05 (*s*, 1C, Ti–OCH(*C*H_3)$_2$), 25.29 (*d*, *J* = 10.5 Hz, 1C, P–*C*H(CH_3)$_2$), 24.17 (*br s*, 1C, P–*C*H(CH_3)$_2$), 21.26 (*br s*, 1C, *p*-CH_3), 21.02 (*br s*, 1C, *p*-CH_3), 20.68 (*d*, *J* = 8.4 Hz, 1C, P–CH(*C*H_3)$_2$), 20.43 (*d*, *J* = 12.5 Hz, 1C, P–*C*H(CH_3)$_2$), 20.18 (*d*, *J* = 6.3 Hz, 1C, P–CH(*C*H_3)$_2$), 19.64 (*d*, *J* = 5.5 Hz, 1C, P–CH(*C*H_3)$_2$), 19.48 (*d*, *J* = 11.9 Hz, 1C, P–CH(*C*H_3)$_2$), 19.23 (*d*, *J* = 12.5 Hz, 1C, P–*C*H(CH_3)$_2$), 18.99 (*d*, *J* = 6.3 Hz, 1C, P–CH(*C*H_3)$_2$), 18.91 (*br s*, 1C, P–CH(*C*H_3)$_2$), 16.68 (*d*, *J* = 7.0 Hz, 1C, P–CH(*C*H_3)$_2$), 16.38 (*d*, *J* = 7.0 Hz, 1C, P–CH(*C*H_3)$_2$). $^{31}P\{^1H\}$ NMR of **8** (25 °C, 162 MHz, C_6D_6): δ 34.23 (*d*, $^2J_{P\text{-}P}$ = 48.1 Hz, 1P), 26.07 (*d*, $^2J_{P\text{-}P}$ = 48.1 Hz, 1P).

b) Independent synthesis using [(PNP)Ti=CH^{t}Bu(OTf)] and NaO^{i}Pr in THF. [(PNP)Ti=CH^{t}Bu(OTf)] (0.050 g, 0.072 mmol; 1 equiv.) and NaO^{i}Pr (0.009 g, 0.109 mmol; 1.5 equiv.) were mixed in THF (1 mL) in a sealed NMR tube, and the tube placed in a rotator at room temperature for 24 h, after which time complete conversion ensued. Formation of (PNP)H and Na(PNP) (<10 %), could not be avoided. However, (PNP)H could not be removed during work-up and therefore no isolated yield for **7** is reported for this synthesis.

XI. Summarized NMR data.

Table S2. NMR diagnostic peaks for [(PNP)Ti=CH^{t}Bu(OR)] (R = Me, Et, ^{n}Pr, ^{n}Bu, ^{i}Pr, ^{t}Bu).

Compound	^{1}H		^{13}C{^{1}H}		^{31}P{^{1}H}	
	Ti=C*H*^{t}Bu	Ti–OC*H*$_2$R	Ti=*C*H^{t}Bu	Ti–O*C*H$_2$R	(*P*NP)Ti	(PN*P*)Ti
	δ	δ	δ	δ	δ_1	δ_2
	(*m*)	(*m*, $^2J_{HH\text{-}gem}$)	(*m*, $^1J_{CH}$)	(*m*)	(*m*, $^2J_{PP}$)	(*m*, $^2J_{PP}$)
[(PNP)Ti=CH^{t}Bu(OEt)] (**1**)	10.76 (*s*)	4.70, 4.48 (*dq*, J_{gem} = 11 Hz)	299.13 (*m*, 97.5 Hz)[a]	69.25 (*s*)	35.54 (*d*, 48.1 Hz)	25.73 (*d*, 48.1 Hz)
[(PNP)Ti=CH^{t}Bu(OMe)] (**2**)	11.14 (*s*)	4.39 (*s*)	301.94 (*m*, 98.8 Hz)[a]	61.64 (*s*)	36.7 (*d*, 48 Hz)	25.5 (*d*, 48 Hz)
[(PNP)Ti=CH^{t}Bu(O^{t}Bu)] (**3**)	9.34 (*s*)	--	290.80 (*m*, 94.8 Hz)[b]	--	31.62 (*d*, 47 Hz)	25.69 (*d*, 47 Hz)
[(PNP)Ti=CH^{t}Bu(O^{n}Pr)] (**4**)	10.63 (*s*)	4.67, 4.44 (*ddd*, J_{gem} = 10.8 Hz)	298.16 (*m*, 96.5 Hz)[b]	76.16 (*s*)	35.18 (*d*, 48.1 Hz)	25.73 (*d*, 48.1 Hz)
[(PNP)Ti=CH^{t}Bu(O^{n}Bu)] (**6**)	10.61 (*s*)	4.77–4.71, 4.54–4.47 (*m*)	298.04 (*m*, 99.0 Hz)[b]	74.03 (*s*)	35.2 (*d*, 47.8 Hz)	25.8 (*d*, 47.8 Hz)
[(PNP)Ti=CH^{t}Bu(O^{i}Pr)] (**8**)	9.95 (*s*)	4.86 (*septet*, *J* = 6.0 Hz)[c]	293.11 (*m*, 96.0 Hz)[b]	74.85 (*s*)[b]	34.23 (*d*, 48.1 Hz)	26.07 (*d*, 48.1 Hz)

([a]) $^1J_{CH}$ measured by 1D-HSQC. ([b]) $^1J_{CH}$ measured from the carbon satellite peaks around the alkylidene singlet in the ^{1}H NMR spectrum. ([c]) Ti–O*C*H*H*Me$_2$.

XII. Catalysis trials.

1) Follow-up of reaction between 2 with LiCH$_2$^{t}Bu (1.2 equiv.) in C$_6$D$_6$. In a Young tube, compound **2** (0.033 g, 0.058 mmol; 1 equiv.) was dissolved in C_6D_6 and to it was added LiCH$_2$^{t}Bu (0.006 g, 0.069 mmol; 1.2 equiv.). The tube was placed in a rotator to ensure constant mixing and the reaction followed at r.t. for the following 24h, by ^{31}P{^{1}H} NMR spectroscopy. Transient formation of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)] (δ 28.39 (*d*, $^2J_{P\text{-}P}$ = 46 Hz, 1P), 20.15 (*d*, $^2J_{P\text{-}P}$ = 46 Hz, 1P)) took place after 1h, which further decayed in C_6D_6 to [(PNP)Ti=CD^{t}Bu(C_6D_5)] (δ 30.26 (*d*, $^2J_{P\text{-}P}$ = 45 Hz, 1P), 22.41 (*d*, $^2J_{P\text{-}P}$ = 45 Hz, 1P)).[5]

2) Catalysis screening: reaction between [(PNP)Ti=CH^{t}Bu(OTf)] and LiCH$_2$^{t}Bu (6 equiv.) in ^{t}BuOMe. [(PNP)Ti=CH^{t}Bu(OTf)] (0.005 g, 0.007 mmol; 1 equiv.) was dissolved in ^{t}BuOMe in a Young tube and to it was added LiCH$_2$^{t}Bu (0.0036 g, 0.046 mmol; 6.5 equiv.) The reaction was followed by ^{31}P{^{1}H} NMR spectroscopy for the next 24h. Complete conversion to [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)] and then **2** was confirmed over time, without turnover. Extensive transmetallation to form Li(PNP) (δ -5.86 (1:1:1:1 *q*, *J* = 57 Hz, 2P)) took place instead.

3) Catalysis screening: reaction between [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)] and KCH$_2$Ph (10 equiv.) in ^{t}BuOMe. [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)] (0.010 g, 0.016 mmol; 1 equiv.) was dissolved in ^{t}BuOMe in a Young tube and to it was added KCH$_2$Ph (0.021 g, 0.16 mmol; 10 equiv.) The reaction was followed by ^{31}P{^{1}H} NMR spectroscopy. Complete conversion to **2** was confirmed after 14 h, without turnover. Extensive transmetallation to K(PNP) (δ -1.01 (*s*, 2P)) took place.

4) Catalysis screening using 2 and PhSiH$_3$ (10 equiv.) in ^{t}BuOMe. Compound **2** (0.010 g, 0.016 mmol; 1 equiv.) was dissolved in ^{t}BuOMe in a Young tube and to it was added PhSiH$_3$ (10 μL, 0.08 mmol; 10 equiv.) The mixture was followed by ^{31}P{^{1}H} NMR spectroscopy over a period of 13 h, at r.t. No reaction took place.

XIII. X-Ray Crystallography. Data for [(PNP)Ti=CH^{t}Bu(O^{t}Bu)] (**3**) was collected on a Bruker KAPPA APEX II diffractometer equipped with an APEX II CCD detector. The data collection for complex 8 was carried out using Mo Kα radiation (graphite monochromator) with a frame time of 20 seconds and a detector distance of 5.0 cm. A randomly oriented region of reciprocal space was surveyed to achieve complete data with a redundancy of 4. Sections of frames were collected with 0.50º steps in ω and ϕ scans. Data to a resolution of 0.74 Å were considered in the reduction. Final cell constants were calculated from the xyz centroids of 4176

strong reflections from the actual data collection after integration (SAINT).[6] The intensity data were corrected for absorption (SADABS). [7] The final full matrix least squares refinement converged to R1 = 0.0484 and wR2 = 0.1312 (F2, all data). The remaining electron density for solvent was modeled unsuccessfully, thus the structure was treated with Platon SQUEEZE. [8]

The structure was solved using SIR-92[9] and refined (full-matrix-least squares) using the Oxford University Crystals for Windows system. [10] A direct-methods solution was calculated, which provided most non-hydrogen atoms from the electron density map. Full-matrix least squares / difference Fourier cycles were performed, which located the remaining non-hydrogen atoms. All ordered non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were placed in idealized positions and refined as riding atoms. The *tert*-butoxide and neopentylidene ligands of **3** exhibit positional disorder in the asymmetric unit which resulted in overlap of the two groups and their *tert*-butyl moieties. Additionally, the methyl carbons of the *tert*-butyl fragment of the neopentylidene substituent are further disordered over two positions. Disordered atoms were refined isotropically and hydrogens were not assigned.

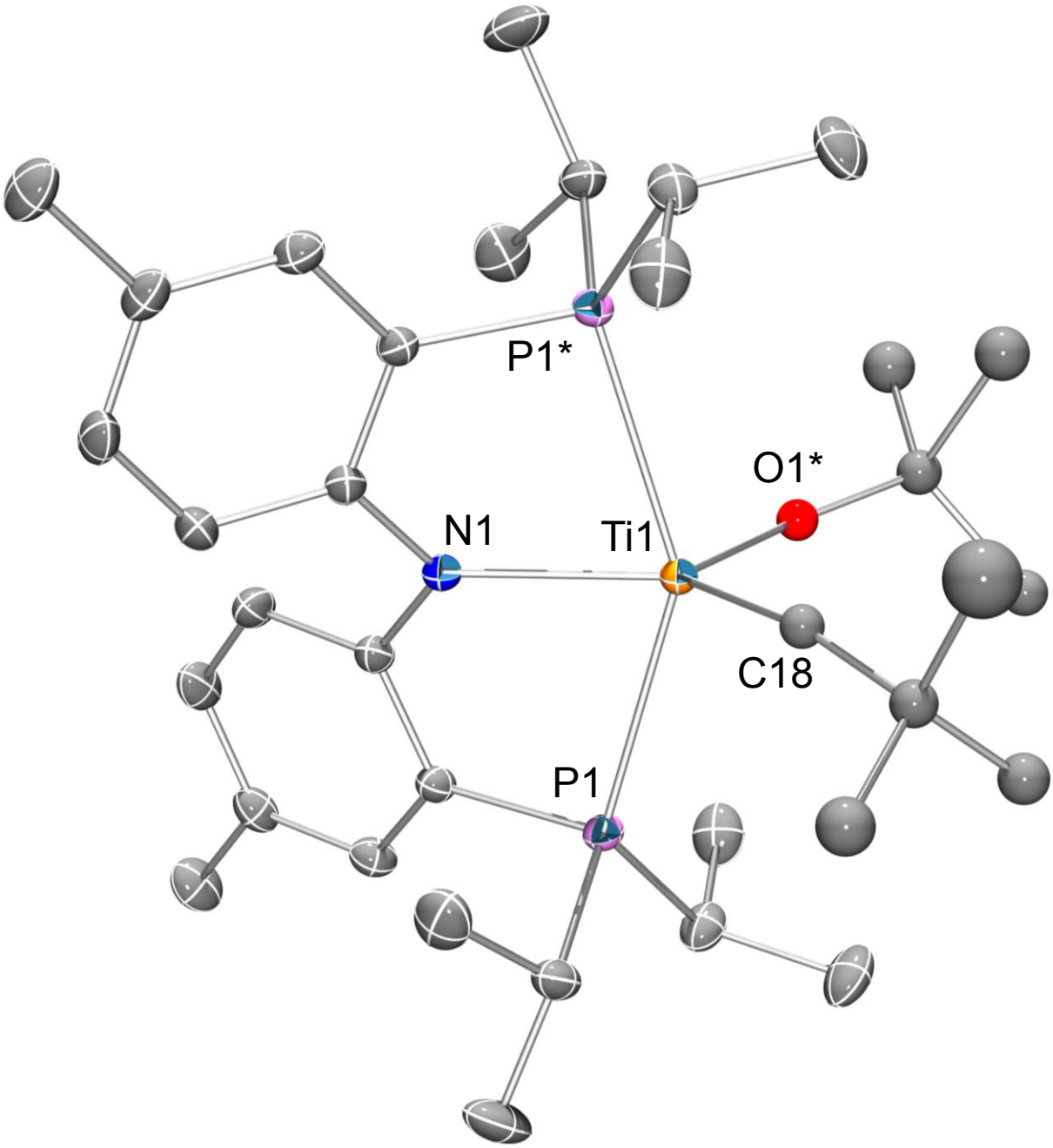

Figure S1. Solid state molecular structure of [(PNP)Ti=CH^{t}Bu(O^{t}Bu)] (**3**) with 50% probability ellipsoids. Asterisks denote symmetry generated atoms.

Table S3. X-ray crystallographic data for **3**.

	3
Empirical formula	$C_{35}H_{58}N_1O_1P_2Ti_1$
Crystal Habit, color	plate, yellow
Crystal size (mm)	0.503 × 0.268 × 0.040
Crystal system	Monoclinic
Space group	*C*2/*c*
Volume (Å^3)	4199.1(7)
a (Å)	11.4434(8)
b (Å)	30.85(2)
c (Å)	11.941(1)
α(°)	90
β(°)	94.996(1)
γ(°)	90
Z	4
Formula weight (g/mol)	618.70
Density (calculated) (Mg/m^3)	0.979
Absorption coefficient (mm^{-1})	0.302
F_{000}	1340
Final *R* indices ($I > 2\sigma(I)$]	R_1 = 0.0484, wR_2 = 0.1312
Largest diff. peak and hole (e$^-$Å^{-3})	0.72 and -0.73
GOF	0.9990

XIV. References-Experimental Section.

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XV. Selected NMR spectra of isolated compounds.

Unless otherwise stated, all spectra were obtained in C_6D_6 solution, at 296 K.

1) [(PNP)Ti=CH^{t}Bu(OEt)] (1).

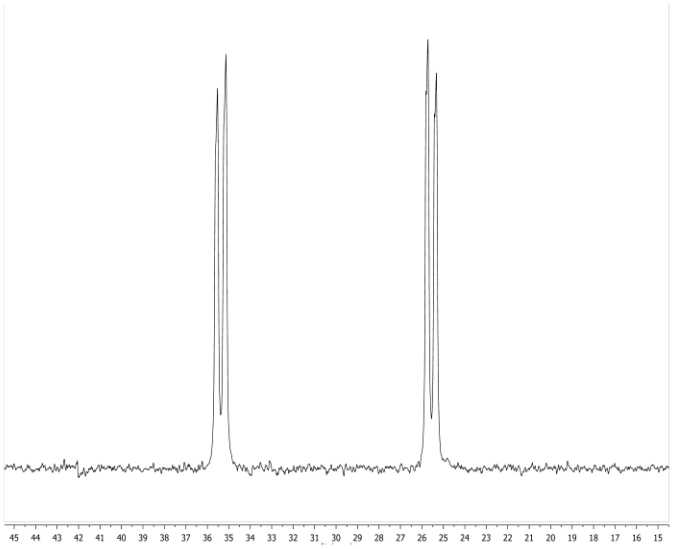


Fig. S2. $^{31}P\{^1H\}$ NMR spectrum of **1** at 121 MHz, showing two phosphorus environments.

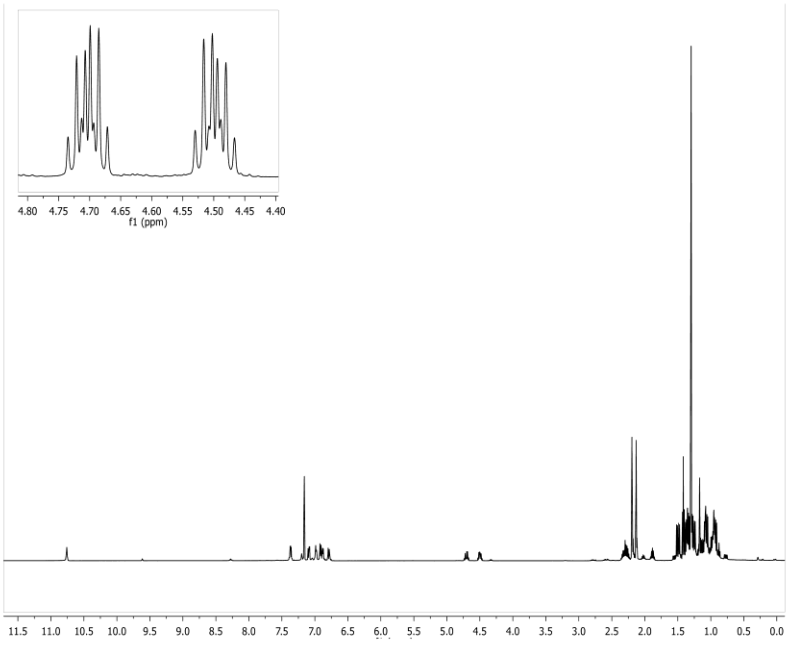


Fig. S3. ^1H NMR spectrum of **1** at 500 MHz showing in the inset, the multiplicities of the Ti–OCH_2CH$_3$ protons

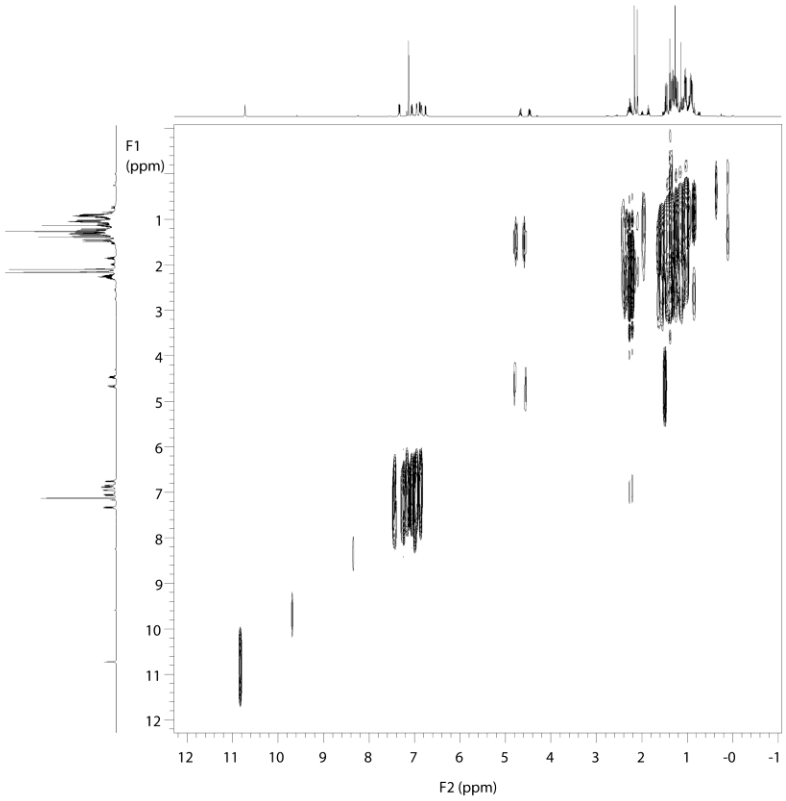


Fig. S4. gCOSY spectrum of **1** at 500 MHz

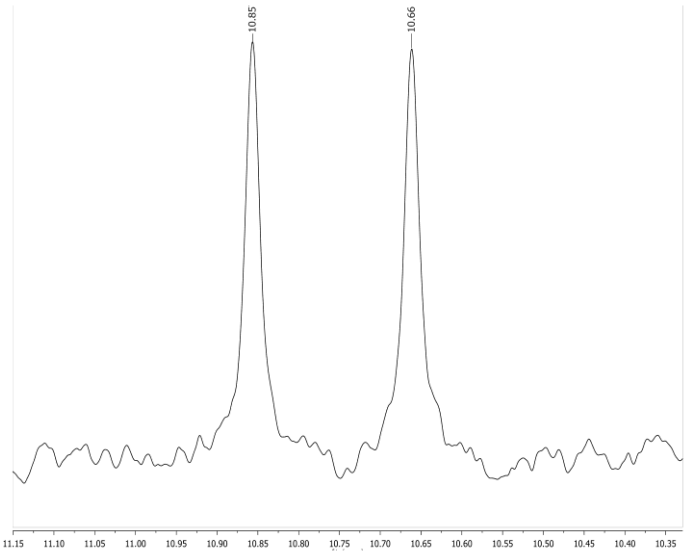


Fig. S5. Expansion of the 1D-HSQC spectrum (500 MHz) of **1** showing the 13C-splitting of the alkylidene peak

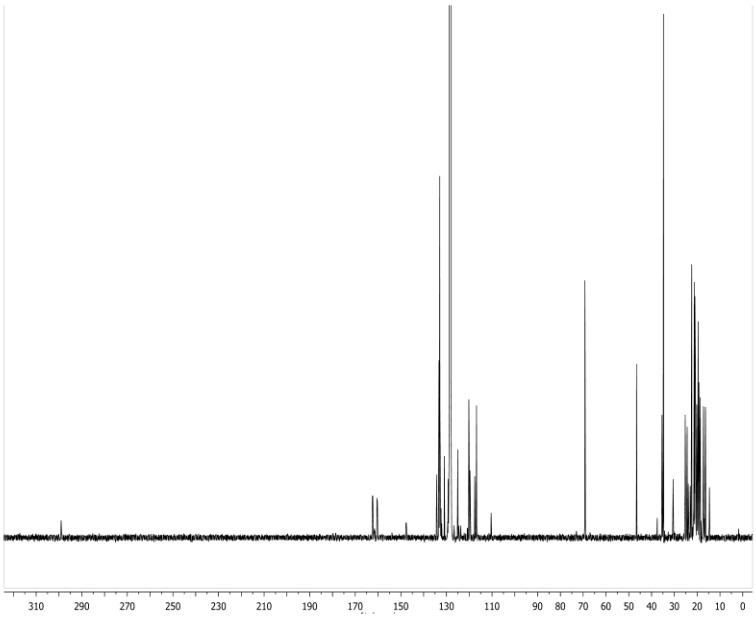


Fig. S6. $^{13}C\{^{1}H\}$ NMR spectrum of **1** at 100 MHz

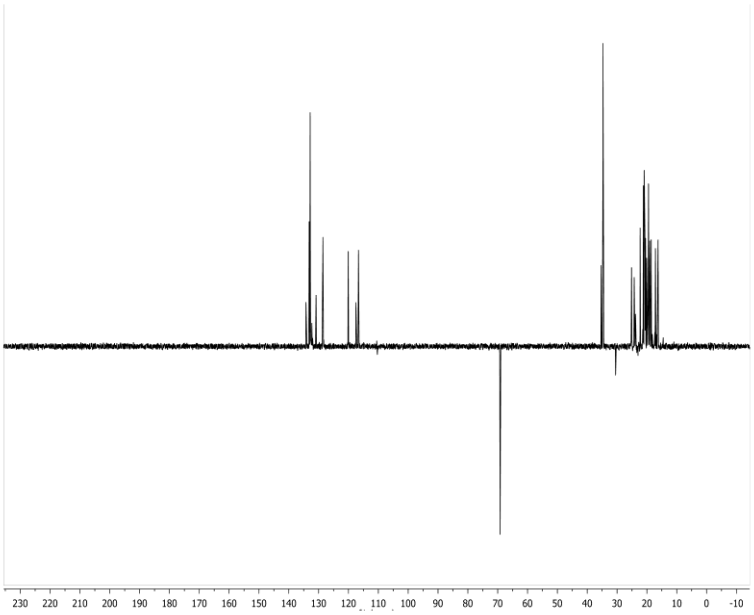


Fig. S7. DEPT-135 spectrum of **1** at 125 MHz, showing an intense negative peak for the Ti–OCH_2CH_3 carbon at 69.2 ppm

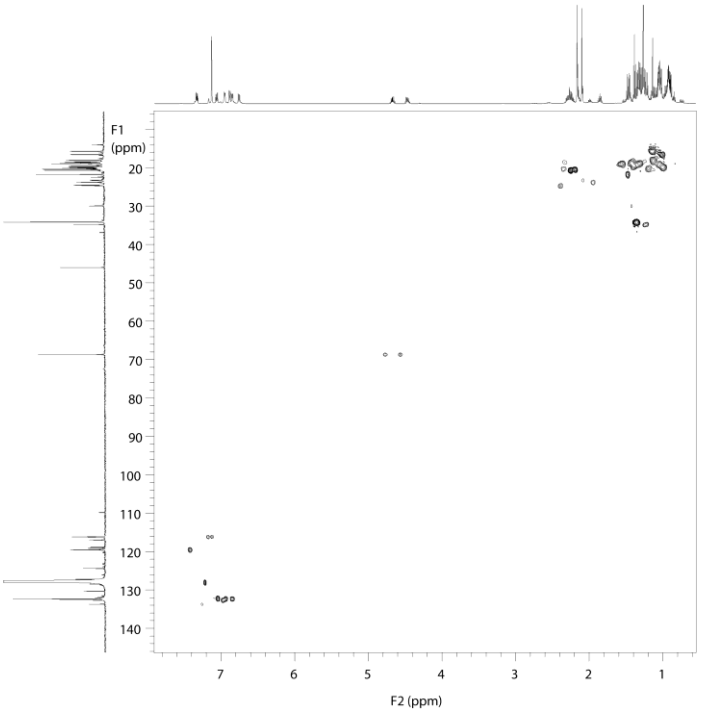


Fig. S8. Expansion (0-150 ppm) of the 2D-gHSQC spectrum of **1** at 500 MHz

2) [(PNP)Ti=CH^{t}Bu(OMe)] (2).

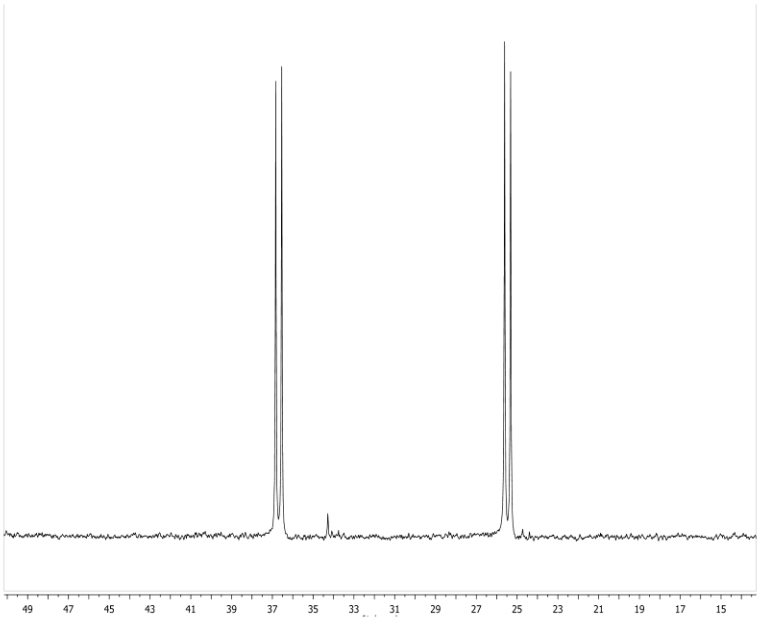


Fig. S9. $^{31}P\{^1H\}$ NMR spectrum of **2** at 162 MHz, showing two phosphorus environments.

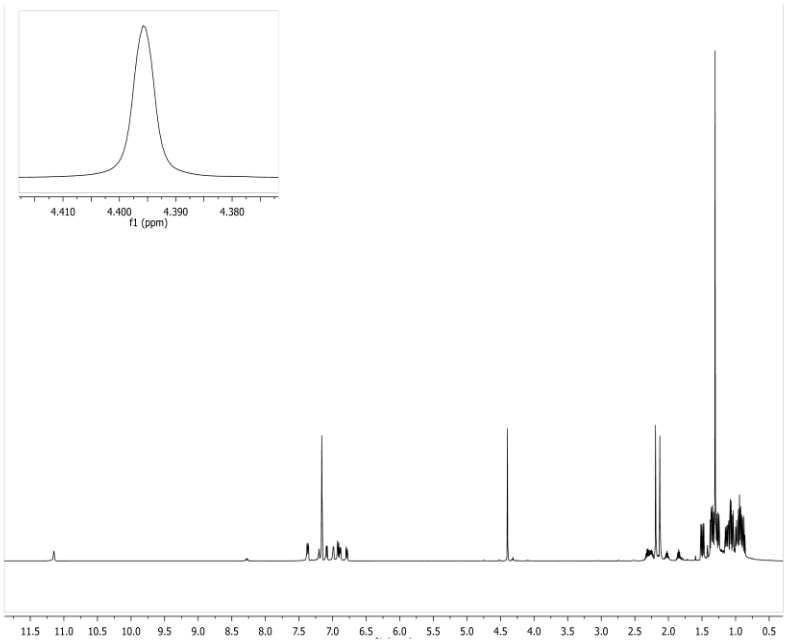


Fig. S10. ^{1}H NMR spectrum of **2** at 500 MHz showing in the inset, the multiplicity of the Ti–OCH_3 protons

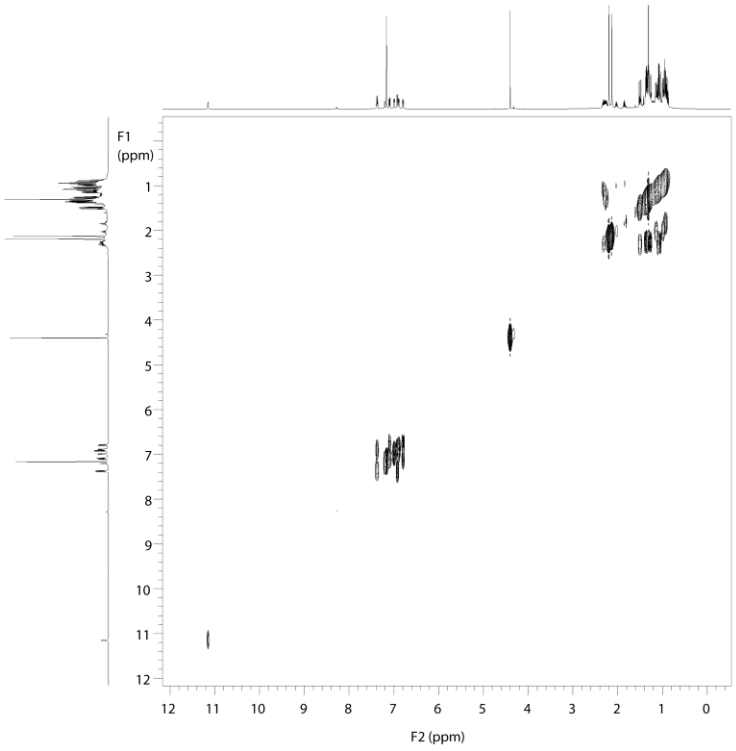


Fig. S11. Expansion of the gCOSY spectrum of **2** at 500 MHz

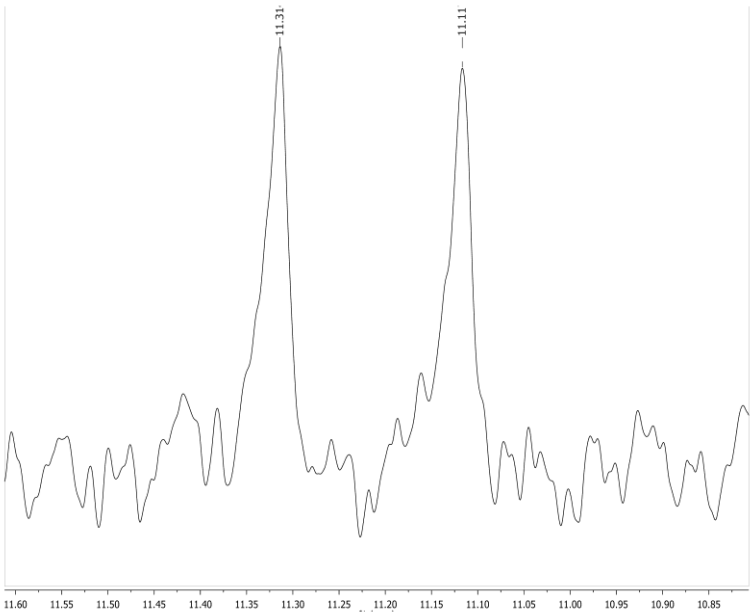


Fig. S12. Expansion of the 1D-HSQC spectrum (500 MHz) of **2**, showing the 13C-splitting of the alkylidene peak

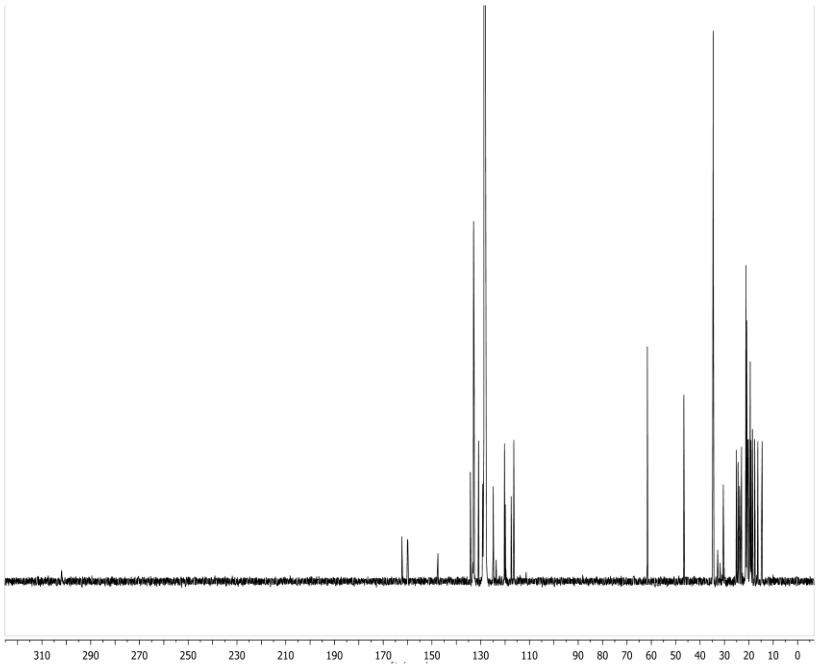


Fig. S13. $^{13}C\{^{1}H\}$ NMR spectrum of **2** at 125 MHz

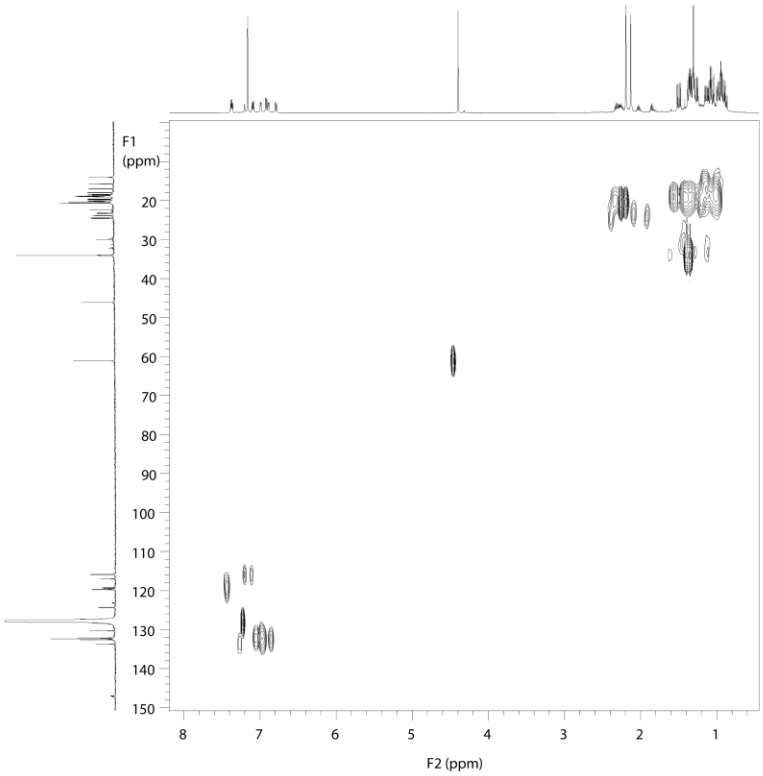


Fig. S14. Expansion of the 2D-gHSQC spectrum of **2**

3) [(PNP)Ti=CH^{t}Bu(O^{t}Bu)] (3).

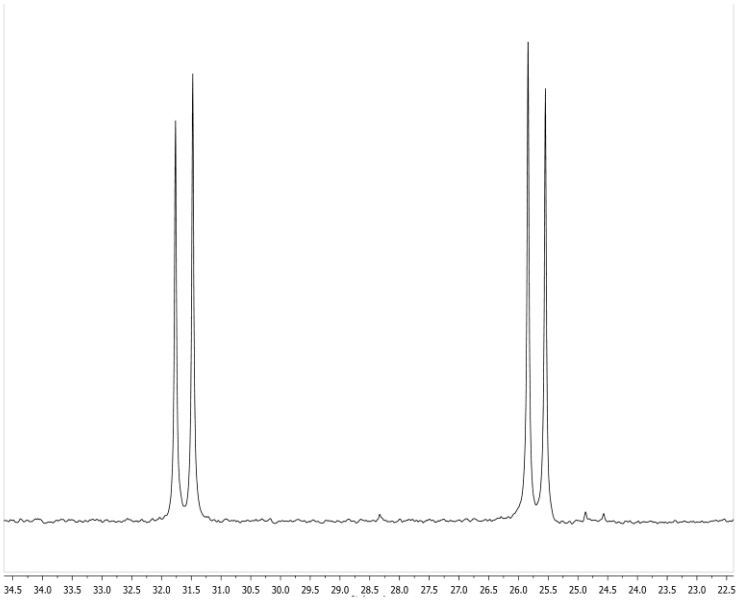


Fig. S15. $^{31}P\{^1H\}$ NMR spectrum of **3** at 162 MHz, showing two phosphorus environments.

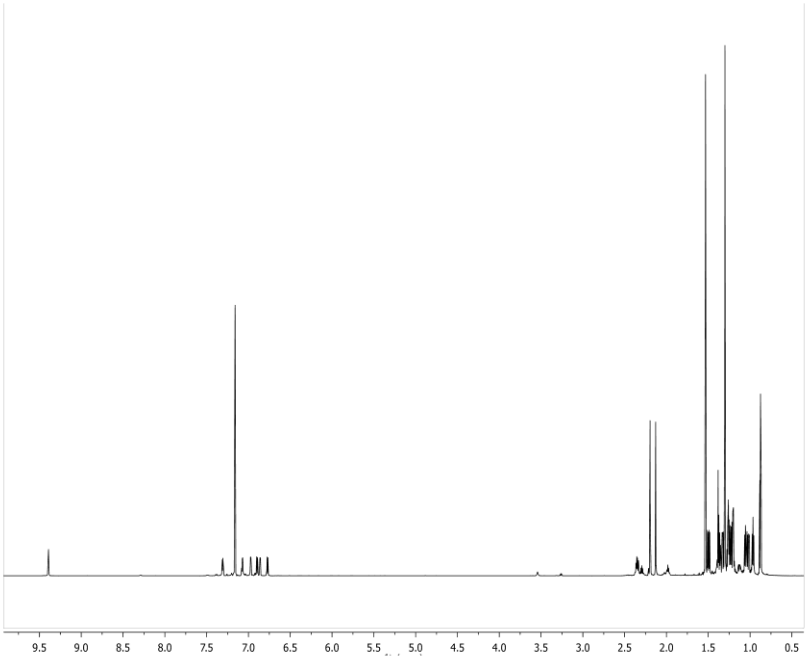


Fig. S16. ^{1}H NMR spectrum of **3** at 800 MHz

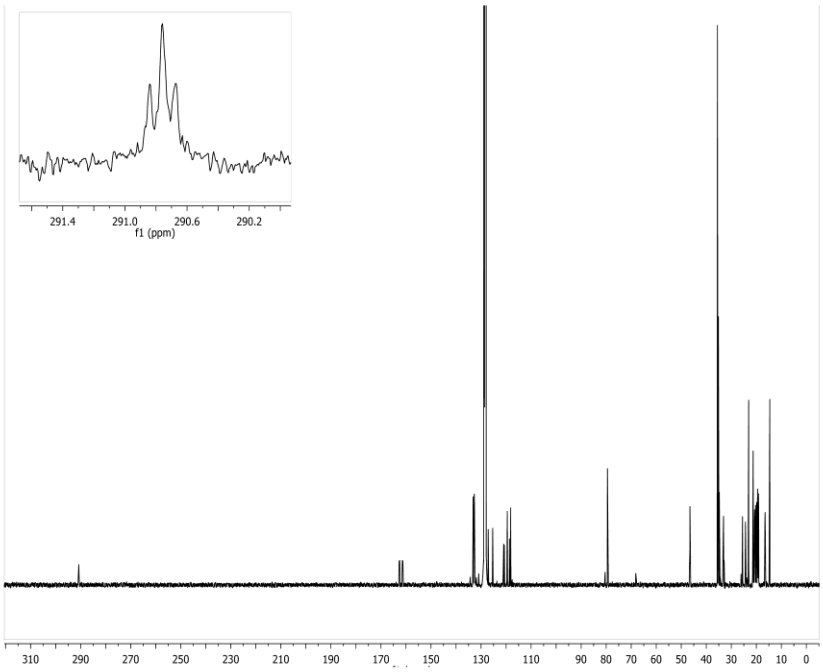


Fig. S17. ^{13}C{^{1}H} NMR spectrum of **3** at 100 MHz showing in the inset, the multiplicity of the alkylidene peak

3) [(PNP)Ti=CH^{t}Bu(O^{n}Pr)] (4).

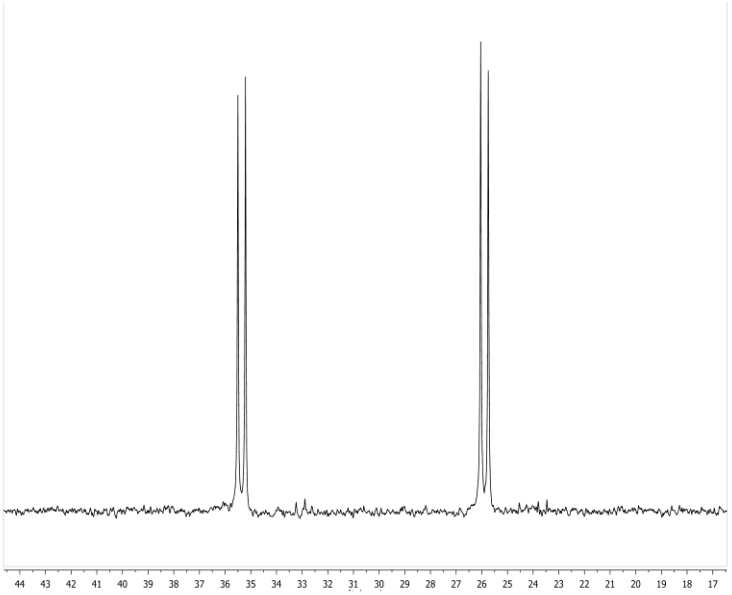


Fig. S18. $^{31}P\{^{1}H\}$ NMR spectrum of **4** at 162 MHz, showing two phosphorus environments.

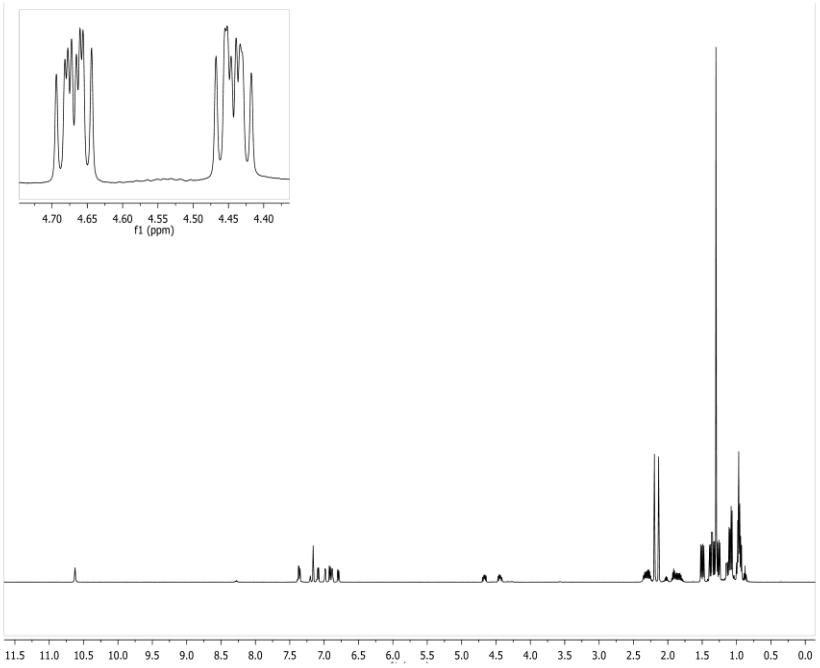


Fig. S19. ^{1}H NMR spectrum of **4** at 500 MHz, showing in the inset the multiplicities of the Ti–OCH_2CH$_2$CH$_3$ protons

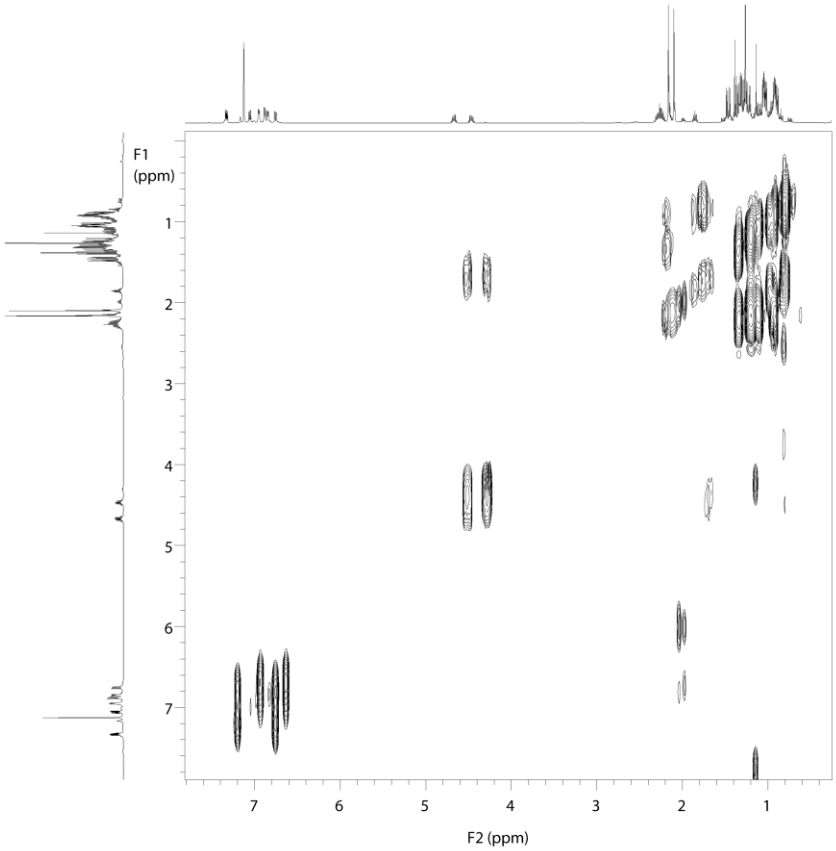


Fig. S20. dqCOSY spectrum of **4** at 500 MHz

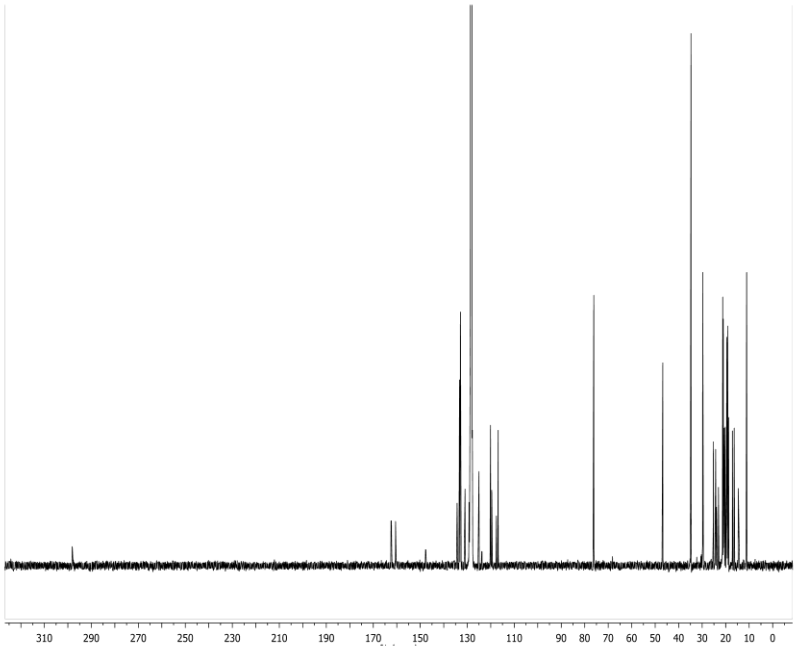


Fig. S21. $^{13}C\{^{1}H\}$ NMR spectrum of **4** at 125 MHz

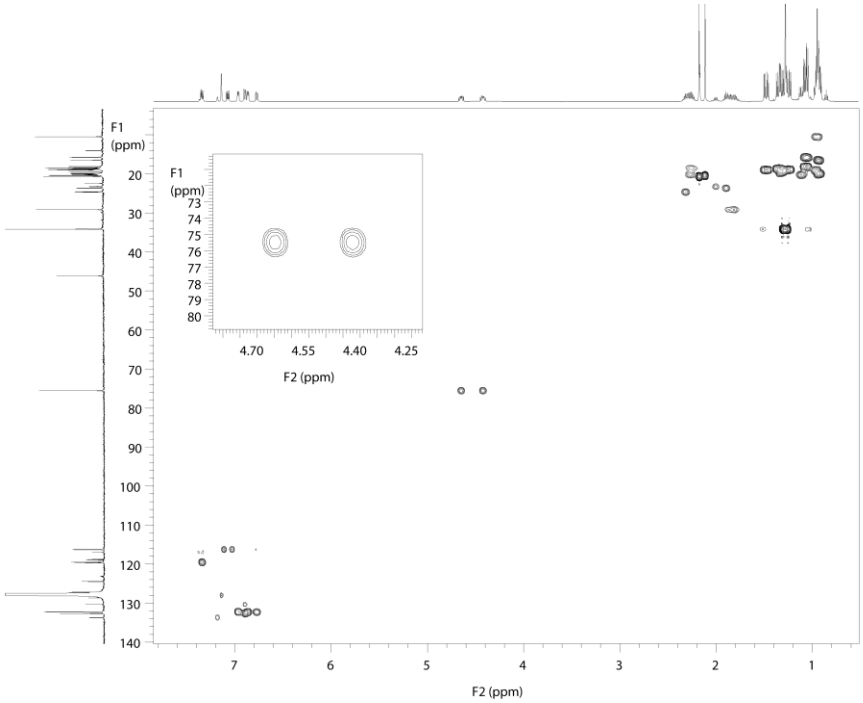


Fig. S22. 2D-gHSQC spectrum of **4** showing in the inset, the contour for the Ti–O*CH*$_2$CH$_2$CH$_3$ fragment

4) [(PNP)Ti=CH^{t}Bu(O^{n}Bu)] (6).

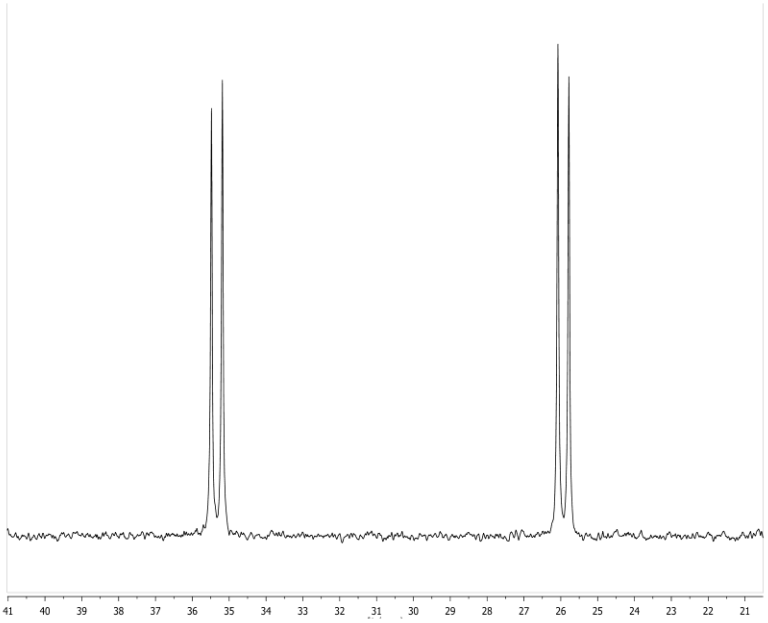


Fig. S23. $^{31}P\{^1H\}$ NMR spectrum of **6** at 162 MHz, showing two phosphorus environments.

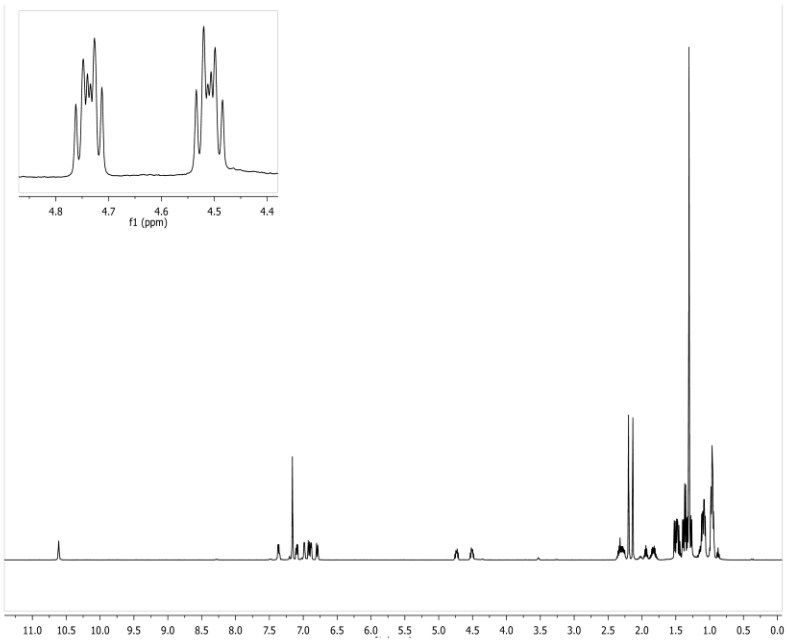


Fig. S24. ^{1}H NMR spectrum of **6** at 500 MHz showing in the inset, the multiplicities of the Ti–OCH_2CH$_2$CH$_2$CH$_3$ protons

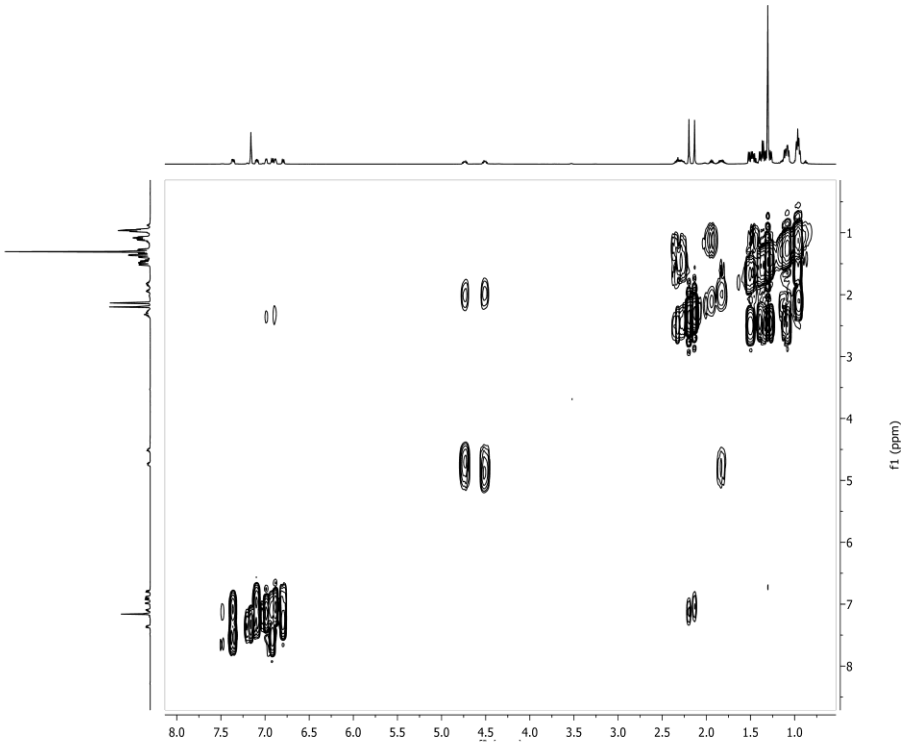


Fig. S25. dqCOSY spectrum of **6** at 500 MHz

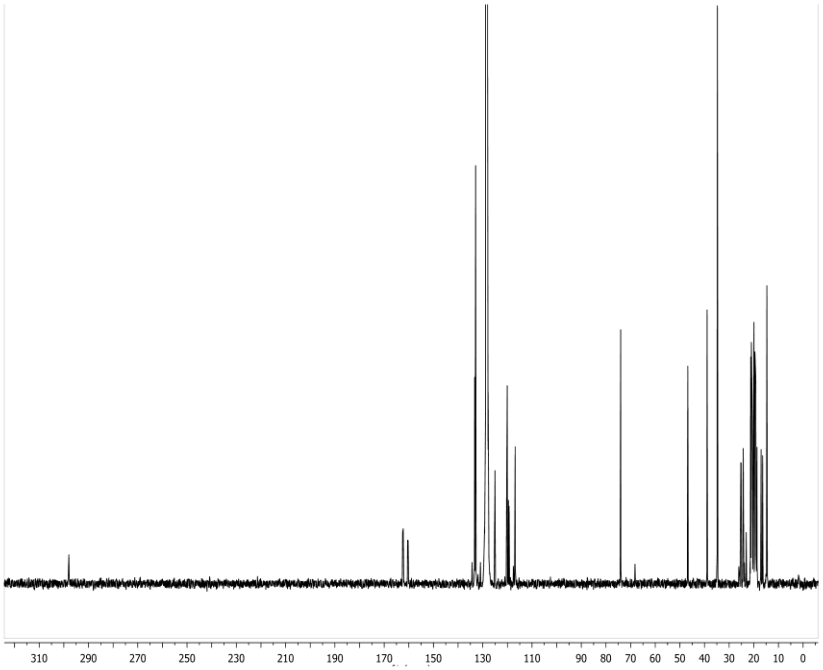


Fig. S26. $^{13}C\{^{1}H\}$ NMR spectrum of **6** at 100 MHz

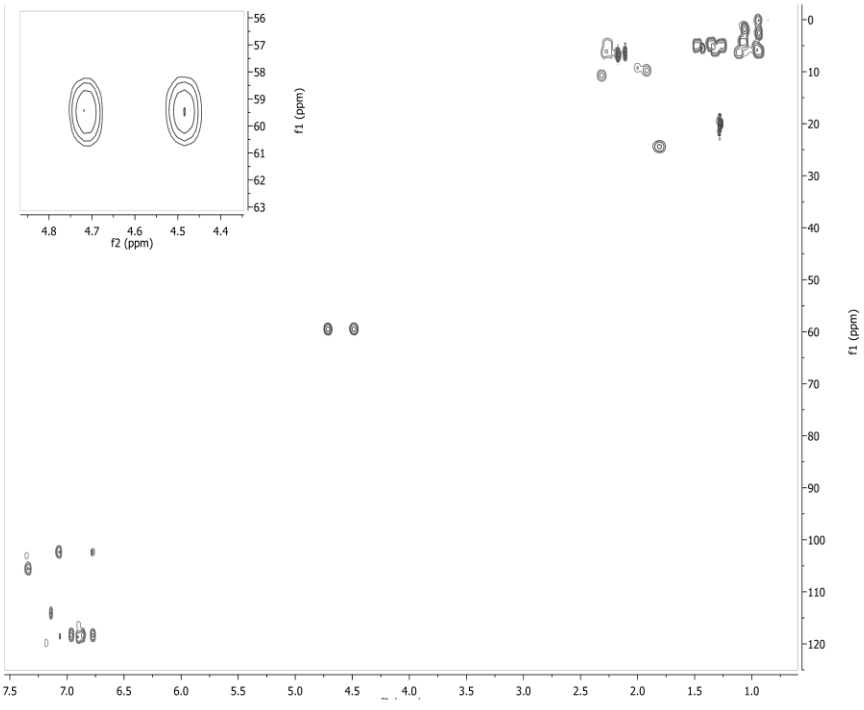


Fig. S27. Multiplicity edited gHSQC spectrum of **6** at 500 MHz, showing the diastereotopic methylenic protons in Ti–O$CH_2CH_2CH_2CH_3$ in the inset.

5) [(PNP)Ti=CH^{t}Bu(O^{i}Pr)] (8).

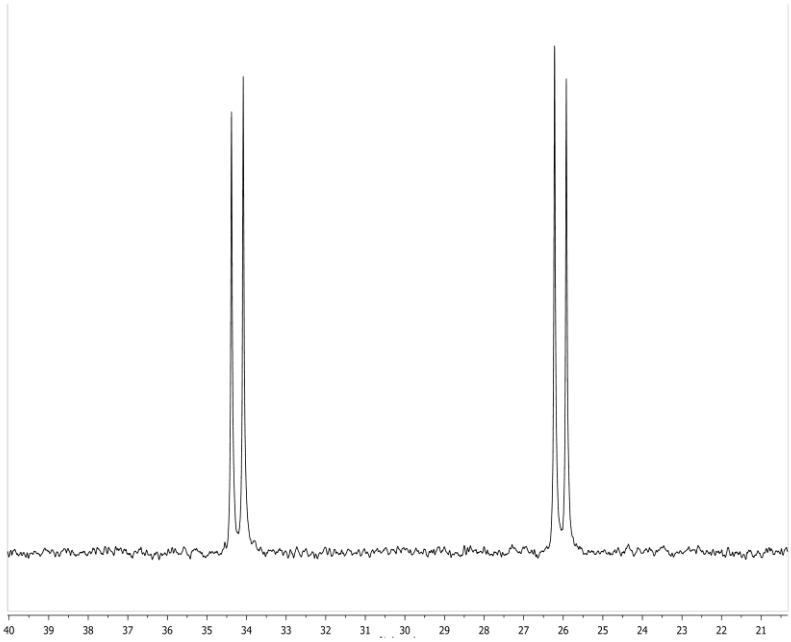


Fig. S28. $^{31}P\{^1H\}$ NMR spectrum of **8** at 162 MHz, showing two phosphorus environments.

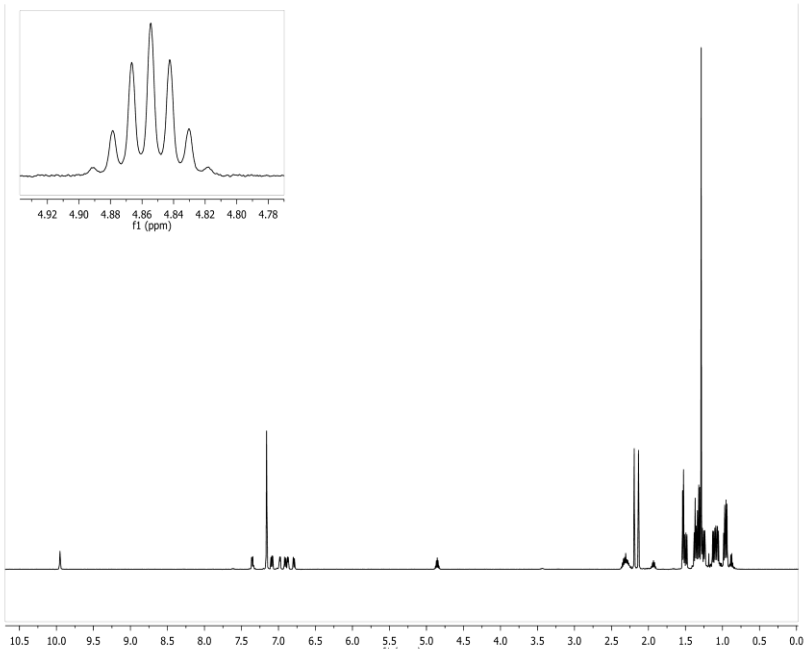


Fig. S29. ^1H NMR spectrum of **8** at 500 MHz showing in the inset, the multiplicity of the Ti–OC*H*$(CH_3)_2$ proton

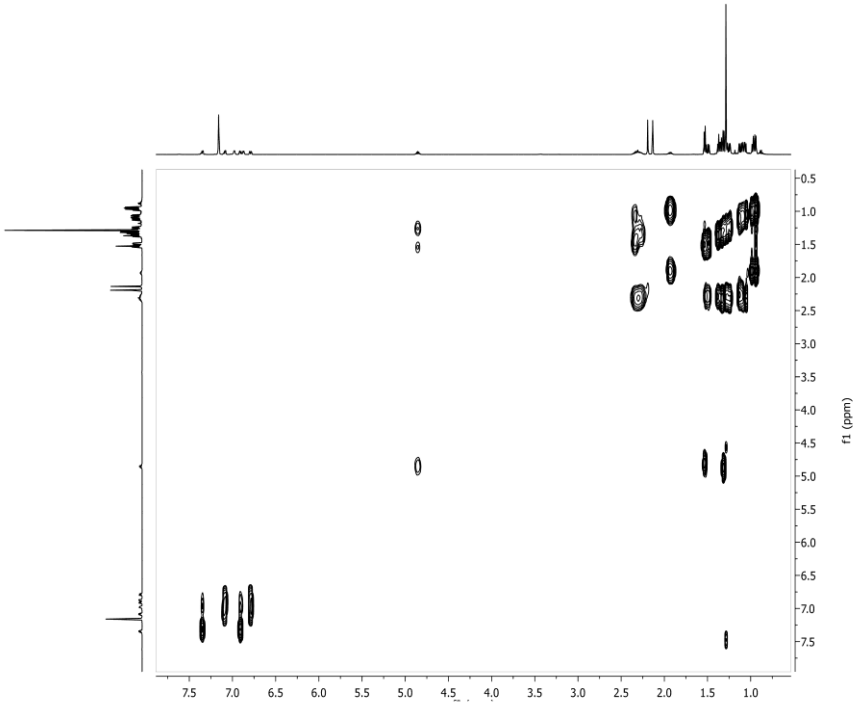


Fig. S30. dqCOSY spectrum of **8** at 500 MHz

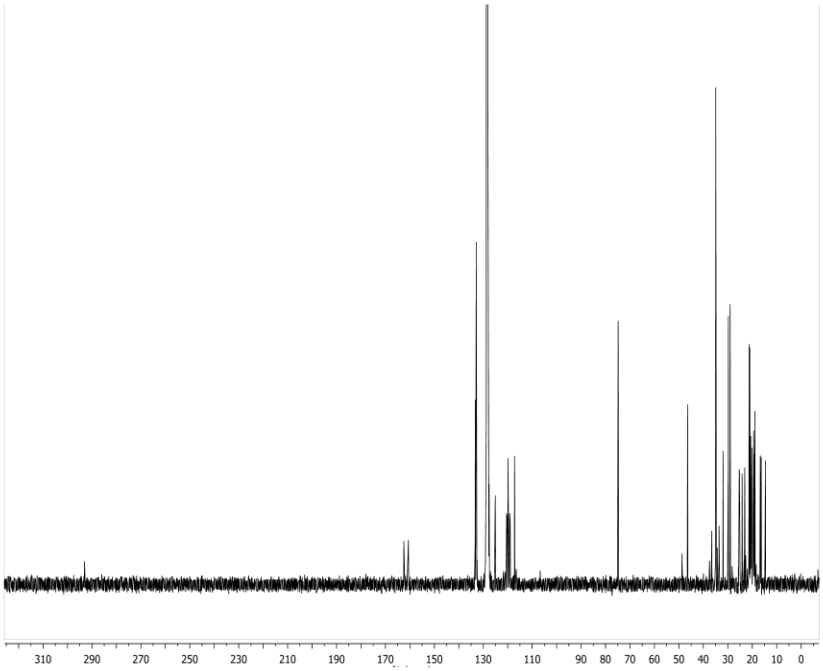


Fig. S31. $^{13}C\{^{1}H\}$ NMR spectrum of **8** at 125 MHz showing in the inset, the multiplicity of the alkylidene peak

XVI. Kinetics experiments, selected NMR spectroscopic data.

Unless otherwise stated, all spectra were acquired at 162 MHz, at 29.5 ± 0.1 °C in neat ether solutions. The peak for the internal standard (PMe_3 in C_6D_6, δ = -61.9 ppm, *s*) is not shown.

1) ^{t}BuOMe activation

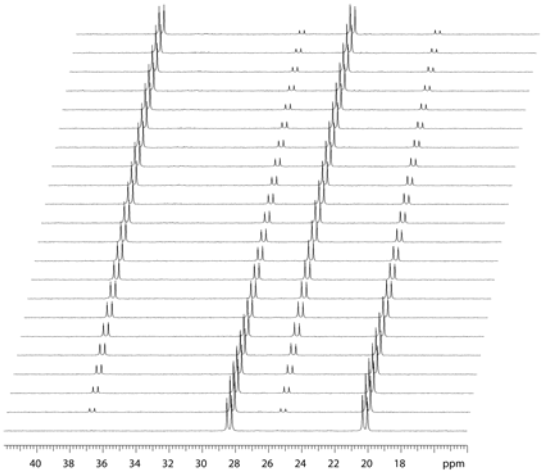


Fig. S32. Expanded view of arrayed $^{31}P\{^1H\}$ NMR stacked spectra from a typical ^{t}BuOMe activation run, showing the decay of [(PNP)Ti=CH^{t}Bu($CH_2{}^t$Bu)] and the exclusive formation of **2**

2) Et_2O activation

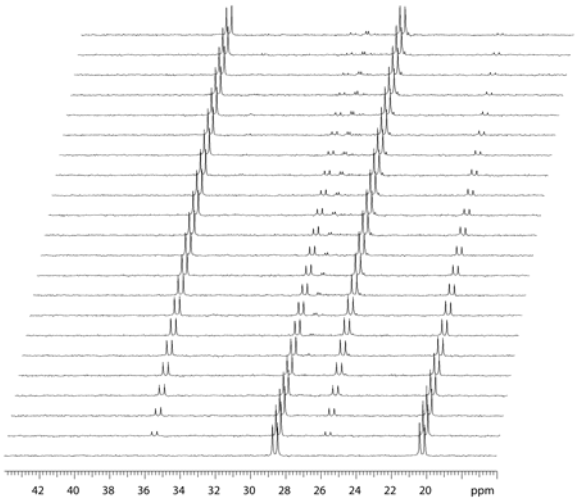


Fig. S33. Expanded view of arrayed $^{31}P\{^1H\}$ NMR stacked spectra from a typical Et_2O activation run, showing the decay of [(PNP)Ti=CH*t*Bu(CH_2*t*Bu)] and simultaneous formation of **1** and [(PNP)Ti(η^2-H_2C=CH_2)(CH_2*t*Bu)] (barely visible)

3) Et_2O-d_{10} activation

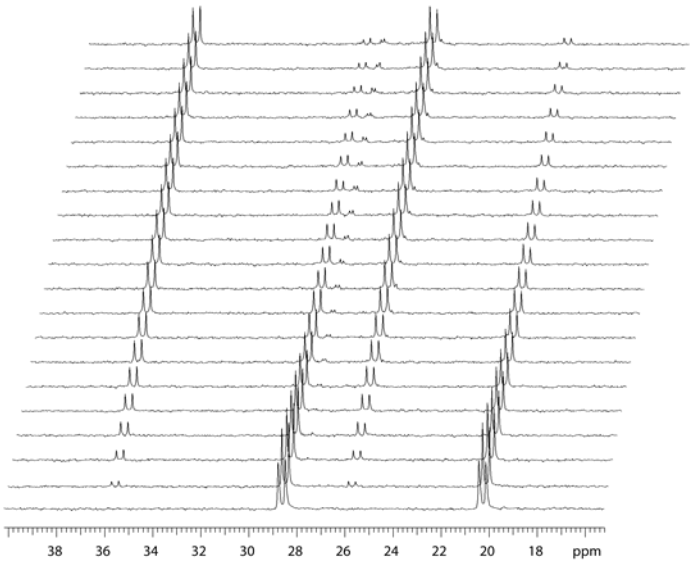


Fig. S34. Expanded view of arrayed $^{31}P\{^1H\}$ NMR stacked spectra from a typical Et_2O-d_{10} activation run, showing the decay of [(PNP)Ti=CH^{t}Bu($CH_2{}^t$Bu)] and the simultaneous formation of [(PNP)Ti=CD^{t}Bu(OCD_2CD_3)] and [(PNP)Ti(η^2-D_2C=CD_2)($CD_2{}^t$Bu)] (barely visible)

4) $^n Pr_2O$ activation

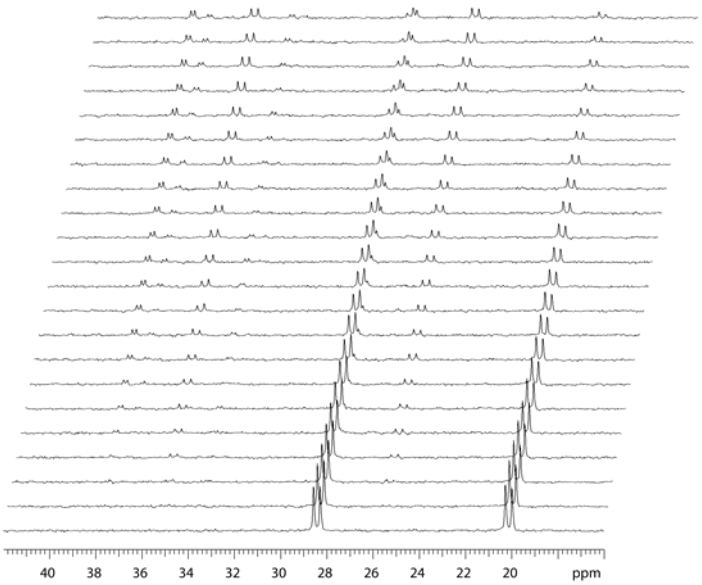


Fig. S35. Expanded view of arrayed $^{31}P\{^1H\}$ NMR stacked spectra from a typical $^nPr_2O$ activation run, showing the decay of [(PNP)Ti=CH^{t}Bu($CH_2{}^t$Bu)] with concomitant formation of **4**, **5a** and **5b**

5) $^{n}Bu_2O$ activation

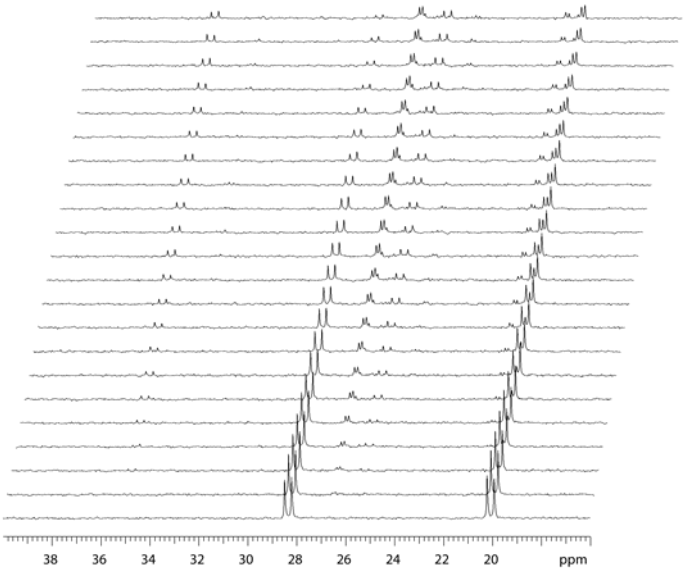


Fig. S36. Expanded view of arrayed $^{31}P\{^{1}H\}$ NMR stacked spectra from a typical $^{n}Bu_2O$ activation run, showing the decay of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)] with concomitant formation of **6**, **7a** and **7b**

6) ^{t}BuOEt activation

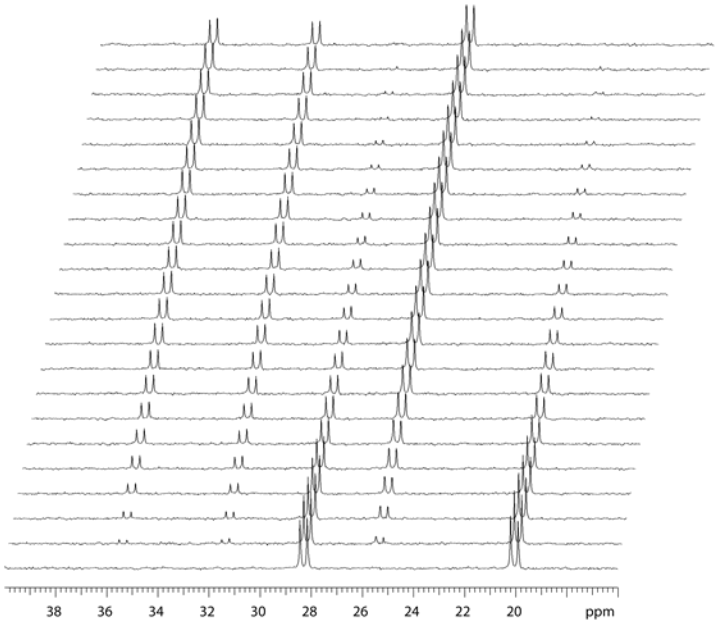


Fig. S37. Expanded view of arrayed $^{31}P\{^{1}H\}$ NMR stacked spectra from a typical ^{t}BuOEt activation run, showing the decay of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)] and simultaneous formation of **1** and **3**; the doublets at δ = 25.5 ppm of either product overlap

7) $^{i}Pr_2O$ activation

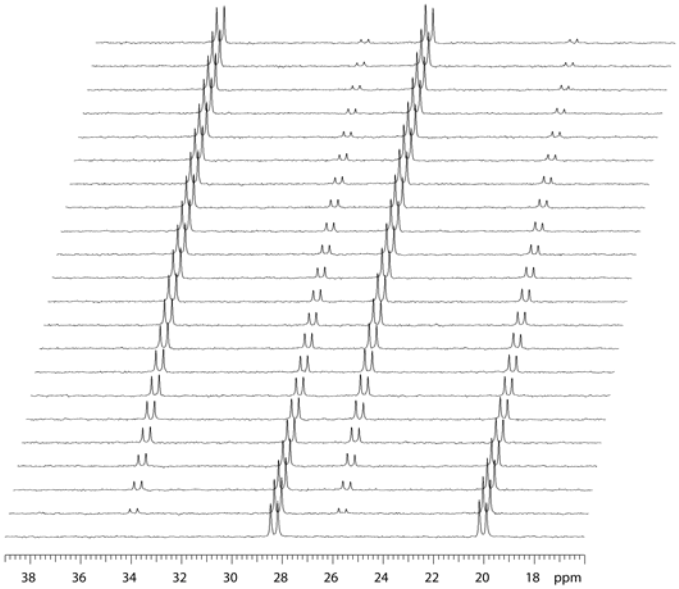


Fig. S38. Expanded view of arrayed $^{31}P\{^{1}H\}$ NMR stacked spectra from a typical $^{i}Pr_2O$ activation run, showing the decay of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)] and exclusive formation of **8**.

7) Competing ^{t}BuOMe:Et$_2$O activation

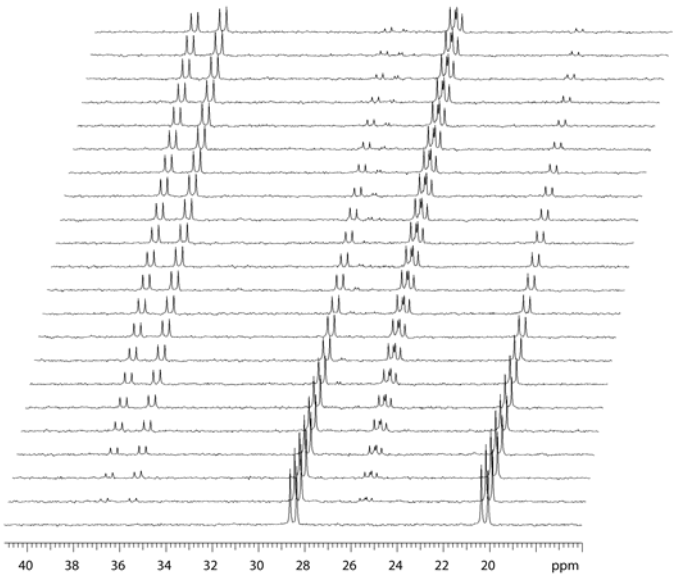


Fig. S39. Expanded view of arrayed $^{31}P\{^{1}H\}$ NMR stacked spectra from a typical competing ^{t}BuOMe:Et$_2$O activation run, showing the decay of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)] and simultaneous formation of **3** and **4**.

8) Pentane activation(*)

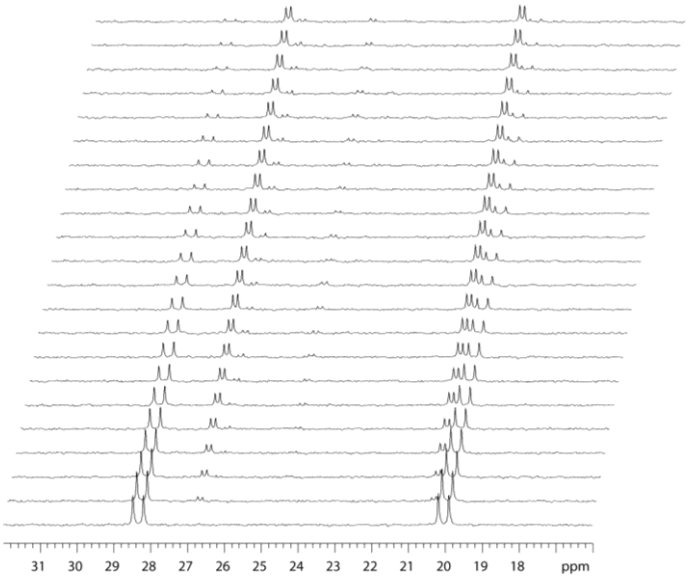


Fig. S40. Expansion of arrayed $^{31}P\{^{1}H\}$ NMR stacked spectra from a typical pentane activation run, showing the decay of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)] and the exclusive formation of diastereomers of the type, [(PNP)Ti(CH$_2$^{t}Bu)(η^2-*C*H$_2$=*C*H-(CH$_2$)$_2$CH$_3$)], in ~4:1 ratio.

9) Cyclohexane activation(*)

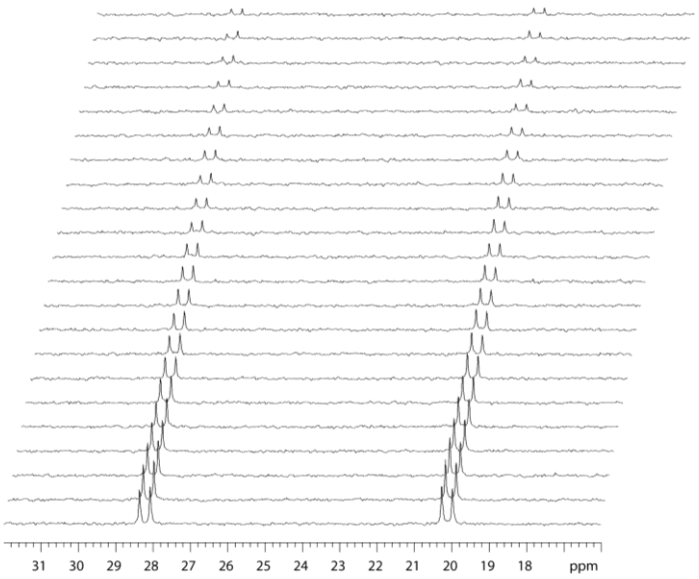


Fig. S41. Expansion of arrayed $^{31}P\{^{1}H\}$ NMR stacked spectra from a typical cyclohexane activation run, showing the decay of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)]. No products are observed, indicative of the large instability of [(PNP)Ti(CH$_2$^{t}Bu)(cyclohexene)] adducts.

XVII. Kinetics experiments plots.

1) ^{t}BuOMe activation

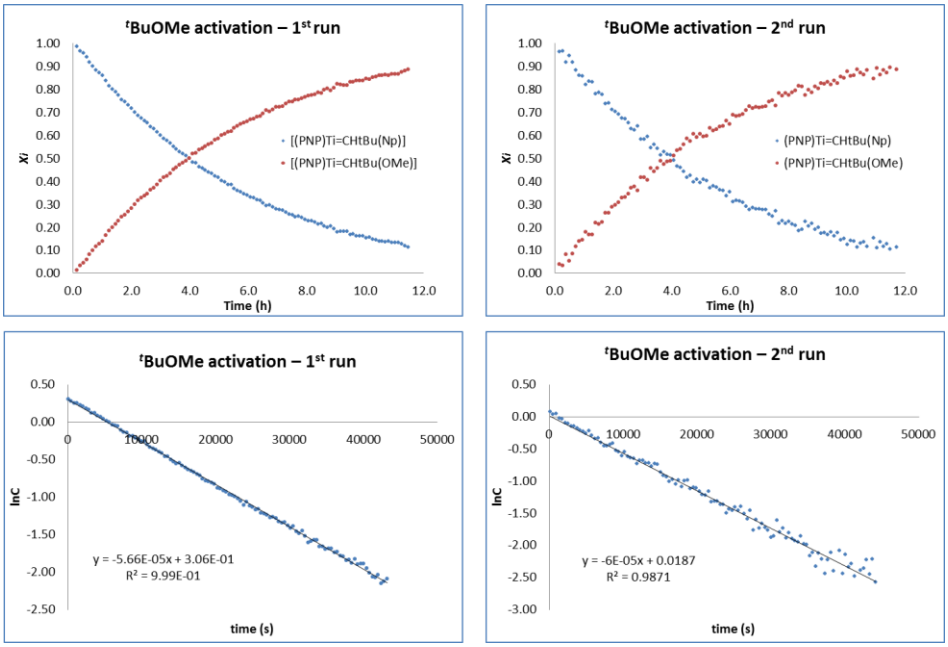


Fig. S42. Substrate decay and product formation curves in ^{t}BuOMe with the respective logarithmic plots for decay of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)]

2) Et_2O activation

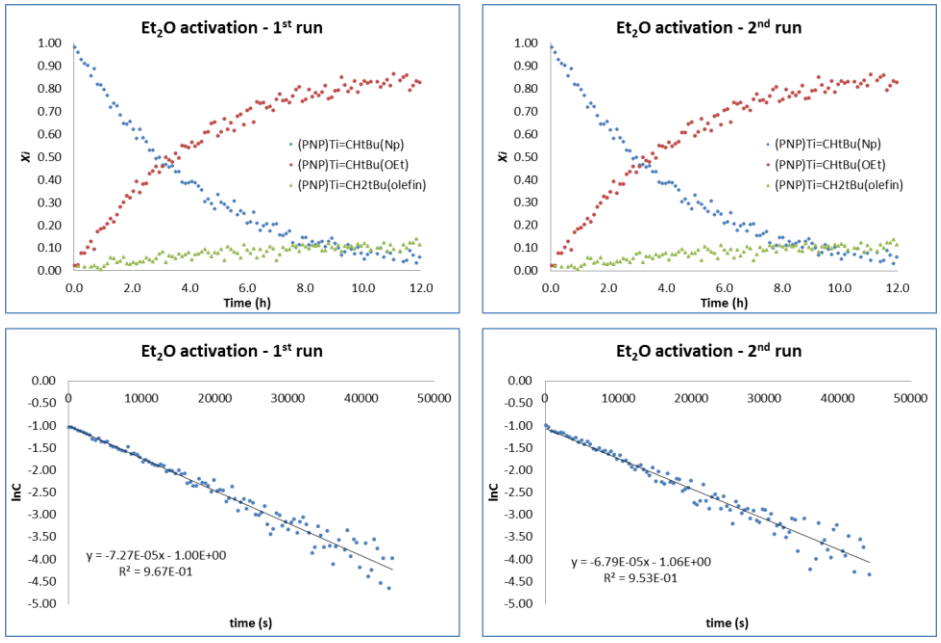


Fig. S43. Substrate decay and product formation curves in Et_2O with the respective logarithmic plots for decay of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)]

3) Et_2O-d_{10} activation

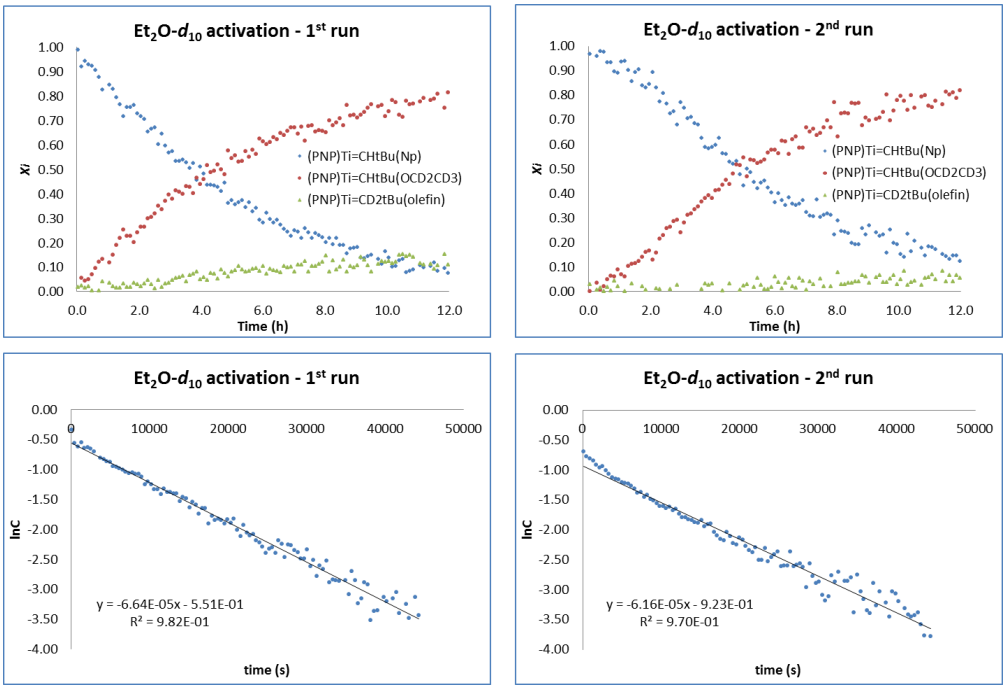


Fig. S44. Substrate decay and product formation curves in Et_2O-d_{10} with the respective logarithmic plots for decay of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)]

4) ^{n}Pr$_2$O activation

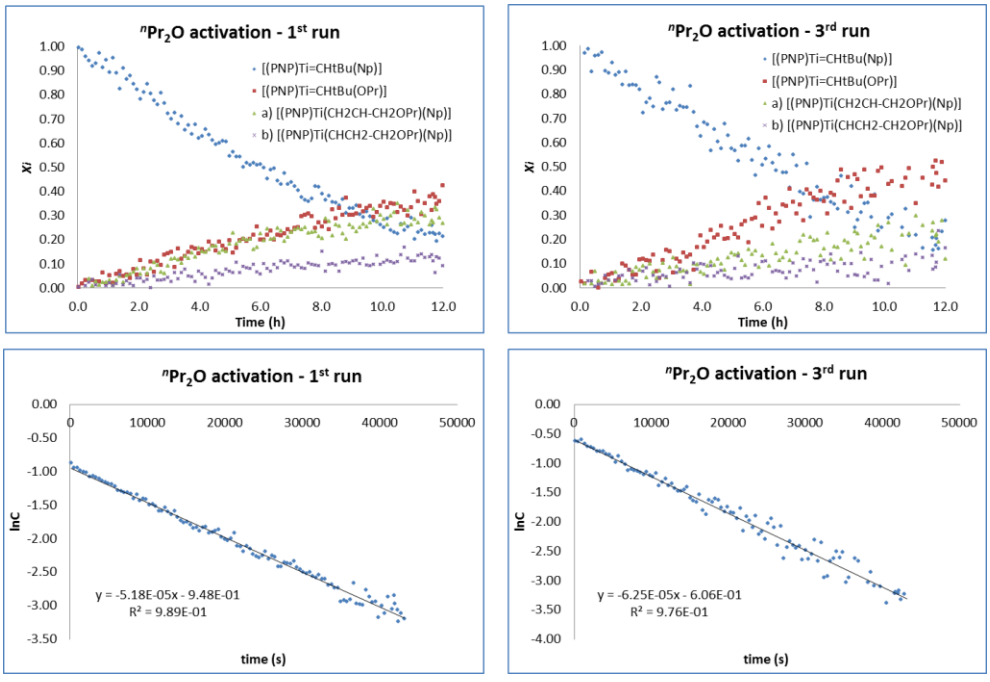


Fig. S45. Substrate decay and product formation curves in ^{n}Pr$_2$O with the respective logarithmic plots for decay of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)]

5) $^{n}Bu_2O$ activation

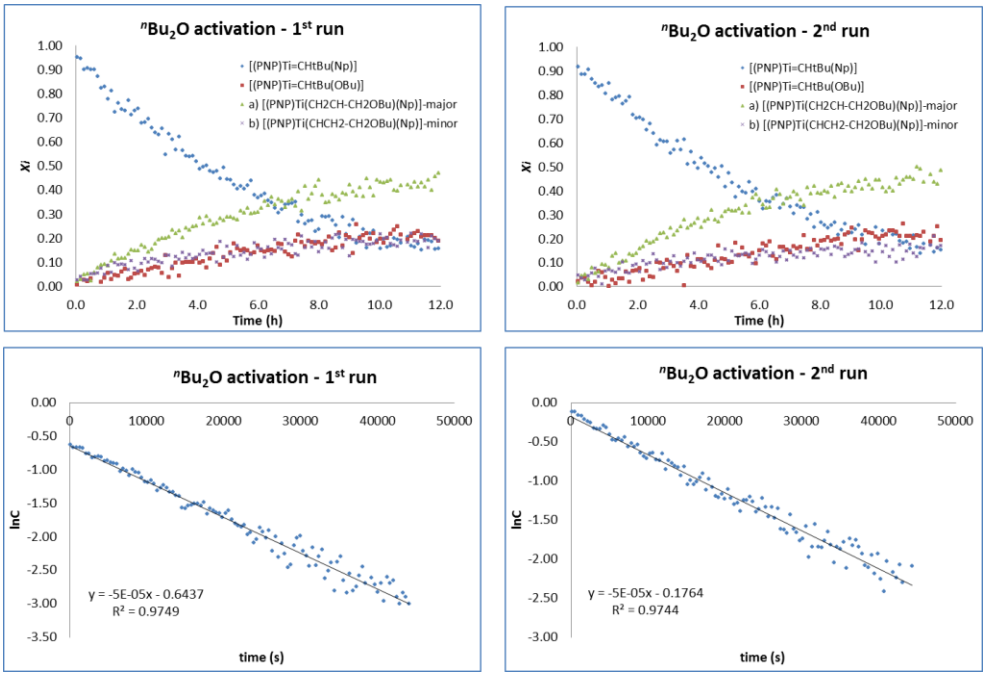


Fig. S46. Substrate decay and product formation curves in $^{n}Bu_2O$ with the respective logarithmic plots for decay of [(PNP)Ti=CH^{t}Bu(CH_2^{t}Bu)]

6) ^{t}BuOEt activation

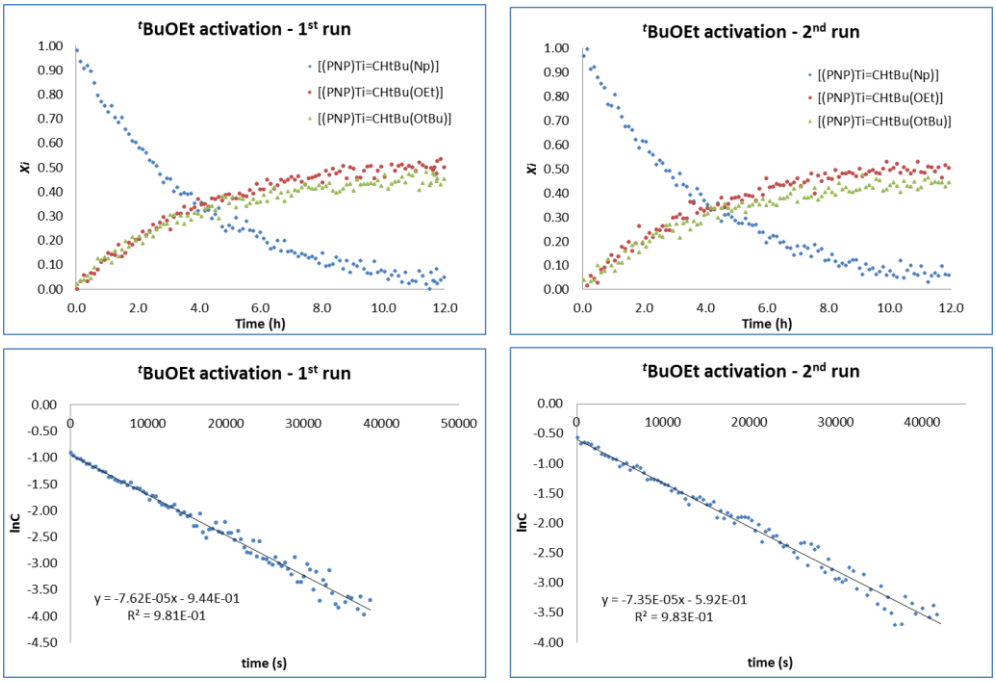


Fig. S47. Substrate decay and product formation curves in ^{t}BuOEt with the respective logarithmic plots for decay of [(PNP)Ti=CH^{t}Bu(CH_2^{t}Bu)]

7) $^{i}Pr_2O$ activation

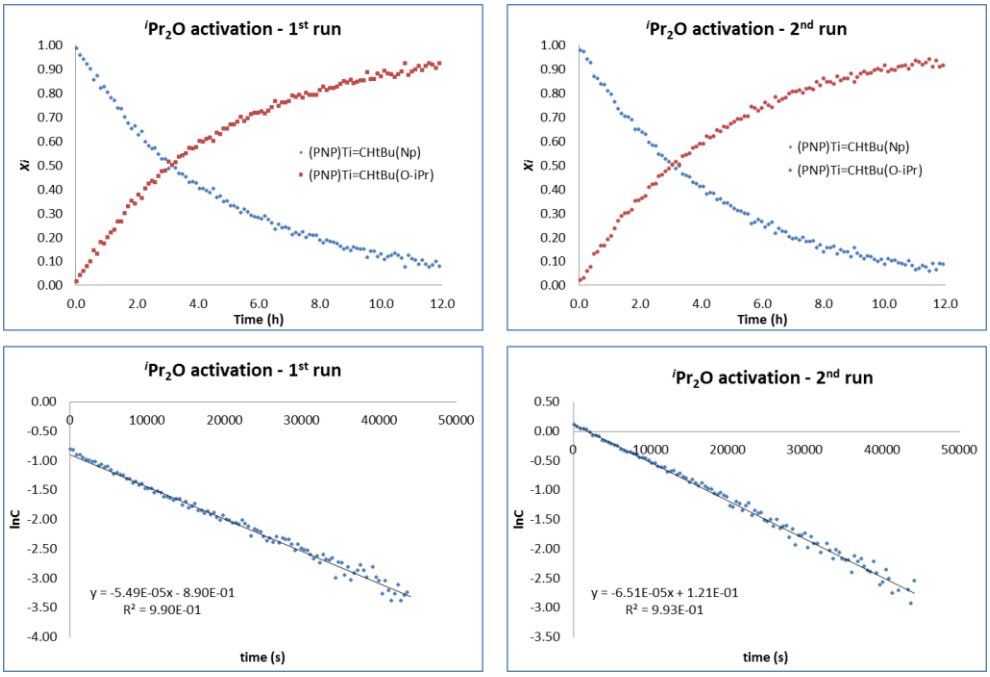


Fig. S48. Substrate decay and product formation curves in $^{i}Pr_2O$ with the respective logarithmic plots for decay of [(PNP)Ti=CH^{t}Bu($CH_2{}^{t}$Bu)]

8) Competing ^{t}BuOMe:Et_2O activation

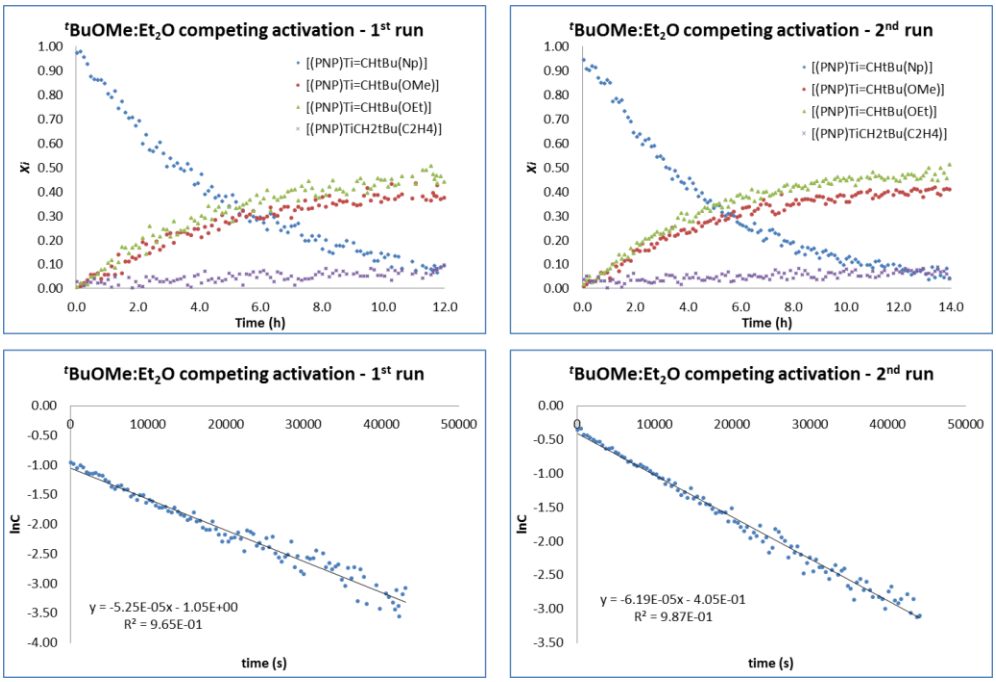


Fig. S49. Substrate decay and product formation curves in ^{t}BuOMe:Et_2O with the respective logarithmic plots for decay of [(PNP)Ti=CH^{t}Bu($CH_2{}^{t}$Bu)]

9) Pentane activation(*)

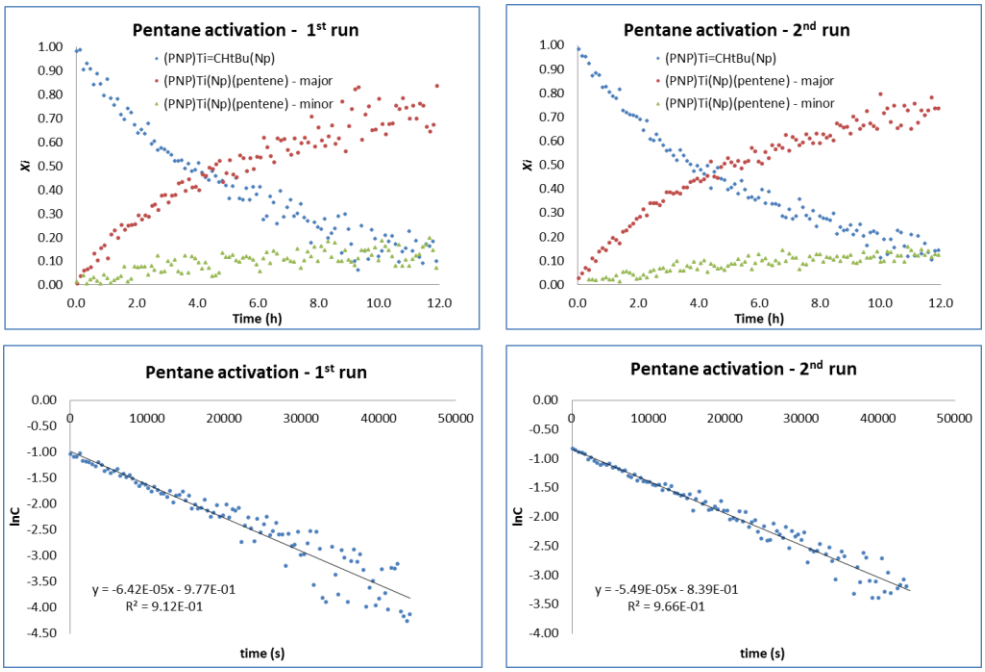


Fig. S50. Substrate decay and product formation curves in Pentane with the respective logarithmic plots for decay of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)]. (*)For comparison with ether-activations.

10) Cyclohexane activation(*)

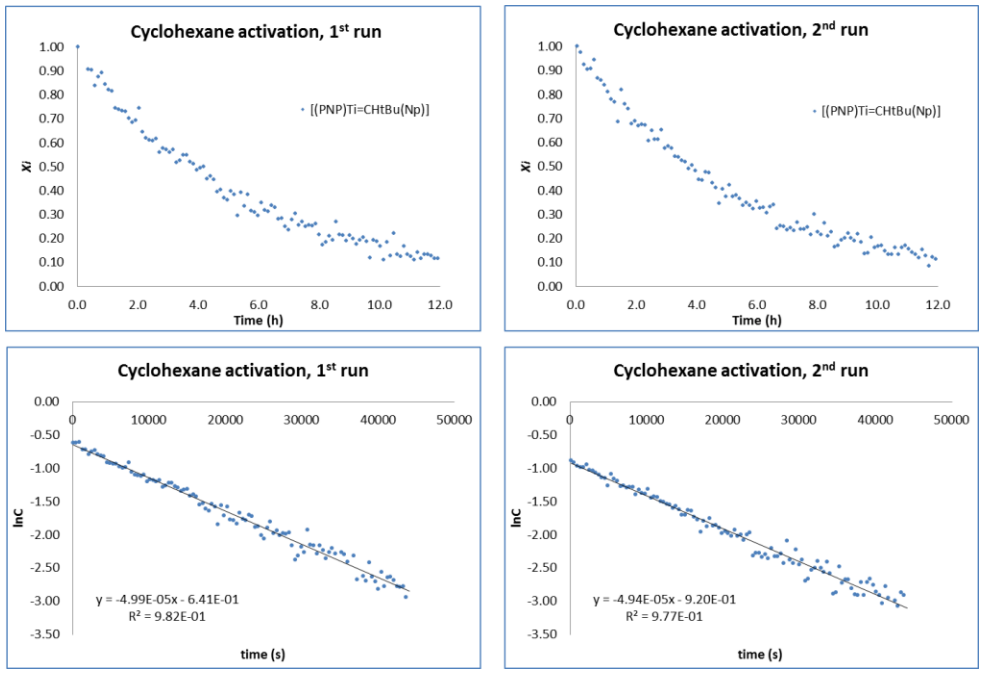


Fig. S51. Substrate decay and product formation curves in Cyclohexane with the respective logarithmic plots for decay of [(PNP)Ti=CH^{t}Bu(CH$_2$^{t}Bu)]. (*)For comparison with ether-activations.

XVIII. Evidences of volatile organics from ether activation reactions.

1) ^{t}BuOMe activation: evidence of isobutene

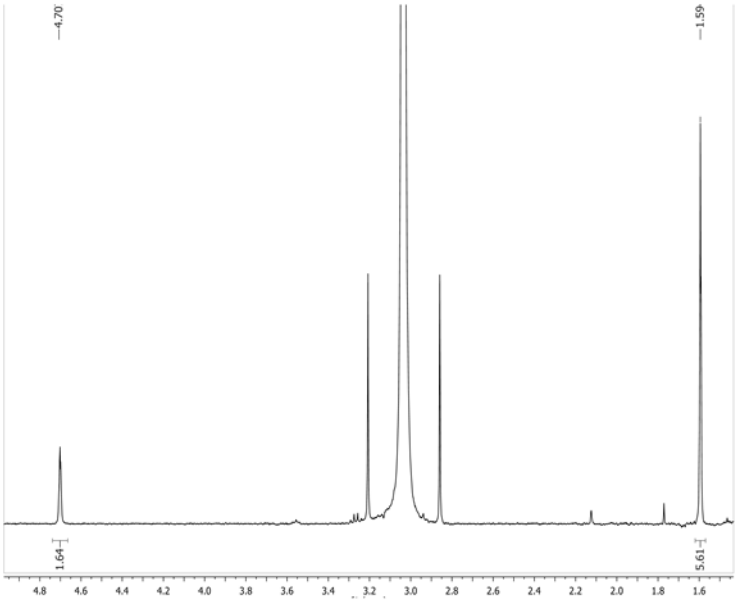


Fig. S52. Blow-up of the ^{1}H NMR spectrum of transferred volatiles from ^{t}BuOMe activation, showing the peaks of isobutene at δ = 4.71 and 1.59 ppm

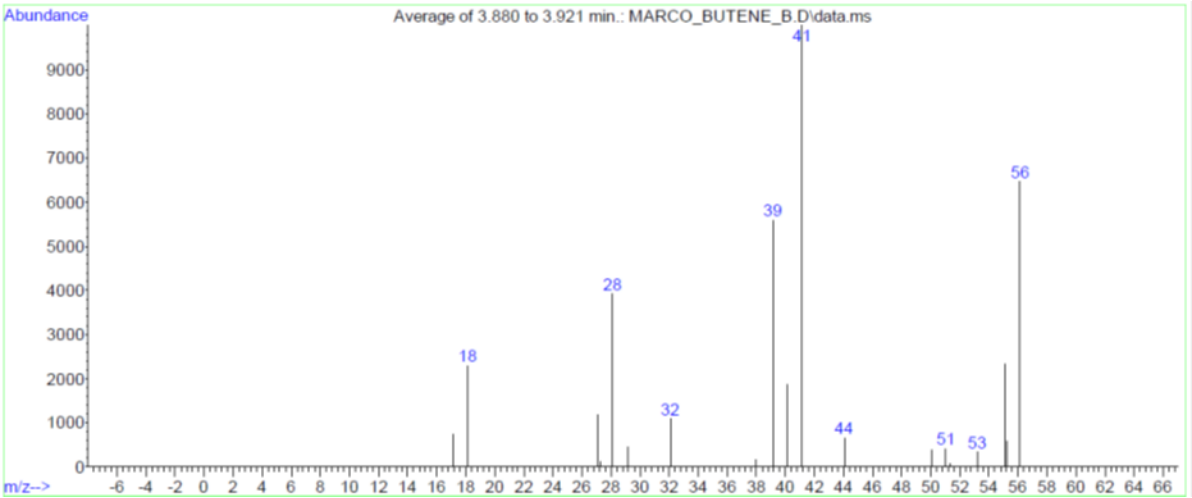


Fig. S53. MS spectrum of isobutene detected by GC-MS

2) Et_2O activation: evidence of ethylene

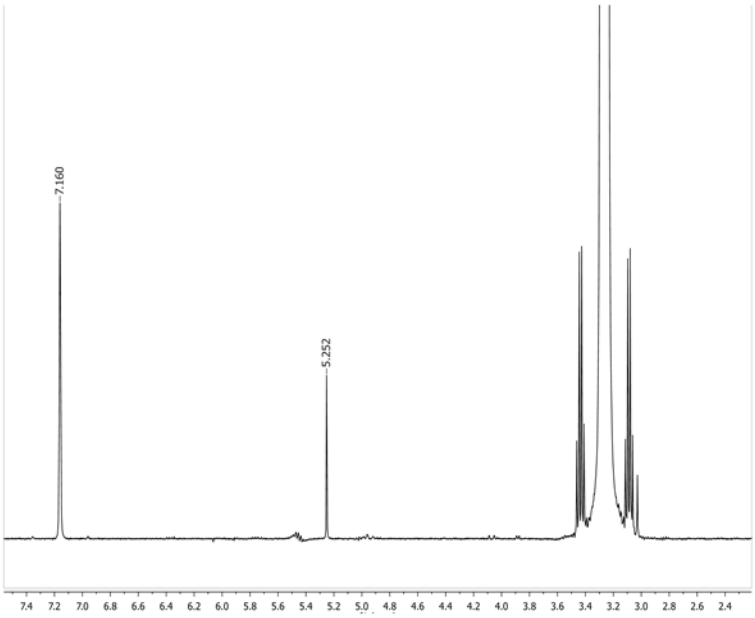


Fig. S54. Blow-up of the ^1H NMR spectrum of transferred volatiles from Et_2O activation, showing the singlet for ethylene at δ = 5.252 ppm (C_6D_5H: δ = 7.16 ppm)

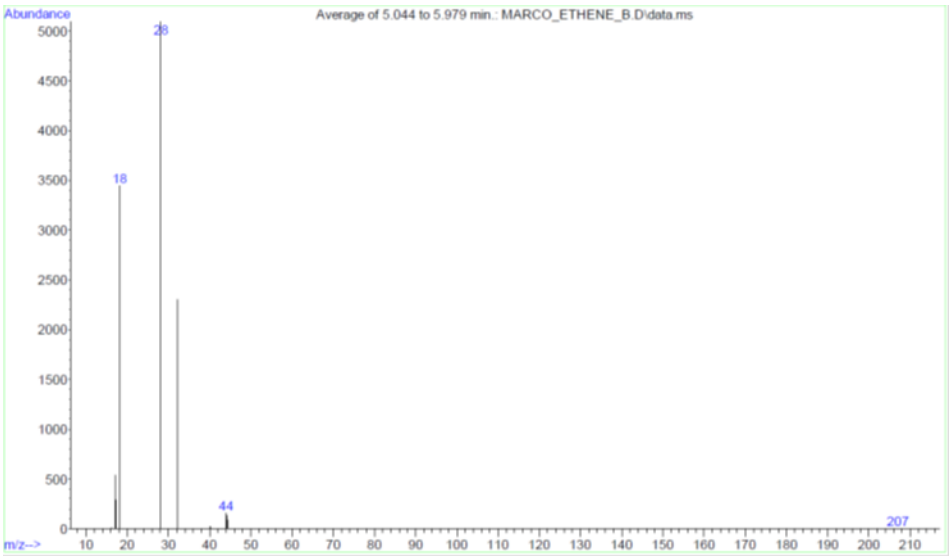


Fig. S55. MS spectrum of ethylene detected by GC-MS

3) ^{t}BuOEt activation: evidence of ethylene and isobutene

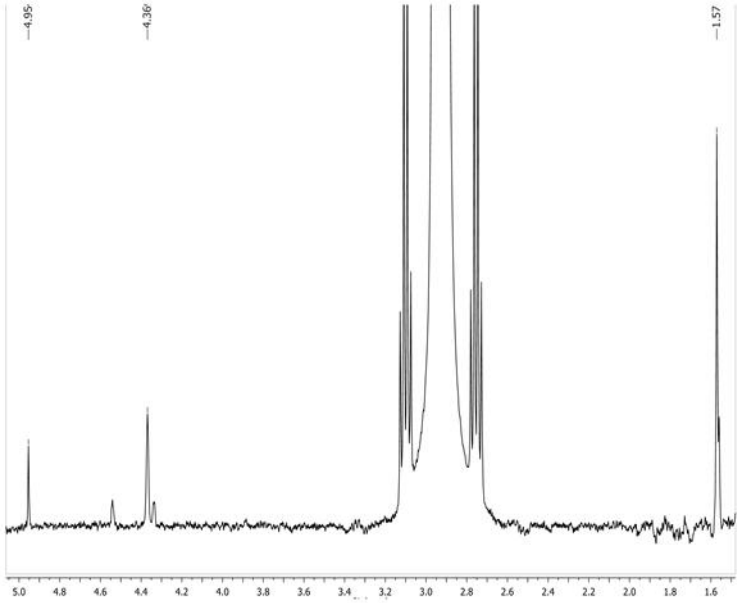


Fig. S56. Blow-up of the ^{1}H NMR spectrum of transferred volatiles of ^{t}BuOEt activation, showing peaks due to ethylene (5.252 ppm) and isobutene (4.71 and 1.59 ppm)

4) Competing activation of a 1:1 mixture of ^{t}BuOMe:Et_2O: evidence of ethylene and isobutene

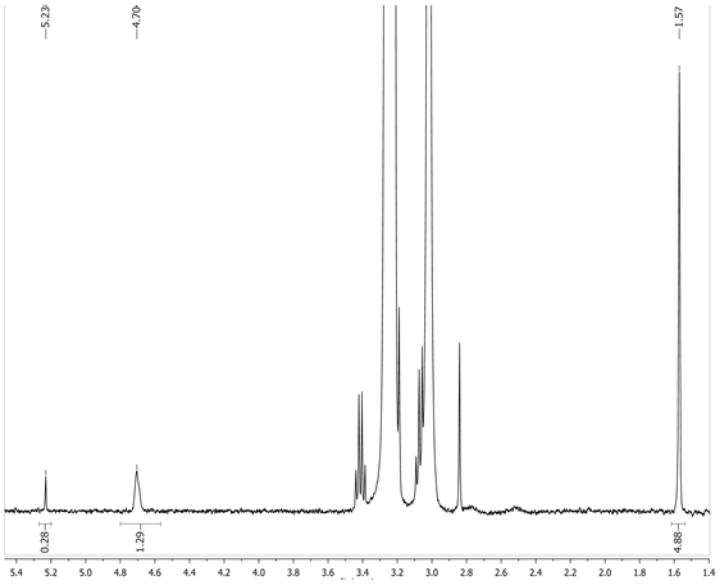


Fig. S57. Blow-up of the ^{1}H NMR spectrum of transferred volatiles of competing ^{t}BuOMe:Et_2O activation, showing peaks assigned to ethylene (5.23 ppm) and isobutene (4.7 and 1.57 ppm)

5) $^{i}Pr_2O$ activation: evidence of propene

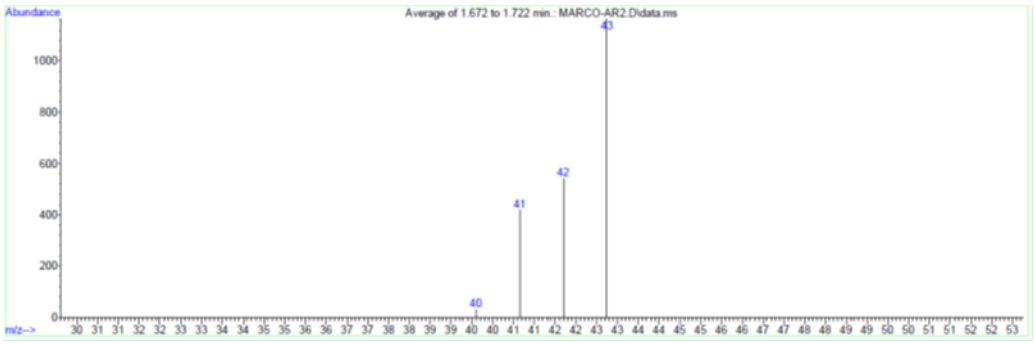


Fig. S58. MS spectrum of propene detected by GC-MS

XIX. Oxidative release of organics from C-H activation reactions: $^{n}Pr_2O$

1) $^{31}P\{^{1}H\}$ NMR spectra

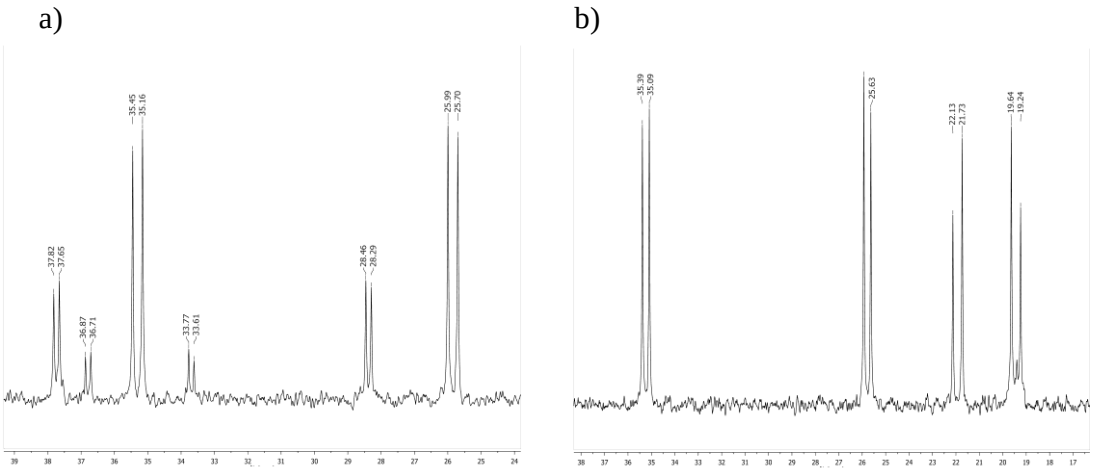


Fig. S59. Expansions of $^{31}P\{^{1}H\}$ NMR spectra of the $^{n}Pr_2O$-activation mixture a) before and b) after N_2O oxidation. The first spectrum shows the peaks due to C-H activation diastereomers **5a** and **5b** in addition to those of the alkylidene-alkoxide, **4**. The second spectrum shows the peaks of **4** unaltered, accompanied by a new set of doublets assigned to the ether-olefin oxidative-release product.

2) ^{1}H NMR spectra

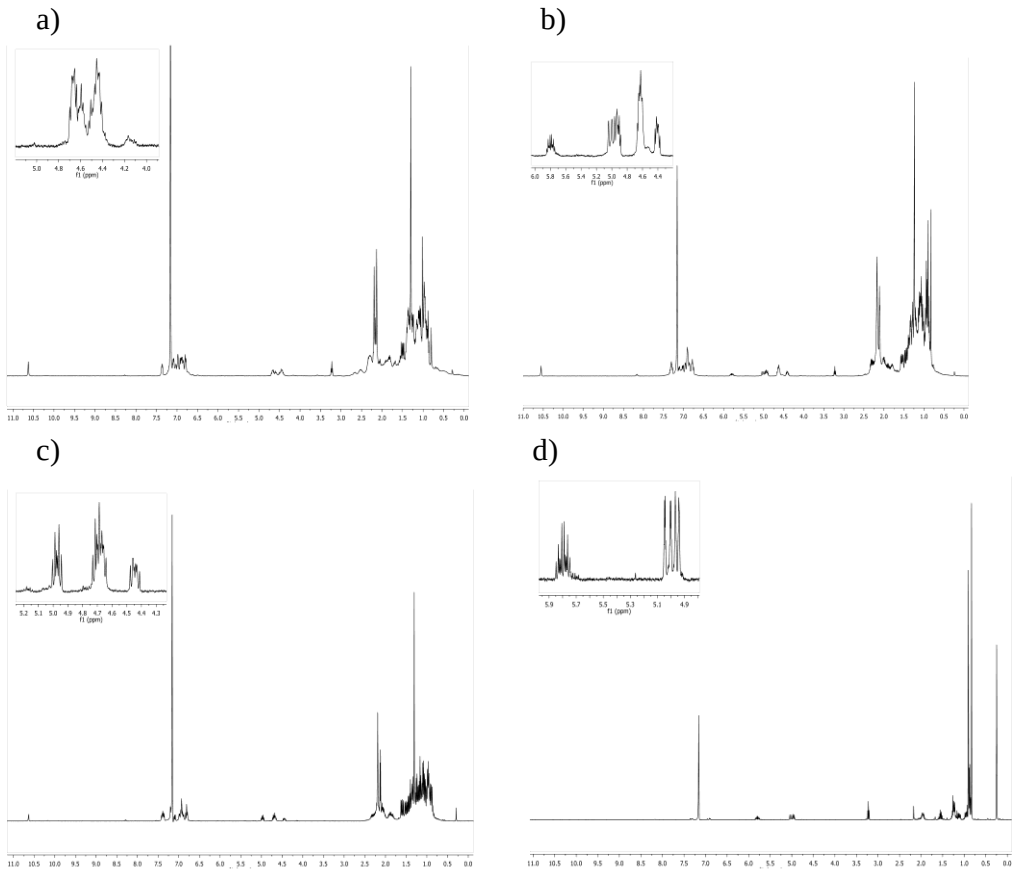


Fig. S60. ^{1}H NMR spectra of the $^{n}Pr_2O$-activation mixture: a) before and b) after N_2O oxidation, c) organometallic residue after vacuum transfer of volatiles, and d) transferred organics, with the inset showing olefin peaks.

XX. Oxidative release of organics from C-H activation reactions: $^{n}Bu_2O$

1) $^{31}P\{^{1}H\}$ NMR spectra

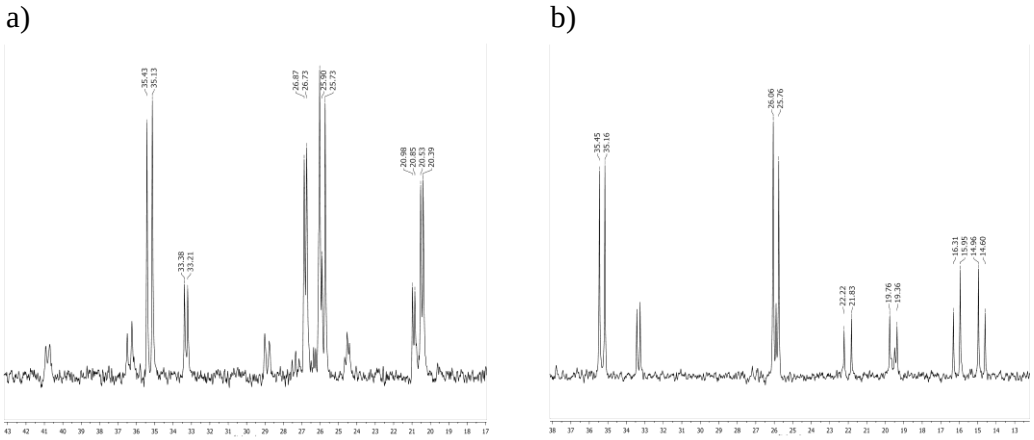


Fig. S61. Expansions of $^{31}P\{^{1}H\}$ NMR spectra of the $^{n}Bu_2O$-activation mixture: a) before and b) after N_2O oxidation. The first spectrum shows a complex mixture resulting from C-H activation products in addition to formation of the alkoxide, **6**. The second spectrum shows the unaltered peaks of **6** accompanied by a new set of doublets assigned to the oxo product, [(PNP)Ti=O($CH_2{}^{t}$Bu)] (16.1 and 14.8 ppm), and the same type of ether-olefin oxidative-release product noted in Figure S55-b.

2) ^{1}H NMR spectra

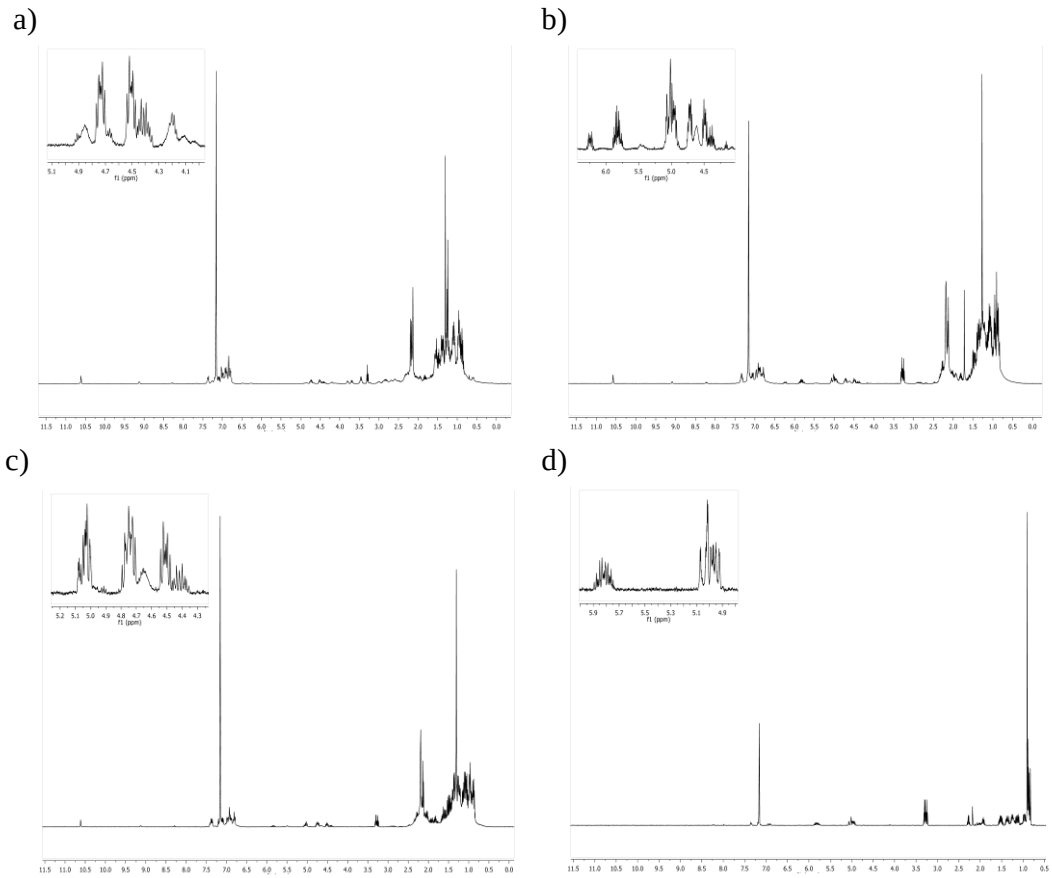


Fig. S62. ^{1}H NMR spectra of the $^{n}Bu_2O$-activation mixture a) before and b) after N_2O oxidation, c) organometallic residue after vacuum transfer of volatiles, and d) transferred organics, with the inset showing olefin peaks.

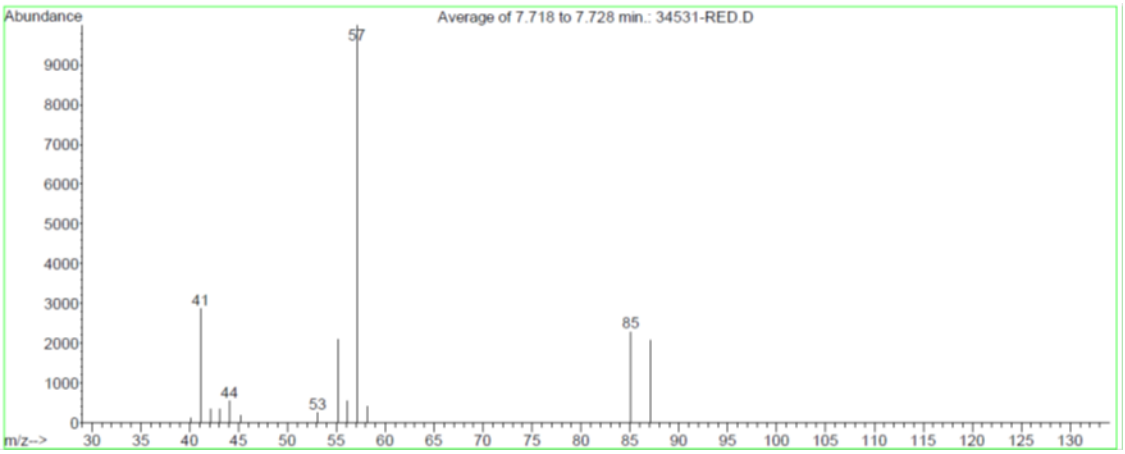


Fig. S63. MS spectrum of 4-butoxy-4-butene, detected by GC-MS

Theoretical Calculations.

XXI. Computational Details. All calculations were carried out using Density Functional Theory as implemented in the Jaguar 7.7 suite[11] of *ab initio* quantum chemistry programs. Geometry optimizations were performed with B3LYP[12] functional and the 6-31G** basis set. Titanium was represented using the Los Alamos LACVP basis[13] that includes effective core potentials. The energies of the optimized structures were reevaluated by additional single point calculations on each optimized geometry using Dunning's correlation consistent triple-basis set[14] cc-pVTZ(-f) that includes a double set of polarization functions. For Ti, we used a modified version of LACVP designated as LACV3P, in which the exponents were decontracted to match the effective core potential with triple-ζ quality. Solvation energies were evaluated by a self-consistent reaction field[15] (SCRF) approach based on accurate numerical solutions of the Poisson-Boltzmann equation. In the results reported, solvation calculations were carried out with the 6-31G**/LACVP basis at the optimized gas-phase geometry employing the dielectric constants of ε = 4.34 for diethyl ether and ε = 3.40 for dipropyl ether. Activation of diethylether was modeled in diethy ether whereas that of dipropylether was calculated in dipropylether. As is the case for all continuum models, the solvation energies are subject to empirical parametrization of the atomic radii that are used to generate the solute surface. We employed the standard set of optimized radii in Jaguar[16] for H (1.150 Å), C (1.900 Å), N (1.600Å), P (2.074 Å), O (1.600) and Ti (1.587 Å). Analytical vibrational frequencies within the harmonic approximation were computed with the 6-31G**/LACVP basis to confirm proper convergence to well-defined minima or saddle points on the potential energy surface. The energy components have been computed with the following protocol. The free energy in solution phase G(sol) was calculated as follows:

$$G(sol) = G(gas) + G(solv) \quad (1)$$

$$G(gas) = H(gas) - TS(gas) \quad (2)$$

$$H(gas) = E(SCF) + ZPE \quad (3)$$

$$\Delta E(SCF) = \sum E(SCF) \text{ for products } - \sum E(SCF) \text{ for reactants} \quad (4)$$

$$\Delta G(sol) = \sum G(sol) \text{ for products } - \sum G(sol) \text{ for reactants} \quad (5)$$

Where G(gas) is the free energy in gas phase, G(solv) is the free energy of solvation as computed using the continuum solvation model, H(gas) is the enthalpy in gas phase, T is the temperature (298.00K), S(gas) is the entropy in gas phase, E(SCF) is the self-consistent field energy (i.e., "raw" electronic energy as computed from the SCF procedure) and ZPE is the zero point energy. Note that by entropy here we refer specifically to the vibrational/rotational/translational entropy of the solute(s). The entropy of the solvent is incorporated implicitly in the continuum solvation model.

To locate transition states, the potential energy surface was first explored approximately using the linear synchronous transit (LST) method,[17] followed by a quadratic synchronous transit (QST) search[18] using the LST geometry as an initial guess.

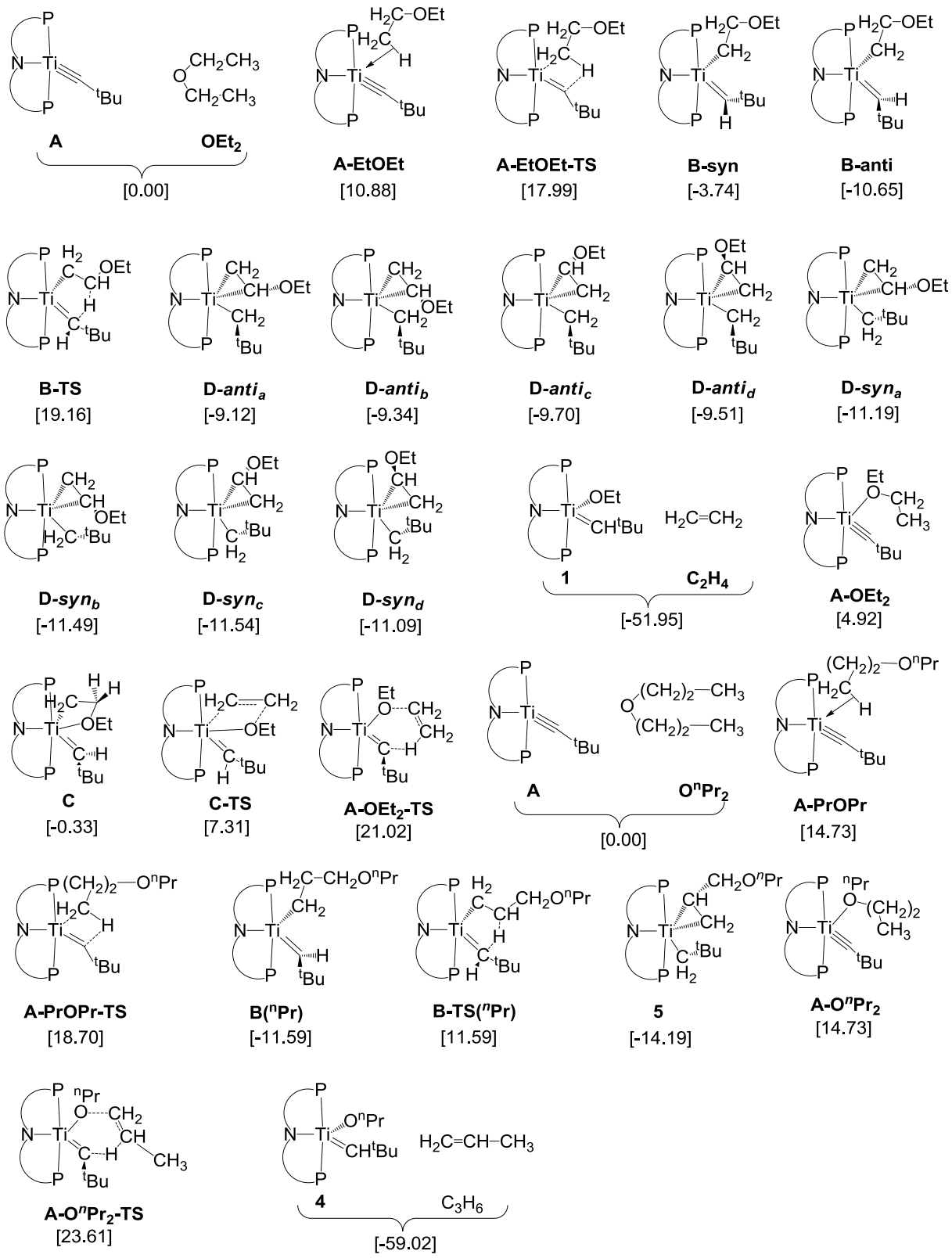
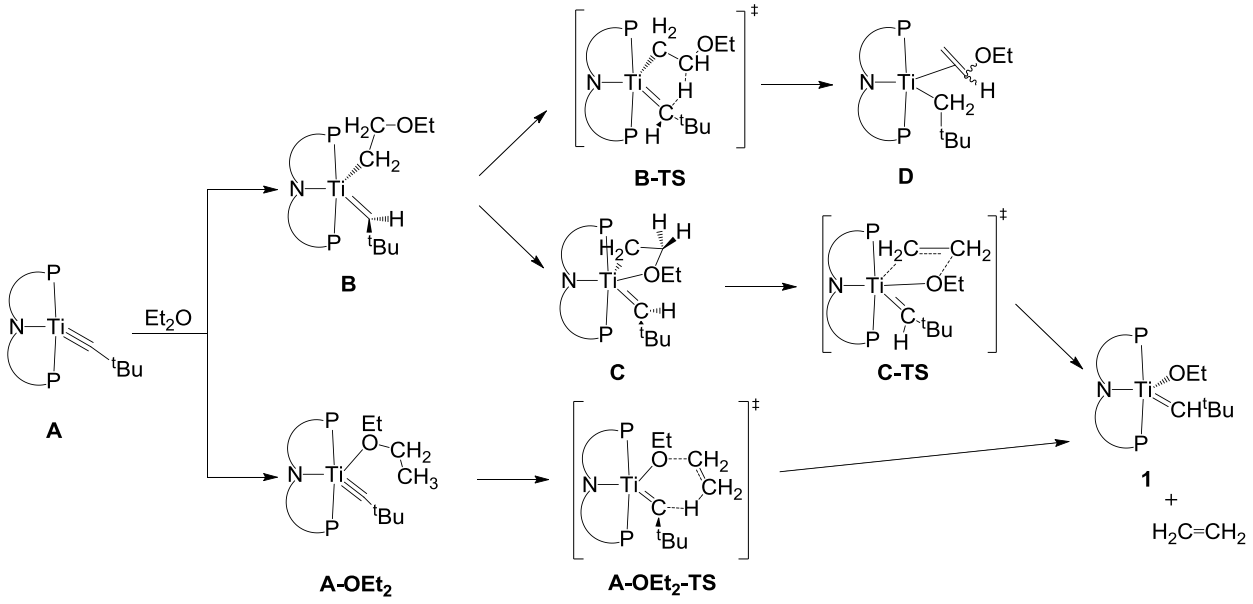
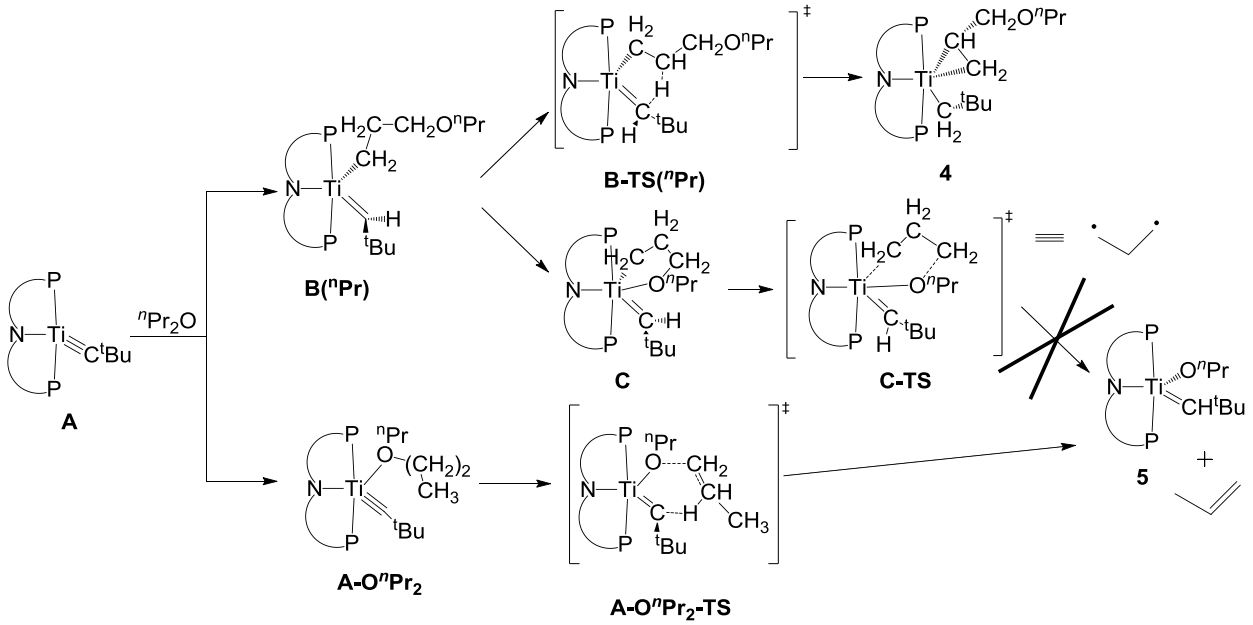


Figure S64. The alkylidyne precursor, intermediates, products, including their rotamers, and transition states with their respective energies.



Scheme S1. Computed pathways for Et_2O dehydrogenation and dehydroalkoxylation



Scheme S2. Computed pathways for $^{n}Pr_2O$ dehydrogenation and dehydroalkoxylation

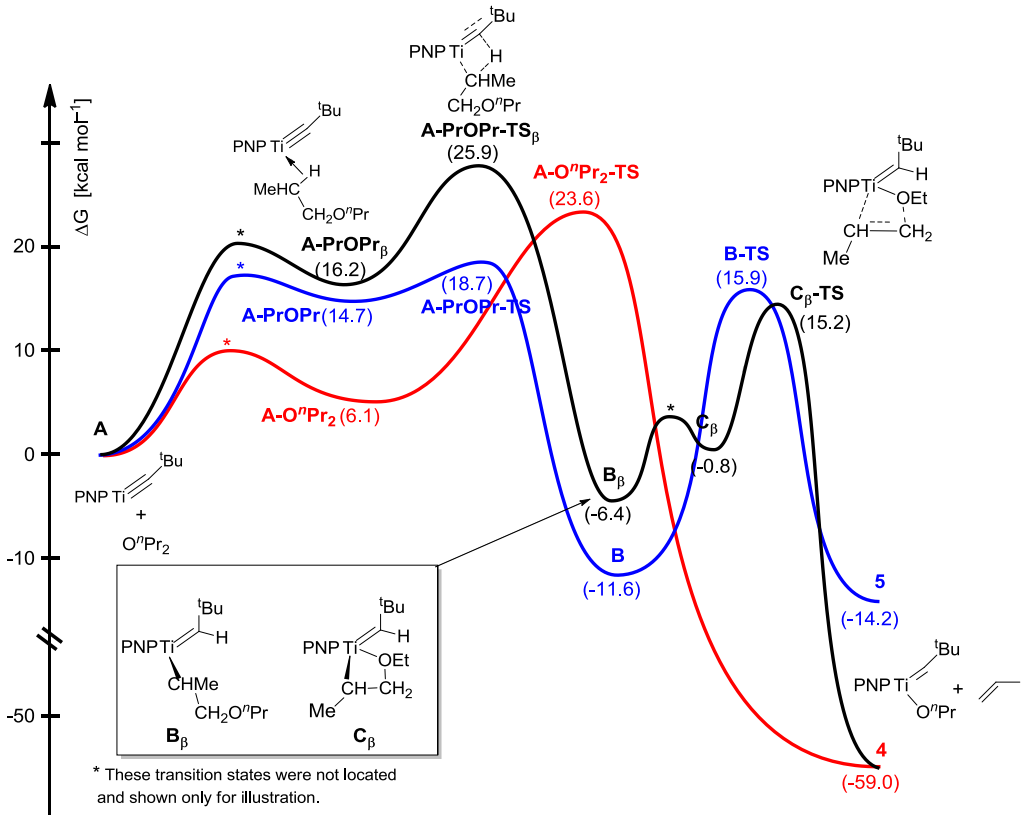


Figure S65. Energy profiles for ^{n}Pr$_2$O dehydrogenation and dehydroalkoxylation. The black curve represents the dehydroalkoxylation process through β-C-H activation.

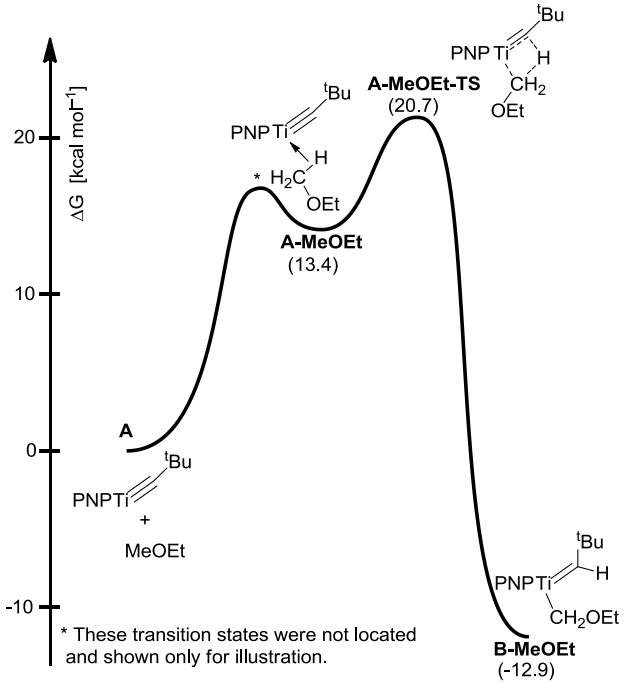


Figure S66. C-H bond activation of methyl-ethyl ether. No dehydrogenation and dehydroalkoxylation processes can further occur from the **B-MeOEt** intermediate.

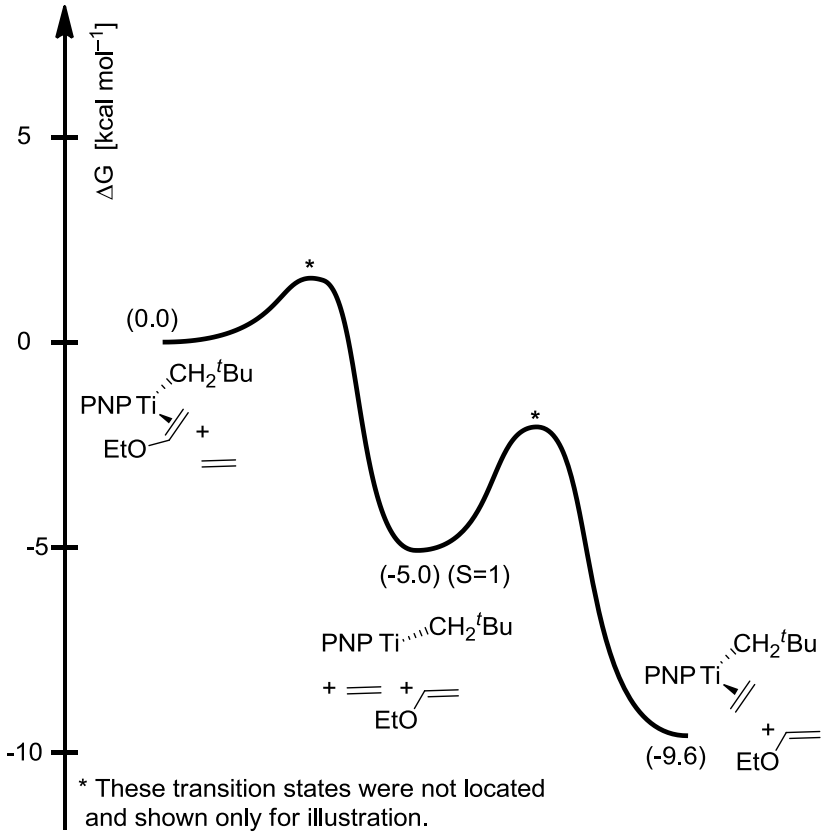


Figure S67. Dissociative mechanism for olefin exchange to form the ethene adduct **F** from **D**.

XXII. References - Computations

[11] Jaguar, version 7.7, Schrödinger, LLC, New York, NY, 2010.

[12] A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098; A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648; S. H. Vosko, L. Wilk, and M. Nusair, *Can. J. Phys.*, 1980, **58**, 1200; C. Lee, W. Yang, and R. G. Parr, *Physical Review B: Condensed Matter and Materials Physics*, 1988, **37**, 785.

[13] P. J. Hay, W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 270; W. R. Wadt, and P. J. Hay, *J. Chem. Phys.*, 1985, **82**, 284.

[14] T. H. Dunning, *J. Chem. Phys.*, 1989, **90**, 1007.

[15] B. Marten, K. Kim, C. Cortis, R. A. Friesner, R. B. Murphy, M. N. Ringnalda, D. Sitkoff, and B. Honig, *J. Phys. Chem.*, 1996, **100**, 11775; M. Friedrichs, R. H. Zhou, S. R. Edinger, and R. A. Friesner, *J. Phys. Chem., B* 1999, **103**, 3057; S. R. Edinger, C. Cortis, P. S. Shenkin, and R. A. Friesner, *J. Phys. Chem., B* 1997, **101**, 1190.

[16] A. A. Rashin, and B. Honig, *J. Phys. Chem.*, 1985, **89**, 5588.

[17] T. A. Halgren, and W. N. Lipscomb, *Chem. Phys. Lett.*, 1977, **49**, 225.

[18] C. Y. Peng, and H. B. Schlegel, *Isr. J. Chem.*, 1993, **33**, 449.

XXIII. Cartesian coordinates of the optimized structures. Values are in Å.

A			
Ti	0.330529231	0.529268590	-1.846424034
P	2.353144773	-0.661416487	-0.734724688
C	1.400601176	-1.554084733	0.559663339
C	2.003465197	-2.208039077	1.646946416
C	1.271336787	-2.813180696	2.669451830
C	-0.126611179	-2.725448240	2.585481233
C	-0.755867755	-2.085610842	1.528411971
C	-0.024291742	-1.489239348	0.469901227
N	-0.635870934	-0.796120899	-0.572611852
C	-1.984147832	-1.007025916	-0.907730100
C	-2.594516864	-2.278827130	-0.931771086
C	-3.909609317	-2.442178235	-1.346988347
C	-4.687171072	-1.355070040	-1.774510078
C	-4.084151865	-0.095693364	-1.773153475
C	-2.765030268	0.101822442	-1.339375550
P	-1.908540750	1.732224836	-1.375498330
C	3.526426052	0.494948236	0.207337770
C	3.295464671	-1.950644612	-1.736154537
C	-2.110410406	2.378400227	0.393939283
C	-2.831180008	2.816054052	-2.611880586
C	-0.040191610	-0.544735870	-4.872235724
C	-0.042838376	-2.086283309	-4.733701470
C	1.034840567	-0.130082847	-5.905147444
C	-1.427631958	-0.090352375	-5.385562159
H	3.087249552	-2.250894332	1.700236679
H	-0.737950342	-3.158899021	3.375203649
H	-1.838215755	-2.018438308	1.519890299
H	-2.011095625	-3.146128427	-0.639511271
H	-4.340413979	-3.441777941	-1.353646508
H	-4.667549667	0.753720008	-2.115809222
C	4.847931654	-0.076906190	0.743545672
C	4.171304607	-1.263558895	-2.796219386
C	-1.446803607	3.753535424	0.571465275
C	-4.113760034	3.520594390	-2.140738812
H	0.930845299	-2.445384097	-4.382004687
H	-0.255620624	-2.573243348	-5.695958657
H	-0.800467854	-2.406944810	-4.011364294
H	1.057183311	0.958406458	-6.024761324
H	0.835951980	-0.580485919	-6.887671328
H	2.029923709	-0.451089568	-5.578580626
H	-2.213458733	-0.382857415	-4.681521553
H	-1.655239595	-0.541424300	-6.361287553
H	-1.459486077	0.998819999	-5.499914774
C	3.787138479	1.762129000	-0.630077302
H	2.907058748	0.782189400	1.067538608
C	4.055004017	-3.042010417	-0.969269546
H	2.458524941	-2.427100080	-2.263306856
C	1.944561832	-3.532289364	3.814686341
C	-6.118777585	-1.546404891	-2.220325960
C	-3.521092685	2.337868575	1.001149208
H	-1.500974020	1.640112333	0.932903041
C	-1.846635517	3.826643818	-3.229809740
H	-3.092285705	2.092365326	-3.393987964
H	-6.572242735	-0.598406126	-2.525512416
H	-6.738465195	-1.966725005	-1.418484988
H	-6.186934284	-2.235103562	-3.071262900
H	1.813226080	-4.620029355	3.745927113
H	1.531718113	-3.222684855	4.781815591
H	3.020682712	-3.333805629	3.834985702
H	4.372287039	2.487305797	-0.051322042
H	2.853841884	2.257171630	-0.924844850
H	4.345727224	1.538821065	-1.544625442
H	5.370114680	0.691039924	1.327960553
H	5.517478713	-0.377664617	-0.067982561
H	4.698078986	-0.938395648	1.397969798
H	4.555940121	-2.009497169	-3.501214135
H	5.037652236	-0.764452470	-2.347639978
H	3.597083598	-0.525374165	-3.364374493
H	4.439420528	-3.783890101	-1.680153165
H	3.407189440	-3.566375686	-0.262697158
H	4.912811735	-2.643802190	-0.419289554
H	-3.459640377	2.497317592	2.085053117
H	-4.004577410	1.371647548	0.833585072
H	-4.168209309	3.119278021	0.594035690
H	-1.412378726	4.022355673	1.633855137
H	-2.002981234	4.543198541	0.054717678
H	-0.418774541	3.765168512	0.192347072
H	-2.338685014	4.388289850	-4.033136460
H	-0.975258132	3.317038703	-3.651272165
H	-1.496592578	4.554359506	-2.488038987
H	-4.599792571	4.006336991	-2.995565257
H	-3.894807111	4.303537470	-1.407494778
H	-4.839075691	2.837617253	-1.691955448
C	0.251723585	0.101193090	-3.539023228

A-EtOEt			
C	1.188420567	3.710130677	-0.729047835
C	1.550245343	2.402114291	-0.432716301
C	2.885256438	1.967757476	-0.553419143
C	3.850729934	2.918578748	-0.988468155
C	3.462084096	4.238478327	-1.257858105

C	2.134132001	4.657194356	-1.148829665
N	3.333313880	0.688963302	-0.172625453
C	2.652244444	-0.470702371	-0.526701326
C	1.655643785	-0.498678274	-1.536015362
C	1.008040669	-1.671363018	-1.897418302
C	1.303907997	-2.897655974	-1.283408637
C	2.304868086	-2.888409738	-0.309229585
C	2.992293588	-1.725327024	0.072766670
P	5.589534855	2.312029002	-1.065394438
P	4.363316990	-1.728936433	1.299235278
C	5.671261145	1.438452298	-2.745940322
C	6.710575885	3.826403624	-1.032748522
C	5.746179103	-2.776995060	0.529604672
C	3.685525666	-2.498588679	2.886775014
C	6.962224211	-2.820134125	1.473318825
C	5.416762088	-4.170666367	-0.025719519
C	5.120394202	2.201544850	-3.960589906
C	7.069336211	0.859790835	-3.016587521
C	8.073172023	3.436571484	-0.429562488
C	6.897156110	4.615471178	-2.339178513
C	3.579605653	-4.030138556	2.948937169
C	4.458827355	-1.954935550	4.101237603
Ti	5.086860397	0.762543552	0.932456810
C	5.177667896	1.825532088	2.320149496
C	5.017340953	2.870445209	3.399060878
C	3.893584987	3.869839986	3.035501792
C	4.666641560	2.188571716	4.743032909
C	6.346752987	3.645970025	3.569041223
C	0.455288481	0.751741368	3.187054074
H	1.514756928	0.539573985	3.016450606
C	-0.425302948	-0.161122634	2.350512415
H	-0.190872051	-0.053275144	1.278226330
H	-1.489230269	0.106015695	2.478777357
O	-0.215289072	-1.505007242	2.756810740
C	-1.005549410	-2.426791835	2.024965018
C	-0.753700514	-3.824241495	2.566872214
C	1.723932524	6.072438216	-1.483318763
C	0.571289210	-4.164771036	-1.660114940
H	0.148254163	4.009708637	-0.615179157
H	0.801912894	1.704010595	-0.072072749
H	4.207396973	4.965338829	-1.566786458
H	1.406921596	0.421951691	-2.052269133
H	0.257392992	-1.634740071	-2.685109801
H	2.562920166	-3.830266005	0.164960447
H	4.991988083	0.597186861	-2.553598472
H	6.199900717	4.467264230	-0.302679200
H	6.018615998	-2.148115902	-0.332166190
H	2.668994700	-2.083286914	2.911354111
H	7.832324382	-3.231211254	0.947849572
H	7.234593702	-1.827266589	1.848670611
H	6.772539431	-3.459707426	2.341490396
H	6.304882681	-4.583991041	-0.520715935
H	4.614694880	-4.132172893	-0.765851740
H	5.126247937	-4.871029420	0.762003093
H	4.995516913	1.509840630	-4.803257405
H	4.144627961	2.646876141	-3.748296201
H	5.794491280	2.996753157	-4.289747725
H	7.802424248	1.646870004	-3.223809267
H	7.042223789	0.202182184	-3.893518266
H	7.441104292	0.270446116	-2.170795681
H	8.694342616	4.330450343	-0.295791041
H	7.949279411	2.957246255	0.545623200
H	8.622868015	2.751127763	-1.085205811
H	7.458403344	5.535432571	-2.135044834
H	5.952064603	4.900804923	-2.807564676
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H	2.998266271	-4.451296160	2.125009253
H	4.567029860	-4.503712069	2.948433539
H	3.955902342	-2.258615881	5.027223281
H	4.523367117	-0.864414801	4.079624683
H	5.480379450	-2.350723471	4.136419763
H	3.777959128	4.639448922	3.811939141
H	4.110217186	4.372391675	2.086834567
H	2.936834269	3.349955808	2.923436392
H	4.561210853	2.929974115	5.547317395
H	5.449224036	1.479226320	5.033366517
H	3.723232980	1.638197293	4.662662698
H	7.164435935	2.962857404	3.823126972
H	6.616302789	4.160929621	2.640295453
H	6.267350508	4.399195980	4.365334090
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H	-0.753210252	-2.376237952	0.952819407
H	-2.074639297	-2.167382622	2.121447613
H	0.298284062	-4.099744212	2.445913275
H	-1.001150102	-3.874673876	3.631660754
H	-1.366855178	-4.558037897	2.033264260
H	2.593142281	6.731671457	-1.567372572
H	1.180894630	6.120717206	-2.436053087
H	1.061952338	6.489610804	-0.716198203
H	0.449234545	-4.251071838	-2.746016006
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H	-0.434983338	-4.200972903	-1.222131452

A-EtOEt-TS

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C	2.007486708	0.767340966	4.942808649
C	0.976349116	0.226575109	4.181601851
C	1.170951464	-0.116749169	2.825390228
N	0.150251921	-0.551524306	1.981844384
C	-0.995958235	-1.163066380	2.514841679
C	-0.945744125	-2.226243131	3.437313567
C	-2.105279039	-2.873542409	3.846499547
C	-3.367259088	-2.502064746	3.356478327
C	-3.423881534	-1.432984051	2.458037823
C	-2.271531361	-0.749132227	2.048959480
P	-2.219785416	0.685082274	0.903115857
C	4.194591356	0.339846654	-0.137640789
C	2.908175023	-2.364958564	0.707753365
C	-2.058142684	2.163668307	2.081652944
C	-3.868825500	0.732815946	-0.008998369
C	-0.426396654	-1.298070124	-1.271251883
C	-0.875520686	-2.328651025	-2.278724672
C	-2.315541010	-2.028806029	-2.758295977
C	-0.855494108	-3.724870224	-1.612023169
C	0.061699198	-2.341886448	-3.510296379
C	0.379779487	1.500447525	-1.732481987
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H	1.811295548	1.029748722	5.981092576
H	-0.002390851	0.083903192	4.628468661
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H	-2.029929145	-3.699683989	4.551218189
H	-4.394911029	-1.129218688	2.077554009
C	5.556270725	-0.229025790	0.300885728
C	3.224647788	-3.006697772	-0.650871821
C	-2.034225664	3.500010200	1.322041161
C	-5.092434225	1.274909293	0.748496390
H	-3.012098680	-2.027912190	-1.913699853
H	-2.654826092	-2.783856680	-3.479958521
H	-2.371155443	-1.048818590	-3.244933206
H	0.154599394	-3.982214785	-1.277835811
H	-1.192052663	-4.499931101	-2.313691637
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H	0.049841083	-1.374037934	-4.024039756
H	-0.249235827	-3.108910466	-4.231966743
H	1.094871246	-2.552917310	-3.216698982
C	4.134491016	0.433499317	-1.674129624
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C	3.871835017	-2.831214339	1.808401877
H	1.894874187	-2.674919584	0.992221392
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C	-4.614666173	-3.243425846	3.777682308
C	-3.013894885	2.208197142	3.283827382
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C	-3.698820141	1.463328220	-1.354194521
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H	-0.401501843	2.158698747	-1.328589406
H	1.340171203	1.827829773	-1.312884891
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H	5.367954513	1.342534539	4.879049631
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H	3.655949389	-2.352928460	2.767268686
H	4.916772028	-2.630533954	1.555495088
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H	-5.240362340	0.801105457	1.721718538
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H	-2.882698983	1.033534397	-1.939888423
H	-3.492289336	2.529937586	-1.211179733
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H	-3.063242008	1.244857112	3.798472764
H	-4.028963382	2.492173692	2.993385212
H	-1.756321926	4.313009062	2.003247319
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C	0.435635313	1.688186599	-3.240949518
H	1.214701275	1.039459806	-3.678471053
H	-0.524273763	1.391548999	-3.700046239
O	0.715528861	3.048504781	-3.537092788
C	0.787151089	3.315790717	-4.926675125
H	-0.167180476	3.054359210	-5.416793230
H	1.569787604	2.694259852	-5.396304610
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H	1.159326260	5.037037235	-6.184189556
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H	2.048651064	5.050208776	-4.646085152

B-anti

C	1.944104785	2.705103253	-1.304934866
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H	3.254257120	0.748355255	1.677184075
C	3.371522074	2.713130435	-0.736667783
C	1.107070918	-4.729531315	0.498711433
H	4.019087448	-0.822925443	1.951208024
C	0.611594678	3.509106348	1.400180173
C	1.660641258	3.964099977	-2.138946877
C	2.287803862	-3.870696470	-1.550463348
C	-3.846154941	4.834840204	-1.560039298
C	-1.979117178	-3.507407962	-1.046647382
C	0.914384090	-4.187257071	-0.931397562
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C	-0.927708221	2.430276972	-0.913042247
C	-2.644376632	-1.311992769	3.227174834
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C	-3.265235589	2.522219415	-2.428233339
C	2.193666868	-0.917332147	0.755390467
C	3.038010898	-0.316109099	1.869897764
C	-0.012664282	-0.874485307	-5.200849249
C	-0.146553813	-2.035996507	-2.667535305
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N	-0.485660825	0.147990411	-1.635877158
C	-0.295938300	-0.632440842	-2.786567976
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C	-3.052408590	-2.433334104	-1.280094994
C	-1.274185078	1.311007224	-1.714471366
C	-2.954089311	3.616281381	-1.606100859
C	1.515704068	3.054665641	2.560195455
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C	-2.455295559	1.396201032	-2.481427270
C	-0.931660158	-0.241237947	1.745116742
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H	0.056414294	-0.404433679	-6.180194298
C	0.034081010	-2.821233146	-3.813880862
C	-1.772938624	0.975805277	3.779965719
C	-0.212395249	-0.075088202	-4.082555774
C	0.895000502	4.977762747	1.041289949
C	0.311167672	-3.130346683	-6.321315864
H	3.607879745	1.785961896	-0.207840904
P	0.652040961	2.240219215	0.005675621
H	1.855509942	1.838755924	-1.973934475
H	-1.418704116	1.938800324	3.397295001
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H	-2.851356933	-1.843282266	-2.177537474
H	2.340257097	3.991679515	-2.999957722
H	0.636768229	3.978763016	-2.521278268
H	-2.954445211	-2.005557894	2.439348493
H	2.073900385	-1.297491885	5.614352001
H	0.284182352	5.347708746	0.214702633
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H	3.515224864	0.977084667	4.121066350
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H	-1.935135845	-4.151824536	-1.935763743
H	0.120717185	-3.901227351	-3.709033848
H	3.529668442	3.548028110	-0.045193501
H	1.632526444	-4.003938804	1.126406736
H	-4.160999350	0.837959784	2.409860253
H	1.823862896	4.881750098	-1.567195659
H	-2.958861483	1.609030092	1.354664815
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H	-3.112591464	-1.747325447	-0.429940795
C	2.394198904	-0.256552846	5.507013274
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H	2.216969831	-3.543603893	-2.589222322
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H	3.006368745	0.009228890	6.375454858
H	0.694291177	5.612124326	1.913472159
H	1.319137775	2.018885318	2.848099861
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H	-3.505308066	-1.139688936	3.886772247
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H	2.168339053	-2.004702160	0.903816833
H	0.168766995	-4.975683883	0.998235654
P	-0.263663280	-2.700707743	-0.955711221
H	4.096290467	2.825991310	-1.551796144
H	-3.617218713	5.466279300	-0.696194559
H	-3.730211838	5.453722687	-2.459086265
H	1.155147976	-2.777791755	-6.926405385
Ti	0.183989388	-0.311296696	0.275894977

H	-4.033122613	-2.909474897	-1.402557684
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B-syn

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C	0.349787794	4.395974962	-1.806973828
C	-1.886538042	1.487083442	-0.625053173
C	2.476098318	-0.386230777	-0.229303254
N	-1.009277340	0.477091058	-1.069001065
H	-1.810447187	1.136186993	-5.554738308
C	0.077029333	-0.449903041	4.397470469
C	-0.234379012	-1.469833622	3.276182044
H	-0.339151392	-2.684302940	-4.327791555
C	1.104011062	3.171945027	-1.265179194
C	-1.583541087	-2.152900293	3.603517117
C	-4.521380734	4.523688544	1.054439773
C	2.006304238	-3.988768952	-0.559607196
C	-1.054201721	0.051059480	-2.401338148
C	0.986893945	-4.562230873	-2.789615932
H	3.242377178	1.227766085	1.033082370
C	-1.479405794	0.454788708	-4.773083075
C	-3.271838834	1.470033489	-0.875166744
C	-3.604164386	3.469672450	0.479063379
C	-0.621767190	-1.262997590	-2.737018107
C	-1.482139948	0.891064156	-3.454295818
C	-0.301369450	-0.771237608	1.927491158
C	1.289986617	-3.420097162	-1.803527095
C	2.622558636	3.410342723	-1.227643340
C	0.394793318	3.133253351	3.096324539
C	3.523887757	0.209867082	0.706416074
C	4.714266970	-0.161101976	2.712096856
H	-3.687507472	0.673628529	-1.484771727
H	4.509430133	0.306746335	0.208197944
C	-1.656262945	-3.423825214	-1.109869728
C	-0.641424907	-1.673396558	-4.076446162
C	1.028281340	3.576944950	1.767036975
H	-1.815064305	1.897888758	-3.223132426
H	-5.174107923	2.393901239	-0.534545659
C	0.927111482	5.100289022	1.569011374
C	-1.472988854	-4.499757886	-0.029804144
C	-1.043211822	-1.299379378	-6.555913377
C	-4.105496015	2.441543539	-0.333969551
C	-1.362503040	2.538288788	0.170867374
C	-1.056167879	-0.836915590	-5.117553834
H	-0.686739564	-5.217308166	-0.277951095
H	3.961757026	-1.225123673	4.442172508
H	2.892753835	4.232793406	-0.556692098
H	1.418814873	-4.781804758	-0.087540575
H	3.172284208	2.521278291	-0.908940171
H	2.828420308	-1.380663889	-0.524098188
H	-1.228247339	-4.048984999	0.936929164
H	-1.855498580	-2.881356138	2.832249958
H	2.097143067	3.327863322	1.824885303
H	0.990519169	-3.011782081	4.238631642
H	-2.392406102	-1.415101693	3.665963861
H	-1.308944113	-0.345281455	1.702672383
H	5.686702842	-0.811780282	4.528788357
H	0.883371738	3.648622635	3.931815867
H	0.634391949	-4.211539481	-3.761083496
H	-4.874283843	5.217113523	0.280340178
H	0.526012080	5.292803785	-1.206304477
H	-4.015874110	5.117816847	1.821576637
H	0.662349483	-3.314448166	2.522121058
H	-3.099176155	-1.856592822	-1.623738572
H	0.913484612	2.340101714	-1.954879394
H	0.690887959	4.612535619	-2.826971745
H	1.973661496	-2.712873443	-2.290682030
H	2.209009617	-3.228715707	0.196746960
H	2.475619901	0.211072592	-1.160718009
H	0.499359316	2.057393423	3.247505754
H	1.309773369	5.606678211	2.464129320
H	0.242922377	-5.259796290	-2.392141796
P	0.463390882	2.443038379	0.368197401
H	-3.790364937	-3.247134116	-0.773299545
H	-0.685033684	0.336047549	4.440088231
P	-0.146347617	-2.297176699	-1.286693537
H	2.964198252	-4.429938987	-0.860733107
H	1.049943598	0.022275830	4.228981590
H	-0.100896454	5.440175772	1.417729585
H	1.903601772	-5.137570403	-2.968406935
H	-2.404992404	-5.065264114	0.091051618
H	-0.848318980	-2.373808413	-6.627798730
H	-0.728757011	4.223924286	-1.844101342
H	-0.671869008	3.372613724	3.136235459
H	5.660409199	-0.063628116	2.150609236
H	-1.826932682	4.293921920	1.333407068
H	2.980008673	3.678686222	-2.228787278
H	-1.536111550	-2.682457912	4.564313265
H	-1.774226051	-3.911978020	-2.086826486
Ti	0.391646831	-0.230085708	0.280209961
H	0.103478040	-0.945452936	5.377421923
H	4.469923424	0.844359931	3.099847522
H	1.841223187	-2.077262373	2.981787155
H	5.138908227	-2.137297300	3.480421670
H	-0.267871664	-0.786205569	-7.139347376
H	1.519770012	5.449220737	0.720369147

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C	-1.140182319	0.035959473	2.660294548
C	-1.777795389	-0.377597861	1.363602247
H	-2.139003402	-1.405113686	1.410631247
H	-2.614465012	0.255543364	1.054151053
H	-1.149804311	-0.727596134	3.454583030
H	-1.521213931	0.972988648	3.088233975
H	1.113739715	-0.302959160	4.062345613
H	2.184551789	0.382028756	2.819772618
C	1.082454114	1.862928436	3.943719464
H	1.862446658	1.987207230	4.703678682
H	0.115128832	2.000295522	4.436828799
H	1.209058587	2.651800762	3.196320652
P	-0.468815958	2.607651143	-0.208839847
C	0.885982754	3.761156925	-0.846100441
C	1.962688369	3.970623516	0.229792126
C	1.503690690	3.234028598	-2.148776798
H	0.752071801	3.117879464	-2.934321265
H	1.989294936	2.265656211	-1.995758551
H	2.436667089	3.019061267	0.487652936
H	2.263620129	3.938345595	-2.509447252
H	2.742870112	4.646508907	-0.140924938
H	1.561429359	4.407946018	1.150085134
H	0.398716521	4.719141938	-1.066766528
C	-1.325855030	3.645349699	1.142227791
C	-1.286642563	5.176377883	0.980123250
C	-2.771105280	3.184525110	1.400608995
H	-0.274221946	5.574147984	0.884090096
H	-1.735815635	5.640380651	1.866941572
H	-1.863740245	5.517154554	0.115486264
H	-3.171061946	3.710950857	2.275873916
H	-3.420580889	3.410306492	0.550259759
H	-2.839762126	2.113559543	1.593779922
C	1.865518393	-0.312847871	-0.141989114
H	1.664203660	0.107607717	-1.160754961
C	3.349298330	-0.642138461	-0.027431666
C	3.865914359	-1.261092751	-1.350331713
C	4.154178197	0.656416684	0.233761998
C	3.644287345	-1.630594538	1.119655772
H	3.264168191	-1.263536536	2.077838521
H	3.185516726	-2.604724038	0.932361852
H	4.725322420	-1.785987439	1.226752652
H	3.320747477	-2.177032634	-1.600154596
H	4.933530635	-1.508764182	-1.281737052
H	3.735003938	-0.564331630	-2.185935355
H	3.855346589	1.122529576	1.178869086
H	3.994230975	1.387000701	-0.566143836
H	5.231131187	0.446106616	0.285515352
C	0.707701087	-3.886324518	-0.335639315
C	0.443085288	-5.295601898	-0.892710649
C	0.769294211	-3.925730743	1.204694440
H	1.681591348	-3.540315337	-0.700998339
H	1.249359774	-5.969283417	-0.577405009
H	1.555704999	-4.616097691	1.534178025
H	-0.173701552	-4.275374292	1.637905358
H	0.986917701	-2.939984457	1.622543212
H	-0.492924241	-5.714751983	-0.511467330
H	0.397537307	-5.330233936	-1.983400311
C	-2.129899902	-3.330046408	-1.128368555
C	-3.139727600	-2.356617343	-1.754931221
C	-2.718189200	-3.960513043	0.145597783
H	-2.792690170	-1.977946734	-2.718832099
H	-3.325731858	-1.498693937	-1.101770245
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H	-3.659203834	-4.468536661	-0.100276850
H	-2.058624392	-4.702880975	0.601784775
H	-1.935973347	-4.133382145	-1.852264480
C	-0.231709295	-0.652468004	-2.909277799
P	-0.443734325	-2.487930463	-0.872600709
C	0.003189289	-2.017436073	-2.592074394
C	0.550546436	-2.875027518	-3.555061892
C	0.880786033	-2.442735626	-4.841475238
C	0.648932228	-1.093198328	-5.144500836
C	0.112871872	-0.218801701	-4.207542345
H	0.730135930	-3.915322478	-3.303305476
C	1.478275277	-3.383267170	-5.861994035
H	1.463969243	-4.418449154	-5.507135238
H	2.521739424	-3.126781906	-6.085350629
H	0.930907537	-3.349854179	-6.811447216
H	0.904665842	-0.715446066	-6.132864270
H	-0.040029963	0.822294384	-4.473171770
N	-0.718587122	0.224934296	-1.917513079
C	-1.632384518	2.479423864	-1.616110283
C	-1.606215486	1.238630033	-2.305883942
C	-2.525412807	1.076718982	-3.370613983
H	-2.548782449	0.134078591	-3.906320223
C	-3.394937469	2.091528386	-3.744916492

C	-3.402688716	3.333097640	-3.090044071
C	-2.508582612	3.494103490	-2.030072890
H	-2.494177848	4.448282847	-1.512253714
C	-4.339113883	4.439178252	-3.518079063
H	-4.088800659	1.914414974	-4.564796713
H	-4.124317535	4.780726990	-4.538677902
H	-5.385445951	4.109798874	-3.506181869
H	-4.259617988	5.308146441	-2.857468029
H	-0.736428080	3.395413560	2.033190851

C-TS

C	0.365403414	-0.086876427	-0.218899890
O	0.160772978	-0.236135909	1.528223591
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Ti	2.102006745	0.070935314	2.049988221
H	1.975355766	1.262822880	-0.704511048
H	2.372113990	-0.507913548	-0.821117381
H	0.026334879	-1.094325995	-0.466307156
H	-0.409558101	0.661759995	-0.381827154
C	-1.102350722	-0.541613821	2.078599589
H	-1.582317262	-1.313838795	1.453647516
H	-0.943192764	-0.973460646	3.072363560
H	-1.543287424	1.445339091	2.816179392
C	-2.008250046	0.684501961	2.181072770
H	-2.974376526	0.411160029	2.621651710
H	-2.200896159	1.126755593	1.197938176
C	1.938454392	-0.431429486	3.847863829
H	2.916740254	0.126098828	3.853888266
C	1.683968892	-0.974288463	5.250181467
C	0.608804461	-2.079701179	5.259400679
H	-0.347346439	-1.707864734	4.877604942
H	0.439305947	-2.437369326	6.282494121
H	0.904500412	-2.937122508	4.650554199
C	2.988942445	-1.546787282	5.856868455
H	2.813871942	-1.934629057	6.868840784
H	3.763300266	-0.774495707	5.921215380
H	3.391450511	-2.361751946	5.247641507
H	1.931448808	0.968942785	6.247283485
H	1.003394197	-0.210095756	7.187173391
H	0.257772578	0.598396310	5.794034982
C	2.468608310	3.695212936	3.712256549
H	2.685403115	4.731826571	3.425512829
C	1.235567416	3.667389026	4.628558131
H	0.961789668	2.638580790	4.875878682
H	1.449231652	4.193781629	5.566745735
H	0.361629489	4.146544216	4.176031292
C	3.707826045	3.142020828	4.428810025
H	4.597215074	3.194401670	3.795365000
H	3.566846142	2.100190186	4.729866352
H	3.903127557	3.728881663	5.334866012
C	0.841985850	5.380817065	1.590058042
C	0.779576305	3.869459609	1.296310228
H	-0.134783713	3.480780937	1.764521128
H	0.466695230	2.602140753	-0.471108356
C	0.650001450	3.645415962	-0.219063464
H	1.551884590	3.963940089	-0.750299165
H	-0.190045612	4.236021289	-0.604239771
H	-0.041087700	5.862848528	1.152956400
H	1.718787995	5.854760757	1.139472447
H	0.845031519	5.616729091	2.655638460
P	2.119269422	2.773016744	2.098589440
C	3.678690752	2.957018934	1.152077049
C	4.081762794	4.123160139	0.484815080
H	3.452171980	5.006152687	0.534358717
C	5.270059494	4.201240261	-0.244864675
C	5.687719804	5.467888125	-0.955281396
H	5.894551200	5.285483725	-2.016948352
H	4.908594458	6.234423490	-0.897685952
H	6.601417423	5.893919998	-0.521330091
C	6.065692525	3.046605181	-0.290054125
H	6.990172031	3.057009753	-0.865030559
C	5.701167372	1.882856525	0.372019715
H	6.340675896	1.009265371	0.305847618
C	4.506427936	1.800479475	1.124494226
N	4.112970956	0.632790093	1.788193253
C	5.095411700	-0.224863643	2.313090348
C	6.285610202	0.248192332	2.911365287
H	6.478645802	1.315956754	2.924548085
C	7.201855637	-0.619065420	3.492507683
H	8.101230403	-0.209509407	3.948648995
C	6.984906720	-2.005671184	3.519401208
C	7.973560446	-2.941715278	4.174821406
H	7.729908276	-3.988322786	3.966990427
H	7.985208908	-2.817891954	5.265385673
H	8.995955782	-2.762043665	3.822045882
C	5.811790446	-2.480807914	2.928485929
H	5.631079893	-3.551480068	2.938592077
C	4.873589223	-1.630198031	2.328392591
P	3.333165875	-2.182717705	1.489619458
C	2.706756948	-3.743018190	2.359052497
H	2.846273200	-3.495722577	3.417346369
C	3.424131525	-5.070986505	2.063986281
H	3.266129462	-5.396426232	1.030801373
H	3.017215931	-5.855819087	2.713367834
H	4.502182359	-5.031910709	2.236723807
H	0.781067284	-4.687817304	2.741860146
H	0.986095844	-4.173217747	1.066502068
H	0.655610336	-2.969065869	2.318623033

H	2.221056669	-2.530468578	-1.389692361
H	3.349750001	-3.730022711	-2.028017407
C	2.903986985	-3.336990599	-1.105757459
H	2.307627725	-4.141159517	-0.665712248
H	4.635759316	-3.698700510	0.117612100
C	4.013016325	-2.839212886	-0.162932614
C	4.928955164	-1.824699613	-0.865999696
H	5.315262907	-2.263707466	-1.794577203
H	5.784942109	-1.559663950	-0.240739516
H	4.404321813	-0.901720194	-1.126251157
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A-OEt$_2$

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C	3.353597513	0.383101589	4.701772352
C	2.040817951	0.232707678	5.165923132
C	0.990322882	-0.070572587	4.305461226
C	1.197703568	-0.250483586	2.918169306
N	0.162945110	-0.463704842	2.008643329
C	-1.000710653	-1.123972727	2.427365720
C	-0.982923749	-2.266267037	3.255573358
C	-2.149284514	-2.959524649	3.553611802
C	-3.393878896	-2.558191409	3.044684902
C	-3.419954348	-1.415977399	2.239947211
C	-2.260914679	-0.686149027	1.940631657
P	-2.200150614	0.832115496	0.907068138
C	4.327299235	0.480819694	0.150639305
C	2.975097872	-2.291627528	0.483879904
C	-2.303974966	2.227614610	2.201341442
C	-3.780874219	0.832311535	-0.130950094
C	-0.351617940	-0.981340211	-1.117491912
C	-0.849900749	-2.185515291	-1.893464580
C	-2.389421227	-2.136746934	-2.042266674
C	-0.485616682	-3.500424884	-1.161426742
C	-0.224716461	-2.209786175	-3.310420381
H	4.585823403	0.288885946	2.955893597
H	1.830376167	0.372244735	6.224765319
H	-0.016991657	-0.154486717	4.700832306
H	-0.031361703	-2.619563217	3.641747088
H	-2.090832502	-3.845389712	4.183838295
H	-4.376343584	-1.093193250	1.839929117
C	5.672975599	-0.207415509	0.438612699
C	3.318771566	-2.685670459	-0.960590790
C	-2.414231471	3.611482734	1.538434918
C	-5.097002370	1.258954805	0.540944554
H	-2.869076799	-2.178520969	-1.059031030
H	-2.755871218	-2.987819342	-2.633696063
H	-2.707784752	-1.216048406	-2.543641610
H	0.599375493	-3.612493403	-1.075104097
H	-0.871270237	-4.377817966	-1.700534906
H	-0.906422634	-3.504562916	-0.151041031
H	-0.508226057	-1.314986224	-3.876803991
H	-0.556774840	-3.089543079	-3.879876254
H	0.868779551	-2.235727807	-3.255188216
C	4.257180413	0.906042006	-1.327474588
H	4.278588017	1.391739407	0.762997221
C	3.903052079	-2.960961295	1.507075112
H	1.950233881	-2.628198121	0.682246981
C	4.492387163	0.740259537	5.629578348
C	-4.652274628	-3.334240691	3.358848570
C	-3.316766956	2.069175034	3.345473104
H	-1.302954285	2.147007466	2.648161154
C	-3.554614995	1.634183633	-1.424872518
H	-3.862474774	-0.223112361	-0.413750380
H	4.175483555	0.706975629	6.676610240
H	4.877097674	1.750416504	5.436890634
H	5.338582596	0.051024140	5.519671408
H	-5.537030323	-2.848920982	2.935178391
H	-4.811422562	-3.426729652	4.440406986
H	-4.610687286	-4.353537649	2.954587105
H	3.241943972	-3.772798482	-1.080517611
H	4.342495672	-2.402788908	-1.229439940
H	2.630959300	-2.220069339	-1.671930606
H	3.784687103	-4.050108324	1.447035390
H	3.667535017	-2.655032635	2.529752932
H	4.957380638	-2.738433306	1.319353994
H	5.115892980	1.539478593	-1.583276104
H	3.342167873	1.462791936	-1.542408209
H	4.277913131	0.037066127	-1.993619081
H	6.494139450	0.487449683	0.221807181
H	5.816389951	-1.084748462	-0.198796033
H	5.777980135	-0.530936820	1.476085777
H	-5.933901223	1.068630979	-0.142632099
H	-5.106299563	2.329530871	0.768530941
H	-5.301018769	0.721195812	1.469269414
H	-4.423624465	1.536591483	-2.087518006
H	-2.674169787	1.269521763	-1.958944827
H	-3.417485595	2.702657040	-1.219821710
H	-3.111201479	2.811707274	4.127353728
H	-3.256159210	1.077767174	3.801323308
H	-4.345397147	2.226586946	3.010128044
H	-2.231235596	4.403445398	2.275165592
H	-3.412940991	3.781319953	1.122890205
H	-1.692880764	3.741869790	0.724494157

C	1.022343226	3.338751689	-0.777194307
H	1.899439257	3.662579900	-1.350048735
H	0.215666531	4.063981642	-0.956595740
C	0.120144033	2.090193179	-2.645092111
H	-0.630899023	2.889231751	-2.720886992
H	-0.361932056	1.120585450	-2.769323291
C	1.235314724	2.279886443	-3.661953389
H	0.800398211	2.242373553	-4.666878799
H	1.750469051	3.240869966	-3.565415204
H	1.969600105	1.473856352	-3.581817572
C	1.360188679	3.265163510	0.700437938
H	2.184570901	2.574076494	0.892688174
H	1.664594560	4.257269202	1.050971905
H	0.499399426	2.951916060	1.297686083
O	0.588451712	2.053695310	-1.266581464

A-OEt$_2$-TS

H	0.022336966	0.129521998	-0.219576744
C	-0.046904569	-0.004333665	1.418425806
Ti	1.739216817	0.005293660	1.519019101
O	2.401359902	0.164349412	-0.362866401
C	3.750004532	0.322238245	-0.798420290
C	4.776115056	0.066576465	0.299664305
H	4.645593801	0.744777707	1.147289310
H	4.724505930	-0.957930533	0.676109688
H	5.784455473	0.226910097	-0.100164369
H	3.936823387	-0.369101296	-1.634499541
H	3.879792484	1.341827272	-1.193985894
C	1.357491839	0.334188884	-1.876810192
C	-0.010510840	0.232545177	-1.468385612
H	1.749359235	1.304856279	-2.170500203
H	-0.610273912	1.128426743	-1.636389667
H	1.817361629	-0.498103496	-2.403083976
H	-0.522880663	-0.672555342	-1.795452876
P	2.422528995	-2.550918082	1.956197903
C	3.247514138	-3.675371543	0.674955133
H	4.253276023	-3.240973081	0.595517541
C	2.552258397	-3.502778217	-0.688547789
H	1.536814682	-3.912543865	-0.671922963
H	3.110988991	-4.034908430	-1.468591909
H	2.478747872	-2.449180169	-0.968369420
C	3.404385835	-5.168987354	1.008617996
H	2.435647052	-5.676819509	1.030874149
H	4.007353002	-5.656397795	0.232268875
H	3.894225878	-5.347329790	1.968154327
C	1.106887377	-3.509692703	2.917578170
C	0.008105791	-4.031732071	1.980074102
H	-0.854628951	-4.371817357	2.565039736
H	0.352565905	-4.884583688	1.384963230
H	-0.334630529	-3.249401714	1.297552917
H	0.676524900	-2.692254269	3.509453049
H	2.391902056	-4.215092909	4.546207769
C	1.599311798	-4.588456160	3.892659360
H	0.765464777	-4.912506864	4.527969961
H	1.975393536	-5.474844404	3.373912946
C	-1.517413920	0.002175880	1.806459502
C	-2.373997189	-0.844644415	0.832219061
C	-2.069996556	1.448888963	1.800918604
C	-1.687122467	-0.572230131	3.233874986
H	-1.374445708	-1.620600791	3.271751471
H	-2.737776716	-0.523667007	3.553293553
H	-1.082485585	-0.013776955	3.954328638
H	-1.571826212	2.050238027	2.567584357
H	-1.914136852	1.929560596	0.829009000
H	-3.147812290	1.458183286	2.014530035
H	-1.999619069	-1.870991770	0.765943024
H	-3.416580067	-0.888795719	1.174535808
H	-2.373924847	-0.420676483	-0.176456429
C	0.831629468	3.922892617	0.255172322
H	0.541433977	2.941495512	-0.128154492
H	0.093369507	4.658734028	-0.086873430
H	1.795736712	4.194173604	-0.190471668
C	1.186315512	5.329443977	2.329296194
H	1.242050558	5.371963265	3.419432827
H	2.123968935	5.730303240	1.932054508
H	0.385748210	6.009077221	2.011795724
C	0.899899079	3.916893085	1.793716482
H	-0.082843504	3.600623240	2.161455476
C	3.774191590	3.142070272	2.647355202
H	4.289485449	2.199286624	2.876853628
H	4.252674778	3.054649499	0.501047277
H	5.468236944	3.869758673	1.494746909
H	3.955828654	4.688987614	1.105215938
C	4.390407044	3.717101632	1.361217729
H	5.074510835	4.193730747	4.025396266
H	3.589016979	5.077038528	3.669678346
H	3.547132121	3.682189897	4.758350087
C	3.998028543	4.078360117	3.845138051
N	2.464367875	-0.117764821	3.514544634
C	3.707664617	-2.191480217	3.217942810
P	2.005716266	2.497693107	2.364724125
C	3.502985482	-0.964221470	3.909388659
C	4.425134957	-0.636092924	4.930188412
C	5.506017639	-1.459611610	5.219757732
C	4.815641092	-2.992892603	3.522865125
C	5.739266249	-2.650489002	4.516259566
C	6.939981703	-3.516273818	4.817287513
H	7.070647064	-3.659979293	5.895857138

H	7.869915054	-3.069978011	4.440759309
H	6.844439320	-4.506062201	4.359931486
H	4.970683066	-3.919359325	2.977334458
H	6.197244466	-1.161382960	6.006587136
H	4.291861986	0.288111222	5.483761025
C	1.476788060	2.040754007	4.061356140
C	1.862440173	0.731685977	4.455707332
C	0.749810420	2.854226952	4.940206389
C	0.409703654	2.435543167	6.230222890
C	0.834843201	1.158454502	6.626450671
C	1.539605801	0.324243076	5.766890195
H	1.828942421	-0.669631650	6.095150927
H	0.591729885	0.802449609	7.626088728
H	0.436975579	3.844103172	4.620385641
C	-0.399599337	3.312243074	7.157302800
H	-1.438493215	2.966182436	7.235350876
H	0.013400881	3.315231243	8.172533447
H	-0.426591381	4.348364207	6.805678086

B-TS

Ti	0.089384552	0.378833756	-2.097109494
P	2.123254153	-1.238729753	-1.202959548
C	1.555656124	-1.181698114	0.542136423
C	2.331343152	-1.228700676	1.704592598
C	1.754876457	-1.226940866	2.982031561
C	0.356560139	-1.199157363	3.060325154
C	-0.437674998	-1.125272012	1.918668855
C	0.141985115	-1.084319941	0.635023188
N	-0.600323491	-0.886359174	-0.540718193
C	-1.852491852	-1.510518215	-0.671220437
C	-2.108546477	-2.831029067	-0.250218595
C	-3.330489942	-3.440117714	-0.518514255
C	-4.343961306	-2.773036846	-1.221503427
C	-4.103896819	-1.448271058	-1.606192220
C	-2.894998460	-0.803182515	-1.323958013
P	-2.423637507	0.932897119	-1.699025105
C	3.978397723	-0.873157933	-1.187175545
C	1.827759843	-3.050064119	-1.682922230
C	-2.736925927	1.815311892	-0.046688916
C	-3.637192177	1.556561861	-3.001068079
C	0.064132166	0.014756564	-5.455691999
C	1.234045437	-0.830966405	-6.015354144
C	0.240522358	1.468951810	-5.934811296
C	-1.263647658	-0.546910320	-6.018926301
C	0.535875913	2.441332561	-1.701578603
H	3.413842944	-1.273003106	1.628890211
H	-0.123344976	-1.215983778	4.036678239
H	-1.518715761	-1.080329759	2.012725795
H	-1.332034596	-3.379075405	0.275787733
H	-3.493735453	-4.464844674	-0.190749219
H	-4.889070700	-0.914628151	-2.133488339
C	4.913574089	-1.967354919	-0.639969285
C	2.417725564	-3.377696177	-3.063349027
C	-2.606531104	3.342815919	-0.166705004
C	-5.074972245	1.869183008	-2.551346331
H	2.193909560	-0.467363457	-5.634035712
H	1.262459998	-0.778224835	-7.111164859
H	1.130824543	-1.885391677	-5.735162674
H	-0.606829124	2.090334614	-5.628351797
H	0.299874437	1.504248010	-7.029784030
H	1.147355027	1.912161444	-5.518311023
H	-1.412500963	-1.591653484	-5.722148101
H	-1.268150265	-0.503390194	-7.115364486
H	-2.118554805	0.031570782	-5.653467226
C	4.464868228	-0.417152234	-2.578290840
H	4.032875633	-0.007670936	-0.512230207
C	2.203257612	-4.110907670	-0.637546222
H	0.733919084	-3.051522143	-1.776709087
C	2.612448605	-1.237674125	4.226291578
C	-5.643226080	-3.465011938	-1.562080107
C	-4.009667833	1.420544823	0.717684684
H	-1.876161667	1.453699955	0.530542309
C	-3.036588452	2.762372099	-3.747353310
H	-3.666976158	0.712467806	-3.703233577
H	-0.061512773	3.142783232	-2.285859616
H	0.628251523	2.721681969	-0.651431285
C	1.703194847	1.898534232	-2.382858462
H	-6.426557584	-2.743549538	-1.814300785
H	-6.006318362	-4.073713934	-0.726589170
H	-5.530110431	-4.137121527	-2.422873626
H	2.121249367	-1.770451551	5.047273101
H	2.822190797	-0.220622101	4.582893578
H	3.578409925	-1.720590904	4.045238689
H	5.507305303	-0.082094579	-2.511422225
H	3.873127143	0.404922566	-2.986804674
H	4.434678972	-1.240464945	-3.299097891
H	5.926071815	-1.560881457	-0.524689167
H	4.982804932	-2.810390330	-1.334216326
H	4.600786322	-2.361137418	0.329166186
H	2.033867497	-4.343546022	-3.412968108
H	3.509419778	-3.457848948	-3.027984617
H	2.157247249	-2.623833527	-3.811061652
H	1.797119118	-5.083552376	-0.942231923
H	1.798211390	-3.872502135	0.349263987
H	3.286273478	-4.226529251	-0.540218676
H	-3.970149779	1.836960637	1.732262781
H	-4.115102947	0.336166422	0.804261142
H	-4.913298852	1.811337759	0.241129782

H	-2.590916972	3.791842796	0.833868653
H	-3.454485681	3.782306089	-0.702591030
H	-1.688412057	3.639184586	-0.678385510
H	-3.666257035	3.026717512	-4.605719557
H	-2.031885458	2.544472172	-4.115460966
H	-2.975523641	3.644924252	-3.101807337
H	-5.699577612	2.068125552	-3.431125708
H	-5.108982057	2.764878982	-1.923571507
H	-5.539482517	1.054702869	-1.991362830
C	0.026411287	-0.080816552	-3.939902132
H	-0.174791084	-1.131340894	-3.613232945
H	1.294747546	0.679863489	-3.284485366
H	2.522466632	1.614853834	-1.712001808
O	2.220033240	2.531268575	-3.547453059
C	2.865029096	3.766569820	-3.247669532
H	3.676987441	3.595453519	-2.520017403
H	2.151284828	4.459710564	-2.778756800
C	3.419735396	4.348120344	-4.537445222
H	3.933251042	5.294619709	-4.337617832
H	4.133249905	3.658141671	-4.998521908
H	2.614426426	4.537030864	-5.253880411

D-antia

Ti	0.175093192	0.440104660	-1.892387916
P	1.931367358	-1.493468567	-1.148492860
C	1.468940243	-1.089765121	0.590046153
C	2.321708479	-1.084869497	1.700478372
C	1.847938547	-0.857564261	2.997839006
C	0.471902246	-0.643267624	3.160798509
C	-0.391045271	-0.599535805	2.071378808
C	0.092439187	-0.790063812	0.764847072
N	-0.709969372	-0.608978800	-0.376661348
C	-1.988656484	-1.183173236	-0.448189063
C	-2.291390080	-2.445151766	0.097995594
C	-3.540221506	-3.025531258	-0.100342095
C	-4.533315319	-2.387921905	-0.855666319
C	-4.241832376	-1.116764246	-1.366783138
C	-3.006280422	-0.494103775	-1.156700538
P	-2.505132413	1.197958959	-1.684973461
C	3.807960706	-1.295956751	-1.253776802
C	1.477356102	-3.342913418	-1.252161676
C	-2.804590312	2.226457599	-0.116267832
C	-3.766054967	1.716644184	-3.000903411
C	-0.391447366	-0.572756006	-5.110177236
C	-1.929752835	-0.628397893	-5.113896128
C	0.144661269	-1.999299817	-4.900770549
C	0.079784434	-0.073980708	-6.496665113
C	1.899164431	1.672191230	-1.486362742
H	3.381844713	-1.277711875	1.566628869
H	0.072245992	-0.483586475	4.160133927
H	-1.446950238	-0.391927333	2.217513898
H	-1.531781304	-2.972145256	0.667788882
H	-3.741371400	-4.005646056	0.328236897
H	-5.011962306	-0.604538944	-1.935017372
C	4.698592776	-2.378045497	-0.618197758
C	2.057712130	-4.031202149	-2.498573040
C	-2.766710677	3.734463784	-0.412626804
C	-5.186711143	2.094071881	-2.543556102
H	-2.315916500	-0.985831659	-4.153422056
H	-2.293798162	-1.306668238	-5.896135680
H	-2.358272363	0.359421209	-5.312913131
H	1.240719854	-2.007208510	-4.905067808
H	-0.195800602	-2.672347713	-5.697700322
H	-0.196597765	-2.409824192	-3.944717484
H	-0.292230163	0.937502376	-6.697374176
H	-0.278209700	-0.729034407	-7.302082914
H	1.174179744	-0.042594181	-6.550925424
C	4.215937380	-1.059370368	-2.720628803
H	3.971422139	-0.356457985	-0.711100607
C	1.739386442	-4.182612349	0.008088136
H	0.389068367	-3.275304655	-1.384733775
C	2.792538144	-0.841268756	4.177557216
C	-5.868249281	-3.050038703	-1.106939683
C	-4.022135930	1.848304312	0.739404699
H	-1.896136034	1.996008672	0.449208080
C	-3.178904992	2.836799839	-3.881642045
H	-3.840080601	0.814661447	-3.618942950
C	0.700393129	2.452931675	-1.348841490
H	-6.595070353	-2.341653799	-1.515919663
H	-6.291061965	-3.465850008	-0.185092819
H	-5.780765962	-3.878882630	-1.821101095
H	2.250490117	-0.942261879	5.122610341
H	3.361168594	0.096303443	4.225372030
H	3.522414798	-1.656787246	4.122703889
H	5.282723532	-0.811334886	-2.780241608
H	3.650740455	-0.237196589	-3.166833813
H	4.052761342	-1.953306141	-3.332297800
H	5.744729244	-2.048092255	-0.638475897
H	4.648122750	-3.318729953	-1.173916357
H	4.441259747	-2.594404845	0.420827998
H	1.583473206	-5.010742450	-2.633499450
H	3.133419797	-4.206318585	-2.399724831
H	1.890112505	-3.455944698	-3.410655986
H	1.294955226	-5.178027970	-0.118197545
H	1.303736986	-3.731640385	0.902567465
H	2.809010225	-4.324247793	0.189629023
H	-3.980629272	2.395336002	1.690152504

H	-4.045426249	0.780281742	0.970400482
H	-4.968705484	2.108366858	0.256746817
H	-2.706177287	4.291773796	0.530090257
H	-3.667968902	4.076755375	-0.931521604
H	-1.894626952	4.007948722	-1.010543709
H	-3.849892791	3.043209148	-4.724678525
H	-2.200719437	2.566160858	-4.287181555
H	-3.061610960	3.769360855	-3.320357692
H	-5.830618204	2.217326619	-3.423565083
H	-5.197740126	3.043863686	-2.001603129
H	-5.647507380	1.341728555	-1.900253590
C	0.141719252	0.365788766	-4.004466096
H	1.249259548	0.386894446	-4.076173514
H	-0.170560493	1.405773655	-4.219202329
H	0.457791393	3.201068037	-2.112453169
H	2.530834925	1.828072394	-2.360772176
O	0.264886901	2.822451876	-0.055808146
C	0.737474207	4.090032236	0.404524330
H	0.607169562	4.841679128	-0.390897701
H	0.070661926	4.364094583	1.230444081
C	2.185559037	4.084555839	0.887087431
H	2.321982297	3.342014400	1.679550989
H	2.873877750	3.850544252	0.071597707
H	2.449879574	5.069764234	1.288949202
H	2.446832028	1.430895160	-0.578963034

D-antic

Ti	0.220686820	0.397451709	-1.908091039
P	1.962769206	-1.543276775	-1.147908214
C	1.468049667	-1.210942569	0.595825380
C	2.295846937	-1.285994132	1.720938882
C	1.806489480	-1.094552898	3.017786357
C	0.439248292	-0.823238415	3.164924949
C	-0.398178479	-0.703406605	2.061117748
C	0.101722598	-0.871397094	0.757015722
N	-0.688114791	-0.637293547	-0.388373228
C	-1.978778347	-1.188691347	-0.465245923
C	-2.307262956	-2.453315797	0.058953641
C	-3.574367312	-2.995677019	-0.133098019
C	-4.562849383	-2.316060543	-0.857436428
C	-4.244224148	-1.043839894	-1.350102124
C	-2.987702552	-0.462786354	-1.148321875
P	-2.424207540	1.207447589	-1.671259785
C	3.837801878	-1.350061934	-1.221808667
C	1.492102836	-3.382627537	-1.341803441
C	-2.608306942	2.220457688	-0.071103046
C	-3.701268717	1.815252273	-2.928746164
C	-0.414965556	-0.651004921	-5.096065107
C	-1.953941446	-0.653512076	-5.045931721
C	0.082969041	-2.092330810	-4.897355439
C	0.026856417	-0.173900686	-6.499760084
C	1.902445304	1.698650552	-1.528918659
H	3.350902308	-1.507188589	1.597311938
H	0.026222964	-0.685378497	4.162178506
H	-1.448961535	-0.464130871	2.196819183
H	-1.555658290	-3.011851649	0.608593945
H	-3.794946694	-3.979246786	0.277758788
H	-5.007787504	-0.498828919	-1.897018679
C	4.721458907	-2.451154783	-0.610150135
C	2.126841774	-4.034712211	-2.581320433
C	-2.460454223	3.730558432	-0.323478836
C	-5.080274242	2.256962041	-2.407216154
H	-2.318079071	-1.005653783	-4.075006400
H	-2.369262536	-1.311520064	-5.819880131
H	-2.354022634	0.351070961	-5.220857780
H	1.176593209	-2.134062366	-4.950180112
H	-0.312768420	-2.759958715	-5.672984316
H	-0.227282237	-2.486231684	-3.923741855
H	-0.319795904	0.847663275	-6.694271515
H	-0.376492749	-0.822013192	-7.289148448
H	1.119499221	-0.176723251	-6.589427396
C	4.270238729	-1.062776154	-2.672334603
H	3.965041059	-0.423442855	-0.650829457
C	1.697206671	-4.266573208	-0.101335375
H	0.411581842	-3.305620323	-1.522148495
C	2.727319767	-1.173471671	4.213946920
C	-5.920176505	-2.936061062	-1.096228552
C	-3.832757205	1.918366165	0.805984857
H	-1.719206799	1.886563124	0.477620564
C	-3.087171066	2.915841741	-3.815260448
H	-3.845287239	0.927953282	-3.556881320
C	0.672902954	2.441057052	-1.476657960
H	-6.629004840	-2.204286202	-1.495619665
H	-6.345967299	-3.341419453	-0.171002823
H	-5.865911947	-3.765022944	-1.813485825
H	2.161536729	-1.241893400	5.148007562
H	3.371656421	-0.287922608	4.285352774
H	3.387658917	-2.046403404	4.159063920
H	5.336575683	-0.806837138	-2.701561373
H	3.711193608	-0.226315414	-3.099665936
H	4.126053000	-1.934101546	-3.320696429
H	5.764291749	-2.110342339	-0.589353677
H	4.697711909	-3.369101006	-1.204877991
H	4.442604820	-2.714261573	0.412357001
H	1.645327005	-5.000307148	-2.777549822
H	3.192632082	-4.231401673	-2.432358901
H	2.016890091	-3.424624027	-3.479340453

H	1.265131107	-5.258477842	-0.285213865
H	1.217457930	-3.851021914	0.787517713
H	2.758317517	-4.409103798	0.125686259
H	-3.719783013	2.421341133	1.774913214
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H	-4.761799775	2.281430994	0.357529073
H	-2.338815580	4.254737719	0.632216066
H	-3.347759405	4.149538798	-0.808657729
H	-1.591816533	3.965557071	-0.943208177
H	-3.775269968	3.169632876	-4.631000065
H	-2.139479877	2.599314749	-4.258773388
H	-2.900529706	3.832844014	-3.246766223
H	-5.754843589	2.426653791	-3.255892954
H	-5.018512733	3.197946967	-1.852939899
H	-5.549326974	1.518109310	-1.754038585
H	0.330780457	2.761804731	-0.493191804
C	0.177415379	0.278761650	-4.014402084
H	1.284685345	0.262996834	-4.100978421
H	-0.106108514	1.324531776	-4.237847081
H	0.416565886	3.129085938	-2.283134058
H	2.547325400	1.831042107	-2.407938457
O	2.643954708	1.519384353	-0.337627541
C	3.320993979	2.699984763	0.090918224
H	2.592143719	3.443994947	0.449792749
H	3.858360646	3.152427591	-0.759519137
C	4.289377453	2.325020798	1.201213407
H	3.755735399	1.833301682	2.021894324
H	5.060979447	1.637955046	0.835878906
H	4.785055083	3.219113948	1.597007115

D-antid

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C	2.307174522	-1.210815629	1.729573387
C	1.814247930	-0.988980510	3.021769674
C	0.439548215	-0.755643630	3.163340919
C	-0.403535786	-0.687618954	2.058779708
C	0.100290386	-0.873651360	0.758577014
N	-0.677691422	-0.670292960	-0.395353991
C	-1.977245004	-1.199619198	-0.474137805
C	-2.327026877	-2.458728667	0.047869803
C	-3.598425284	-2.985591285	-0.160354078
C	-4.567761068	-2.293916247	-0.898671994
C	-4.229587363	-1.023098901	-1.382611475
C	-2.968795547	-0.457420662	-1.164394692
P	-2.380289525	1.211970724	-1.667096479
C	3.844024026	-1.495920162	-1.180717425
C	1.410326322	-3.413956231	-1.277434800
C	-2.562975208	2.201002579	-0.051696858
C	-3.648932485	1.851348845	-2.918755704
C	-0.415241168	-0.619023865	-5.107145373
C	-1.954478204	-0.604565412	-5.072991536
C	0.064739092	-2.069604839	-4.929619617
C	0.045641128	-0.122066249	-6.498379769
C	1.968106649	1.582686365	-1.436523540
H	3.366257923	-1.418227223	1.612849087
H	0.023975457	-0.602961640	4.157364416
H	-1.460079637	-0.472621393	2.190289192
H	-1.588098943	-3.026763257	0.605209516
H	-3.836721939	-3.966577792	0.246528227
H	-4.980620777	-0.467974129	-1.936728628
C	4.645693012	-2.631031359	-0.518494368
C	1.985139820	-4.106959325	-2.523790534
C	-2.380630310	3.711114673	-0.278880221
C	-5.026288709	2.295666451	-2.395000330
H	-2.333225166	-0.970820677	-4.112752955
H	-2.369798158	-1.242324276	-5.863731283
H	-2.340653137	0.408080152	-5.232864066
H	1.158625173	-2.121838230	-4.970222029
H	-0.328845827	-2.718492435	-5.722187227
H	-0.262201283	-2.477599927	-3.967159692
H	-0.288640975	0.906480894	-6.677398261
H	-0.356705120	-0.751258942	-7.303739486
H	1.138891282	-0.134214844	-6.576084357
C	4.310946999	-1.274127043	-2.631787888
H	4.041174638	-0.567328711	-0.629748268
C	1.596000065	-4.289707628	-0.028362767
H	0.330830030	-3.287484399	-1.434274014
C	2.737734425	-1.000857554	4.218080667
C	-5.925804049	-2.900960667	-1.164901735
C	-3.800661150	1.909477861	0.810591522
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C	-3.023122958	2.961243588	-3.785037712
H	-3.798342312	0.975727473	-3.561615424
H	2.499594299	1.372474142	-0.504333126
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H	-6.631875302	-2.152944805	-1.538230776
H	-6.355060832	-3.341230260	-0.257662859
H	-5.870367656	-3.701359666	-1.913947881
H	2.178215179	-1.118549908	5.151037996
H	3.309760002	-0.067264869	4.295436470
H	3.464462363	-1.818774585	4.159416967
H	5.400886544	-1.149931457	-2.655169348
H	3.855049842	-0.375058683	-3.051072631
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H	4.572799035	-3.560196302	-1.091044147
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H	1.465304919	-5.058174000	-2.690074416
H	3.048101333	-4.337534816	-2.404436537
H	1.868040379	-3.505592514	-3.426966324
H	1.098789239	-5.255628067	-0.183739991
H	1.166031022	-3.831077685	0.865171669
H	2.651139997	-4.495499335	0.173833743
H	-3.684231619	2.391136332	1.789892220
H	-3.939477471	0.838541463	0.978658022
H	-4.718041235	2.301626032	0.363163383
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H	-3.250550015	4.155261399	-0.773114031
H	-1.496397194	3.935473274	-0.880406849
H	-3.709634564	3.239010685	-4.594273789
H	-2.080359518	2.641442170	-4.236378852
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H	-4.959621419	3.227324453	-1.825663638
H	-5.503827346	1.550148611	-1.755659034
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C	0.182221544	0.282822917	-4.007500186
H	1.288589819	0.265823246	-4.082415514
H	-0.089181840	1.336961259	-4.206510120
O	2.818564958	1.721364436	-2.563426878
C	3.491467236	2.981044661	-2.667638989
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H	4.261835204	3.109965659	-0.636152314
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H	5.147084810	4.089951934	-1.814941198
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D-antib

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C	2.288220086	-1.149931055	1.735426454
C	1.790991785	-0.968354950	3.031908746
C	0.410664190	-0.774114897	3.177742394
C	-0.434807359	-0.708415409	2.075060335
C	0.071582346	-0.855242359	0.770624512
N	-0.717525589	-0.653995348	-0.376379896
C	-2.002757836	-1.216293666	-0.459672433
C	-2.319668011	-2.488953370	0.049927481
C	-3.576808977	-3.046210414	-0.165164390
C	-4.562109814	-2.372721982	-0.899388480
C	-4.255214679	-1.090132691	-1.373284709
C	-3.010394039	-0.493085694	-1.146934473
P	-2.458527037	1.192641505	-1.641617613
C	3.824964258	-1.229062160	-1.201777488
C	1.545629926	-3.331116621	-1.291773047
C	-2.669171360	2.181311487	-0.030038616
C	-3.723711955	1.802163419	-2.908759610
C	-0.400647846	-0.543598423	-5.100288954
C	-1.940059584	-0.568513310	-5.089608935
C	0.113861463	-1.983732853	-4.932418578
C	0.068054164	-0.017696930	-6.477633218
C	1.846166493	1.692045902	-1.385095254
H	3.352482791	-1.326537144	1.614045317
H	-0.008104873	-0.650704633	4.174434020
H	-1.496365615	-0.523554226	2.211297328
H	-1.566340773	-3.043108667	0.602149410
H	-3.790748438	-4.036485345	0.232701935
H	-5.018384681	-0.550697188	-1.926165710
C	4.734341122	-2.305384849	-0.583007750
C	2.160842729	-3.963609769	-2.550683575
C	-2.509660663	3.693991192	-0.263636369
C	-5.119038058	2.205084287	-2.399396407
H	-2.323042238	-0.968040952	-4.144484330
H	-2.326401001	-1.197661287	-5.901668599
H	-2.349458948	0.437544331	-5.230577744
H	1.208652476	-2.009832654	-4.975820951
H	-0.264611963	-2.636996068	-5.728609539
H	-0.200622432	-2.405901419	-3.971817915
H	-0.287311535	1.005099191	-6.647585804
H	-0.307844868	-0.645606357	-7.296393527
H	1.162517214	-0.003908874	-6.540594437
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H	3.952634007	-0.302509350	-0.628995737
C	1.810357349	-4.202145746	-0.053641111
H	0.457981802	-3.285806296	-1.438567083
C	2.715255022	-0.981947475	4.227604430
C	-5.904756995	-3.011010107	-1.170660928
C	-3.905110929	1.865631191	0.825866391
H	-1.788865373	1.838651343	0.527192467
C	-3.121567341	2.933634097	-3.763074435
H	-3.840357299	0.924571403	-3.555659417
H	2.410440656	1.480845583	-0.478588947
H	2.471484552	1.871730067	-2.260117769
C	0.611374711	2.420768207	-1.264873781
H	-6.622705571	-2.282063822	-1.558645579
H	-6.333143825	-3.449538544	-0.262032024
H	-5.826094798	-3.818774809	-1.909578769
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H	3.286095611	-0.047939540	4.307038230

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H	5.771194403	-1.946825871	-0.576477043
H	4.718558918	-3.230189630	-1.166864490
H	4.467501479	-2.559599317	0.444824471
H	1.719007556	-4.952621170	-2.721435936
H	3.240476547	-4.107908805	-2.444300269
H	1.984645740	-3.365230312	-3.446212083
H	1.388738937	-5.202417725	-0.214786242
H	1.354047256	-3.787197332	0.848003699
H	2.880294495	-4.327118495	0.137294040
H	-3.806111024	2.357899239	1.801848613
H	-4.019762324	0.793016769	1.002208693
H	-4.828565734	2.232709886	0.369906152
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H	-3.407184686	4.126787693	-0.718057204
H	-1.657777850	3.920543370	-0.909667609
H	-3.799949734	3.177213363	-4.590220295
H	-2.152003692	2.657345199	-4.182786030
H	-2.975193131	3.844642351	-3.175017128
H	-5.783850793	2.374077746	-3.255828425
H	-5.083911746	3.138877642	-1.831150604
H	-5.583125067	1.447345827	-1.764444443
H	0.289545749	2.701352589	-0.254685845
C	0.154751827	0.359116670	-3.979855005
H	1.264503513	0.347011032	-4.034771138
H	-0.122814943	1.412386259	-4.167101634
O	0.269665315	3.390788611	-2.240776593
C	1.053613461	4.581635977	-2.149818631
H	2.120524936	4.337981515	-2.255465851
H	0.921787162	5.034432123	-1.152936754
C	0.608837120	5.541366121	-3.241279140
H	-0.448718849	5.798776558	-3.127326834
H	1.195125945	6.465564962	-3.200965881
H	0.744941820	5.089183570	-4.228513644

D-synd

Ti	0.330034039	0.559471822	-1.815552453
P	2.045453105	-1.389798944	-1.053833786
C	1.499026466	-1.152000561	0.691101070
C	2.289587477	-1.279448615	1.839666306
C	1.757906465	-1.133546055	3.127371155
C	0.387932693	-0.858392417	3.241495077
C	-0.411813054	-0.688399343	2.115239472
C	0.130130809	-0.807204522	0.822675135
N	-0.613692518	-0.530690554	-0.341712761
C	-1.884720215	-1.112546747	-0.497256571
C	-2.200918650	-2.400357949	-0.022473217
C	-3.431124735	-2.982944341	-0.311422766
C	-4.392869557	-2.321497479	-1.086146176
C	-4.092401394	-1.024045473	-1.520514854
C	-2.875641337	-0.402067556	-1.220855358
P	-2.343230006	1.300641164	-1.662630262
C	3.934388969	-1.394175225	-0.958282052
C	1.401075579	-3.133456308	-1.449552888
C	-2.703176881	2.276434593	-0.074473325
C	-3.520237442	1.869422006	-3.030452508
C	0.737480357	0.371923451	-5.164773307
C	2.202767113	-0.089280304	-5.072874792
C	0.721614392	1.889411722	-5.436430925
C	0.065298609	-0.349943736	-6.356213256
C	1.960233763	1.853960599	-1.299833185
H	3.345173419	-1.516079686	1.744724850
H	-0.056158960	-0.756370757	4.229373123
H	-1.465675966	-0.448945644	2.224429067
H	-1.466430774	-2.947750061	0.560265489
H	-3.640262798	-3.984866196	0.059071905
H	-4.838176838	-0.494039990	-2.104833962
C	4.605707080	-2.675875406	-0.434537297
C	1.868284508	-3.609772641	-2.834057463
C	-2.573815877	3.793075451	-0.294476932
C	-4.966046842	2.228359744	-2.642963867
H	2.723118426	0.434188030	-4.268202104
H	2.734315732	0.112837844	-6.012011977
H	2.268809838	-1.167560978	-4.886757481
H	-0.302933124	2.261565492	-5.551698023
H	1.261571578	2.127558731	-6.361874836
H	1.197540338	2.436035334	-4.616505443
H	0.070252625	-1.436834700	-6.210857087
H	0.586060835	-0.136341475	-7.299418975
H	-0.979057071	-0.035785379	-6.472105838
C	4.552528602	-0.964539975	-2.299866830
H	4.126227984	-0.585798859	-0.240310962
C	1.598981095	-4.220822124	-0.382267205
H	0.324445148	-2.930155055	-1.516467622
C	2.639948923	-1.261966114	4.347937014
C	-5.701071049	-2.988090886	-1.443193831
C	-3.993677281	1.926138587	0.681438255
H	-1.857067469	1.957853654	0.548060643
C	-2.884800334	3.024124195	-3.827539955
H	-3.549096949	0.988039281	-3.685901321
C	0.729931654	2.595901108	-1.316927023
H	-6.419803542	-2.268048175	-1.846243355
H	-6.161197366	-3.465966917	-0.570723285
H	-5.561811763	-3.770392122	-2.200478897

H	2.047084476	-1.431418680	5.251828620
H	3.234030082	-0.353719167	4.512492468
H	3.346048231	-2.093994577	4.249948302
H	5.643975517	-0.906433092	-2.200657561
H	4.180290185	0.015274400	-2.603880987
H	4.334622514	-1.684120281	-3.096152400
H	5.676174457	-2.489714361	-0.282559131
H	4.521568286	-3.492280003	-1.158616334
H	4.191310803	-3.027375519	0.513107744
H	1.342763661	-4.532686130	-3.107009185
H	2.940931265	-3.830469133	-2.849785960
H	1.664210820	-2.869555173	-3.612448258
H	0.972913840	-5.088386064	-0.626190015
H	1.314512779	-3.873600178	0.614650366
H	2.634186026	-4.569975773	-0.336479188
H	-3.987886378	2.415684368	1.663661940
H	-4.092180688	0.849799620	0.843496972
H	-4.886610185	2.270294670	0.151776543
H	-2.556240699	4.308753774	0.673244793
H	-3.423222069	4.193520997	-0.857452770
H	-1.657704042	4.057653471	-0.828731043
H	-3.489033491	3.246441061	-4.715644359
H	-1.873064154	2.779923932	-4.157837963
H	-2.830222563	3.940573777	-3.230583632
H	-5.562734909	2.379056136	-3.551425417
H	-5.004505061	3.162559020	-2.074434584
H	-5.459280141	1.458375730	-2.046274751
C	-0.040876616	0.056856639	-3.861020999
H	-1.096580190	0.313243330	-4.037493639
H	-0.042955688	-1.041428754	-3.696533709
H	2.454252249	1.689154591	-0.334883960
H	0.321367316	2.951790580	-0.371597633
H	0.523636087	3.249661207	-2.165963126
O	2.871312441	2.013468130	-2.371106830
C	3.575277730	3.256254089	-2.333561446
H	2.860580121	4.091988120	-2.378526409
H	4.115462320	3.343085464	-1.375435938
C	4.541102766	3.307954216	-3.504310327
H	5.086045476	4.258912148	-3.505611730
H	5.270770111	2.493301958	-3.448737723
H	4.002549391	3.219525536	-4.453531199

D-synb

Ti	0.312228442	0.530663284	-1.843340878
P	2.032801428	-1.425015214	-1.038932081
C	1.489532197	-1.172343320	0.705290360
C	2.275052830	-1.314643957	1.855934395
C	1.745922323	-1.151973823	3.142409478
C	0.382258116	-0.845422206	3.253656459
C	-0.412234338	-0.662838303	2.125907605
C	0.127820769	-0.798567564	0.834112238
N	-0.612618535	-0.514306023	-0.329869167
C	-1.893772790	-1.074282097	-0.484899640
C	-2.238985341	-2.348448552	0.004880054
C	-3.475759017	-2.912750592	-0.292493693
C	-4.413436437	-2.246044812	-1.091560826
C	-4.083681406	-0.960536094	-1.540961952
C	-2.861132609	-0.354736670	-1.232277184
P	-2.280159032	1.326715572	-1.703772624
C	3.925553009	-1.378333882	-0.957301709
C	1.426588165	-3.186026642	-1.416329332
C	-2.606843430	2.350232069	-0.141543556
C	-3.426584985	1.902334772	-3.089918819
C	0.692766544	0.215027987	-5.195555009
C	2.211709695	-0.000883215	-5.070808320
C	0.435381296	1.675211572	-5.616136712
C	0.161820286	-0.719165254	-6.309268050
C	1.994582721	1.786916746	-1.454244705
H	3.325289773	-1.574506781	1.763778497
H	-0.060684530	-0.728700848	4.240404040
H	-1.460529928	-0.399326892	2.232677538
H	-1.521591181	-2.900692005	0.604237405
H	-3.708602091	-3.904919533	0.089896798
H	-4.810442967	-0.427937132	-2.146152153
C	4.648064627	-2.636604302	-0.444343527
C	1.887528363	-3.655165404	-2.806086247
C	-2.428377384	3.855506085	-0.406552088
C	-4.874408433	2.272368010	-2.718637923
H	2.653288015	0.694395219	-4.350577656
H	2.710695580	0.156651609	-6.035377441
H	2.445588069	-1.019314273	-4.741036079
H	-0.629570828	1.843213669	-5.813162790
H	0.982738116	1.921973019	-6.535089723
H	0.744041513	2.372810711	-4.831257030
H	0.361375887	-1.771035650	-6.071082956
H	0.634203233	-0.499822053	-7.276268274
H	-0.921804667	-0.607372904	-6.432556973
C	4.521723675	-0.938261565	-2.305632466
H	4.101693151	-0.564982099	-0.241219161
C	1.657947555	-4.265428438	-0.348042271
H	0.344506231	-3.006484734	-1.471320742
C	2.623923530	-1.292544229	4.364643522
C	-5.726963723	-2.895523584	-1.460743874
C	-3.907597652	2.055678548	0.619855925
H	-1.770557250	2.021539707	0.488614391
C	-2.778198962	3.052520697	-3.882363728
H	-3.451815541	1.018370797	-3.742343909

H	2.572610885	1.890140167	-2.375343805
C	0.776636149	2.545467634	-1.339902774
H	-6.434183357	-2.165230179	-1.865718098
H	-6.198899708	-3.371603047	-0.593712806
H	-5.591747593	-3.676180738	-2.220602616
H	2.029981278	-1.494613520	5.261182370
H	3.199692406	-0.377259056	4.554303371
H	3.345982333	-2.108540830	4.250789978
H	5.606192396	-0.804077701	-2.208540358
H	4.092243473	0.005089602	-2.647478421
H	4.352569362	-1.687105812	-3.086618618
H	5.714410073	-2.416352160	-0.309429350
H	4.578464327	-3.456534655	-1.165905768
H	4.260900075	-3.000327629	0.509636706
H	1.376789287	-4.587835920	-3.073790954
H	2.963909846	-3.856383306	-2.832121125
H	1.661796843	-2.919737637	-3.583707096
H	1.051167742	-5.148632967	-0.584324628
H	1.372753735	-3.921417221	0.649677578
H	2.701150568	-4.589933306	-0.309613592
H	-3.893696384	2.579265634	1.584271204
H	-4.032247130	0.988166690	0.819209453
H	-4.790174952	2.402038544	0.074460922
H	-2.346151575	4.392736319	0.546340921
H	-3.291267617	4.272306028	-0.937397691
H	-1.533560353	4.063297722	-0.998985468
H	-3.342675588	3.232182821	-4.805818217
H	-1.741085414	2.838898893	-4.143242905
H	-2.785321188	3.982452075	-3.305693995
H	-5.459360106	2.423906653	-3.634570693
H	-4.908896069	3.210540744	-2.156410770
H	-5.382342889	1.511601493	-2.122485777
C	-0.042290301	-0.092508156	-3.865964086
H	-1.117904727	0.061846261	-4.043831169
H	0.052580944	-1.176571520	-3.648777848
H	2.608525801	1.616694203	-0.571154794
O	0.433961393	3.473781446	-2.355373803
C	1.231971107	4.660298468	-2.325852472
H	1.124432959	5.150190258	-1.343976695
H	2.294097872	4.400652166	-2.443063041
C	0.775695005	5.588016616	-3.440726939
H	0.898625611	5.109291648	-4.416960007
H	-0.279829357	5.850756477	-3.320554324
H	1.363854282	6.512018585	-3.433353179
H	0.480674062	2.879547771	-0.338002276

D-syna

Ti	0.254474598	0.599342444	-1.830934454
P	2.020079235	-1.328554330	-1.060901438
C	1.504461841	-1.068685130	0.689654849
C	2.317232123	-1.170337925	1.825993375
C	1.807419786	-1.002249084	3.118803815
C	0.437007044	-0.735726197	3.250291274
C	-0.385152370	-0.595592791	2.137684852
C	0.135496320	-0.732901303	0.838844326
N	-0.628924048	-0.480136850	-0.314844220
C	-1.884883776	-1.090893514	-0.461693433
C	-2.175086478	-2.376794135	0.035500436
C	-3.387929858	-2.994571790	-0.253255766
C	-4.356776532	-2.372561817	-1.051250329
C	-4.084565444	-1.075424154	-1.505070412
C	-2.887728045	-0.416294172	-1.204750878
P	-2.406944091	1.302015880	-1.655194792
C	3.912626659	-1.275282551	-0.996769241
C	1.419209753	-3.094324275	-1.416444229
C	-2.837431243	2.290627910	-0.093863875
C	-3.568044610	1.805756909	-3.062077322
C	0.659072047	0.392265430	-5.179819678
C	2.148931319	0.021960985	-5.077347425
C	0.546822050	1.896298951	-5.499229909
C	0.043333917	-0.402552486	-6.356011283
C	1.929485773	1.893877748	-1.551762672
H	3.372881657	-1.400734935	1.717795042
H	0.010066472	-0.615393135	4.243890869
H	-1.437493598	-0.356874733	2.260620299
H	-1.433082778	-2.894594537	0.635593169
H	-3.576979461	-3.993450914	0.135826119
H	-4.838164463	-0.575296280	-2.104949848
C	4.636931980	-2.531768545	-0.482908380
C	1.876562581	-3.573977821	-2.803290212
C	-2.818179492	3.806009107	-0.352968752
C	-5.038863653	2.107984284	-2.720204081
H	2.649048787	0.605488776	-4.300134762
H	2.666649073	0.213067500	-6.025848303
H	2.281296581	-1.039006843	-4.837163069
H	-0.497441244	2.190640148	-5.651787372
H	1.094978401	2.145908061	-6.416327545
H	0.954397556	2.509057524	-4.687573186
H	0.125583444	-1.482613757	-6.185852109
H	0.548169780	-0.173257091	-7.303936342
H	-1.020346225	-0.166143627	-6.476481826
C	4.501287239	-0.838679482	-2.348790686
H	4.092064261	-0.459339937	-0.284390081
C	1.660887907	-4.160872431	-0.337574522
H	0.336442262	-2.919595394	-1.467137115
C	2.710045228	-1.092154352	4.327870660
C	-5.643295547	-3.078438367	-1.411682970

C	-4.103785295	1.859787421	0.660269705
H	-1.965774477	2.065831536	0.530942727
C	-2.959864380	2.978460003	-3.854567491
H	-3.541401033	0.918267881	-3.709244630
H	2.528004452	2.009333908	-2.456349069
C	0.710213425	2.646223260	-1.429545350
H	-6.383007460	-2.380061230	-1.815057857
H	-6.090286769	-3.571086309	-0.540672986
H	-5.479438976	-3.855238366	-2.169863706
H	2.139749407	-1.311997347	5.235646557
H	3.246517059	-0.149945476	4.500697058
H	3.466423896	-1.875821835	4.209872403
H	5.588570580	-0.721868452	-2.261891433
H	4.084149777	0.114204634	-2.679091486
H	4.311998339	-1.579286143	-3.132915598
H	5.703012817	-2.310159551	-0.347992433
H	4.567808289	-3.352447271	-1.203864853
H	4.249054867	-2.894121502	0.471386668
H	1.373683502	-4.514394583	-3.058402509
H	2.954981843	-3.764208501	-2.834175569
H	1.638634572	-2.848012158	-3.586224718
H	1.049650955	-5.045614272	-0.555839879
H	1.387105444	-3.803373754	0.658776801
H	2.703817337	-4.487095330	-0.305998370
H	-4.151614512	2.386822892	1.621789723
H	-4.114329176	0.786480775	0.866202940
H	-5.016959235	2.105121668	0.109571388
H	-2.874356340	4.339895734	0.603768207
H	-3.672833513	4.133661102	-0.953820432
H	-1.894588888	4.115316623	-0.846455591
H	-3.543187086	3.160119345	-4.765724035
H	-1.926776738	2.778863525	-4.146597108
H	-2.968880049	3.903716535	-3.269780294
H	-5.613214880	2.225728189	-3.647788485
H	-5.133506466	3.044079234	-2.162194018
H	-5.518915750	1.324309242	-2.131004379
C	-0.108961257	0.059992385	-3.874444297
H	-1.173369305	0.272609436	-4.057032091
H	-0.068566996	-1.036114687	-3.706801542
H	0.435992787	3.357797752	-2.217746044
O	0.310027117	3.057675909	-0.137467568
C	1.059258056	4.165260287	0.361456143
H	0.905636209	5.038869988	-0.294417507
H	2.133699016	3.931308837	0.343911261
C	0.597063135	4.465992138	1.776606143
H	0.749909365	3.596233970	2.423047939
H	1.159491089	5.309629497	2.190591249
H	-0.467050161	4.721128292	1.792600458
H	2.521830546	1.715561941	-0.654850143

D-sync

Ti	0.314979780	0.551322200	-1.839125803
P	2.055181184	-1.373215772	-1.061139924
C	1.511692869	-1.181671608	0.686684826
C	2.303274098	-1.357432823	1.827377980
C	1.781754674	-1.226335409	3.120064135
C	0.420831416	-0.913599748	3.247020238
C	-0.378793045	-0.701711060	2.128056234
C	0.152855745	-0.812006527	0.830377021
N	-0.601171672	-0.509976568	-0.323859697
C	-1.875449624	-1.090049887	-0.466631637
C	-2.189733833	-2.378604198	0.008636919
C	-3.427325021	-2.955070279	-0.260411527
C	-4.400851166	-2.287265173	-1.014908786
C	-4.101021973	-0.991033976	-1.453289975
C	-2.875423801	-0.376663248	-1.175268898
P	-2.336002172	1.316037638	-1.639743265
C	3.943891677	-1.333878045	-0.983484907
C	1.439847001	-3.119150222	-1.491052452
C	-2.635669503	2.307941361	-0.048644813
C	-3.542910953	1.891114122	-2.977371435
C	0.698866101	0.349938458	-5.191598798
C	2.201113198	0.028751365	-5.095444226
C	0.538971267	1.847269179	-5.520679028
C	0.101002358	-0.471783824	-6.358940299
C	1.971566032	1.856241510	-1.554416671
H	3.353758766	-1.610704520	1.720775229
H	-0.015579809	-0.818214650	4.239017990
H	-1.425869633	-0.438669822	2.247857125
H	-1.448406463	-2.930346315	0.578202059
H	-3.633954753	-3.957194399	0.111096483
H	-4.854058854	-0.456069580	-2.023882695
C	4.660526923	-2.606227694	-0.501243232
C	1.893093770	-3.553257088	-2.894151979
C	-2.511972296	3.822602890	-0.285790192
C	-4.974343528	2.263035101	-2.551195589
H	2.685881172	0.622927943	-4.315801032
H	2.709067897	0.243127381	-6.044274913
H	2.369648616	-1.028630798	-4.863946660
H	-0.515308433	2.108558497	-5.664397582
H	1.070199152	2.106152109	-6.445147965
H	0.936068715	2.477682013	-4.717572642
H	0.217347788	-1.547587876	-6.182098810
H	0.592876798	-0.233842827	-7.311577718
H	-0.970275445	-0.269148736	-6.474746552
C	4.539181678	-0.858284082	-2.319132531
H	4.106154372	-0.530044530	-0.256845983

C	1.678966019	-4.227859073	-0.454669559
H	0.357362762	-2.939938541	-1.534153032
C	2.665573566	-1.404674882	4.333299271
C	-5.719686514	-2.945843995	-1.346921032
C	-3.899649604	1.966742864	0.754460668
H	-1.768787035	1.991971241	0.545730203
C	-2.920034607	3.038122688	-3.794960824
H	-3.597250317	1.007765415	-3.628710907
H	2.590495015	1.956257711	-2.456433714
C	0.751945840	2.614047850	-1.493701475
H	-6.442248454	-2.220864652	-1.734075227
H	-6.165095581	-3.422413981	-0.466092530
H	-5.600574045	-3.727783928	-2.108073122
H	2.072853074	-1.580945270	5.236056130
H	3.282566241	-0.515338777	4.515826446
H	3.350794978	-2.251095989	4.212522371
H	5.627132329	-0.753211626	-2.224518203
H	4.131460623	0.110540653	-2.612206976
H	4.347769275	-1.568232710	-3.130760077
H	5.726657257	-2.390858849	-0.355870228
H	4.594180349	-3.409178663	-1.242260599
H	4.269123575	-2.992346627	0.442553122
H	1.387273501	-4.483514708	-3.179137688
H	2.970723921	-3.744962034	-2.933431723
H	1.655662067	-2.802361688	-3.652737473
H	1.070175133	-5.104164518	-0.710652721
H	1.402095155	-3.911508286	0.554444248
H	2.722641243	-4.552731452	-0.433460867
H	-3.857905505	2.462955458	1.732431109
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H	-4.809673175	2.309917169	0.253902125
H	-2.458144447	4.345689816	0.676648634
H	-3.380936093	4.220613631	-0.819991644
H	-1.615951733	4.081501535	-0.855546611
H	-3.544741317	3.260795406	-4.668774352
H	-1.918206119	2.786462416	-4.148529407
H	-2.845086544	3.956678873	-3.203549579
H	-5.594833226	2.416481703	-3.443105214
H	-4.989256308	3.198848986	-1.984293274
H	-5.456568952	1.498260692	-1.938923127
H	0.416583761	2.964027182	-0.517220242
C	-0.050812234	0.004919251	-3.878028117
H	-1.120110769	0.207159897	-4.045506310
H	0.002797739	-1.090917016	-3.711663982
H	0.483821555	3.275222752	-2.317933072
O	2.736179798	1.660381182	-0.382217650
C	3.417770370	2.836324175	0.050497515
H	2.691341503	3.637513893	0.255295925
H	4.081152890	3.197882415	-0.754322541
C	4.215010849	2.499324748	1.298307846
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C	-0.833337530	4.027208312	-0.461752219
C	-0.560778048	2.657062333	-0.560852063
C	-1.554284786	1.699806886	-0.225969404
C	-2.790033387	2.191643792	0.241776455
C	-3.038758892	3.556337031	0.330070710
C	-3.334081218	-0.123276337	-1.568491746
C	-4.343466768	-0.989883262	-1.958122497
C	-4.345461925	-2.340951156	-1.574576879
C	-3.245464861	-2.785808392	-0.842098611
C	-2.191727712	-1.937797051	-0.462490122
P	1.042209533	1.885963258	-0.972517970
P	-0.651879001	-2.524813197	0.324257666
C	0.883805845	1.413808559	-2.799191686
C	2.465632044	3.106245924	-0.795563012
C	0.171191320	-3.545101504	-1.055947809
C	-1.172048594	-3.731152079	1.678464209
C	1.456243924	-4.242029071	-0.581449799
C	-0.720355940	-4.539745650	-1.812570119
C	0.264942383	2.472047098	-3.725499654
C	2.203555135	0.850379130	-3.349529486
C	2.582497778	4.255868862	-1.811863097
C	2.546795604	3.618704160	0.651974371
C	0.020798867	-4.082693854	2.585358206
C	-2.316827729	-3.138274290	2.516494693
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O	2.210153985	-1.027419598	-0.088785278
C	0.321933324	0.785468725	3.609273727
C	1.157541117	2.024750554	4.013078210
C	-1.161180003	1.195641860	3.516200393
C	0.479863314	-0.289697638	4.712225541
C	3.516758690	-1.262811651	0.378134657
C	4.568793099	-0.893980809	-0.665840334
C	-5.477864963	-3.264269704	-1.959285358
C	-2.367607444	5.987249431	0.033154022
H	-4.005596163	3.892277225	0.700245796
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H	-3.200473377	-3.835472098	-0.561455380
H	0.168924122	0.583716292	-2.731465659
H	3.328830493	2.443995957	-0.952304220
H	0.467113642	-2.751035737	-1.754081414
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H	2.081508024	-3.581482720	0.019567118
H	1.228706931	-5.141585021	0.000334673
H	-0.127082146	-5.038019789	-2.589578374
H	-1.566992456	-4.054181858	-2.300379937
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H	0.940990959	3.312083256	-3.908021088
H	2.043302534	0.436489084	-4.352496903
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H	3.469581551	4.857678718	-1.577479384
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H	1.724384361	4.303029346	0.882070073
H	3.487092429	4.162443947	0.801805867
H	2.505321370	2.794956216	1.368722914
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H	-0.305713942	-4.764643513	3.379820190
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H	-2.008187257	-2.197918709	2.986209148
H	-2.589021497	-3.837027419	3.316607602
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H	0.838784611	2.409505288	4.990750730
H	2.223820965	1.778245330	4.080842208
H	1.040708689	2.827559996	3.279024824
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H	-1.308078634	1.972228041	2.760015622
H	-0.109021421	-1.181992410	4.475605842
H	1.527304152	-0.596286484	4.817667369
H	0.140861229	0.092593632	5.684027797
H	3.701809604	-0.695276515	1.304886023
H	3.628163363	-2.328590010	0.634690829
H	4.415020542	-1.463706743	-1.588266589
H	4.520666151	0.172273751	-0.910395605
H	5.574931046	-1.113400991	-0.289401708
H	-6.395932115	-3.035121070	-1.402948576
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H	-5.226716282	-4.310672883	-1.759747895
H	-1.448960637	6.580167624	-0.012917001
H	-3.006397400	6.307874792	-0.800211149
H	-2.890954454	6.253422355	0.958266292

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Ti	0.461897817	0.907360700	0.943482690
P	3.131909119	0.842318366	1.122681315
C	3.159437911	2.251928881	2.308205141
C	4.174363027	3.207095776	2.418275161
C	4.131288467	4.245466939	3.359206928
C	3.024630429	4.283516068	4.215519910
C	1.983598233	3.365351962	4.114417575
C	1.999218586	2.343138852	3.139325315
N	0.931472437	1.480312730	2.902537347
C	-0.033413036	1.251304941	3.898455942
C	0.291462487	0.843790078	5.205527912
C	-0.703285677	0.530045912	6.125840105
C	-2.064215977	0.602851983	5.790023686
C	-2.389711908	1.027791366	4.497382257
C	-1.406157592	1.370295829	3.559607761
P	-1.718505194	2.000696586	1.858909658
C	4.489802968	1.192227069	-0.147361185
C	3.600734142	-0.648256614	2.191361746
C	-1.667445000	3.884168238	2.122761981
C	-3.459515474	1.458016730	1.376030043
C	-0.179899491	-0.717628298	0.896916810
C	-0.672054163	-2.135376208	1.085871860
C	-2.198227282	-2.151513699	1.339238091
C	0.028704886	-2.788525427	2.301542468
C	-0.371493793	-2.969983457	-0.182773452
C	0.444108072	1.779161993	-1.637254846
H	5.036922245	3.150312849	1.760541224
H	2.963548431	5.064118487	4.972061582
H	1.129668735	3.447593293	4.779231458
H	1.338256777	0.755472841	5.482240726
H	-0.417536599	0.207180209	7.125271889
H	-3.439500511	1.097985510	4.226215405
C	5.948338395	0.986530013	0.300224983
C	3.802989883	-1.907201972	1.335229294
C	-1.961346632	4.649392336	0.822952556
C	-4.648316175	2.256545194	1.933934785
H	-2.440391559	-1.598392654	2.252860284
H	-2.566970791	-3.179910893	1.458472646
H	-2.738385516	-1.693738721	0.503408341
H	1.112165683	-2.828524267	2.151413819
H	-0.328205904	-3.815830706	2.460709222
H	-0.164462700	-2.212623275	3.212216022
H	-0.871468077	-2.539055050	-1.057082041

H	-0.715166212	-4.007654866	-0.067206175
H	0.704044442	-2.988602251	-0.389300039
C	4.226263430	0.414902320	-1.451825422
H	4.342992019	2.260086697	-0.359793788
C	4.738992357	-0.441954380	3.201062848
H	2.667899543	-0.776033667	2.753082230
C	5.227732760	5.283520189	3.429302026
C	-3.134201493	0.237908306	6.793215484
C	-2.463613643	4.458267762	3.304811317
H	-0.601051435	4.014973182	2.353575576
C	-3.550721713	1.343859138	-0.156932482
H	-3.499439063	0.440658659	1.782239365
H	0.989645262	0.887366921	-1.279928777
H	-0.434837118	1.968345725	-0.998877277
H	0.040514889	1.485413006	-2.609697960
H	5.247872601	5.775937435	4.406769677
H	5.095023509	6.069974417	2.673740656
H	6.216152304	4.841389187	3.259950721
H	-4.134078548	0.467803041	6.412364501
H	-3.004412820	0.782261394	7.736334925
H	-3.111727811	-0.831946804	7.035581844
H	3.858887658	-2.790857964	1.981821890
H	4.736217981	-1.866765023	0.762547398
H	2.972981145	-2.055027799	0.638180428
H	4.765099100	-1.289902666	3.896731626
H	4.600109175	0.468835266	3.789481747
H	5.718448469	-0.388168592	2.717429196
H	4.951328115	0.714459832	-2.218493268
H	3.224628902	0.597572510	-1.848543552
H	4.330578524	-0.664441564	-1.304546220
H	6.627110301	1.380224015	-0.466646126
H	6.178707062	-0.076216879	0.420558060
H	6.184116376	1.485644048	1.242251536
H	-5.584710678	1.749433707	1.670484959
H	-4.695404611	3.262436901	1.504428453
H	-4.623065180	2.359912578	3.021355909
H	-4.517705840	0.914243810	-0.446316272
H	-2.758544133	0.699675585	-0.548935961
H	-3.471435961	2.325156890	-0.640534038
H	-2.158443183	5.497318585	3.483135059
H	-2.285190769	3.895898731	4.224890417
H	-3.540019198	4.464651387	3.112558624
H	-1.751027154	5.717571597	0.956770153
H	-3.011852841	4.560912869	0.525301646
H	-1.346926035	4.294392258	-0.011104151
C	1.331709820	3.022696690	-1.773994189
H	1.660420691	3.380818942	-0.789406405
H	2.237034606	2.768332851	-2.337367513
C	0.628816147	4.171848325	-2.494057558
H	-0.287170045	4.461708333	-1.949267777
H	1.283065567	5.059792223	-2.522807496
O	0.308165864	3.749288677	-3.805017194
C	-0.409489589	4.711219334	-4.559095121
H	0.176879977	5.642718050	-4.648729471
H	-1.352374861	4.972499175	-4.046947957
C	-0.697431518	4.129806828	-5.938404726
H	-1.256491298	3.195272481	-5.810229077
H	0.256529577	3.862253489	-6.407965467
C	-1.477875711	5.097216624	-6.833268274
H	-0.924969191	6.029876189	-6.994060754
H	-1.670909609	4.654578720	-7.815185935
H	-2.446773604	5.358325406	-6.392313133

A-PrOPr-TS

Ti	0.035848722	-0.099662733	-0.084849664
P	2.607936596	-0.520507962	0.505276736
C	2.470638111	0.081782522	2.236903814
C	3.483300630	0.685312932	2.987676505
C	3.292361291	1.089514410	4.316353115
C	2.035944235	0.844993564	4.882737580
C	0.999563644	0.267061532	4.154740956
C	1.174106004	-0.104127635	2.803610354
N	0.145882517	-0.566480932	1.984241567
C	-0.984223330	-1.183856783	2.542245988
C	-0.907180650	-2.230606285	3.482435172
C	-2.051160021	-2.889838292	3.914698166
C	-3.324675036	-2.548849770	3.431411501
C	-3.408307817	-1.495963962	2.516721741
C	-2.272013875	-0.798344665	2.085440872
P	-2.259951061	0.630680156	0.932605730
C	4.149263842	0.303206939	-0.217061626
C	2.879654375	-2.382418885	0.708497095
C	-2.120730011	2.114702578	2.109257925
C	-3.918224452	0.641948306	0.036365391
C	-0.449800514	-1.265865347	-1.316420171
C	-0.879125949	-2.270411414	-2.357972435
C	-2.305560607	-1.955365581	-2.867416738
C	-0.879964748	-3.681753608	-1.722698803
C	0.087499771	-2.259174173	-3.566320277
C	0.357576608	1.560967205	-1.633691579
H	4.458369949	0.849916778	2.538242881
H	1.854247793	1.130110832	5.917641004

H	0.031896318	0.119063660	4.623698694
H	0.068626368	-2.533520195	3.851269859
H	-1.954625548	-3.701967750	4.632960516
H	-4.387978641	-1.215312331	2.141040776
C	5.518568405	-0.249669955	0.217650018
C	3.179321754	-3.054779346	-0.639067622
C	-2.143453326	3.452218563	1.351792007
C	-5.147079577	1.156425190	0.804707599
H	-3.023124914	-1.961284397	-2.040452650
H	-2.630967900	-2.699259949	-3.606802357
H	-2.343616954	-0.969548840	-3.343763657
H	0.120301423	-3.950064073	-1.368100917
H	-1.199805373	-4.439480068	-2.450668479
H	-1.559586969	-3.718398426	-0.865442324
H	0.095692197	-1.278063170	-4.053673221
H	-0.212424819	-3.004912570	-4.314390242
H	1.111463777	-2.486947701	-3.253721566
C	4.066899100	0.357495253	-1.754521554
H	4.058788631	1.331537720	0.159944463
C	3.859934394	-2.820078201	1.806224172
H	1.871253165	-2.687671536	1.014611186
C	4.392733878	1.777818983	5.091085248
C	-4.555365806	-3.299497114	3.884738209
C	-3.061543669	2.134561916	3.323748077
H	-1.101425854	1.962715761	2.489041006
C	-3.775924951	1.376489941	-1.309789531
H	-4.061878912	-0.424219752	-0.183040354
H	-0.019331030	0.230486969	-1.800877784
H	-0.430067010	2.183878565	-1.182104865
H	1.308062033	1.846839596	-1.156730245
H	4.255892989	1.657103459	6.170584084
H	4.421734048	2.857195311	4.888234864
H	5.379899608	1.377618813	4.834163683
H	-5.471467571	-2.808752395	3.542102306
H	-4.604421473	-3.370485533	4.977723067
H	-4.567252868	-4.325884825	3.496715100
H	3.126115999	-4.144662381	-0.531684640
H	4.185082787	-2.814047025	-1.000984282
H	2.455469702	-2.756195454	-1.402007259
H	3.765687494	-3.901130926	1.967740232
H	3.655697175	-2.320468324	2.756777779
H	4.900552310	-2.621636943	1.534253612
H	4.906312553	0.940211330	-2.153368946
H	3.140331879	0.819852224	-2.101914203
H	4.122540862	-0.643226781	-2.194612416
H	6.313732981	0.414778083	-0.142715139
H	5.701699876	-1.237315596	-0.216379963
H	5.624542400	-0.338632635	1.300710023
H	-6.053660206	0.965127092	0.217491466
H	-5.090826417	2.237613811	0.966744800
H	-5.275761800	0.680302092	1.779456900
H	-4.698840525	1.274329217	-1.893294464
H	-2.953265550	0.967194585	-1.900877693
H	-3.596066058	2.448061278	-1.166641582
H	-2.719160469	2.892016795	4.039970517
H	-3.077795310	1.170864019	3.839570906
H	-4.087709089	2.389882538	3.045763664
H	-1.881143558	4.272086214	2.031055486
H	-3.136604580	3.673369681	0.945924880
H	-1.429519944	3.470519711	0.521715480
C	0.447870579	1.866587386	-3.136093617
H	1.213955261	1.236887710	-3.606025460
H	-0.500265214	1.622468172	-3.631930794
C	0.785034389	3.328147300	-3.416740446
H	0.007958219	3.987453795	-2.988870872
H	1.738201570	3.597469986	-2.926018056
O	0.880699213	3.518339400	-4.815583816
C	1.209847182	4.844398453	-5.184018968
H	0.442022488	5.548925341	-4.815883422
H	2.167343705	5.145385498	-4.721195251
C	1.312481041	4.919158817	-6.703023421
H	0.353034808	4.606395920	-7.132189228
H	2.057548585	4.186305697	-7.035179987
C	1.686002718	6.319771878	-7.198222082
H	1.752747877	6.347005600	-8.290341835
H	0.941326913	7.064734237	-6.894082974
H	2.655817515	6.640272543	-6.799776194

B(^{n}Pr)

Ti	0.402921813	-0.199251704	-0.186702539
P	2.825906189	-0.913216777	0.692357936
C	2.610790467	-0.165080155	2.359333723
C	3.618459918	0.318406921	3.197512203
C	3.345404664	0.850927378	4.467086765
C	2.008506956	0.875846523	4.876061126
C	0.979872821	0.420756168	4.053149616
C	1.250994087	-0.094129516	2.771973885
N	0.251555875	-0.475401785	1.861912260
C	-0.982614659	-0.951080739	2.346436171
C	-1.081362696	-1.910411660	3.374311266
C	-2.314585765	-2.418376138	3.761933882
C	-3.506932063	-2.011841244	3.140713456

C	-3.412428514	-1.053907816	2.128018438
C	-2.182956154	-0.503733939	1.737448965
P	-1.935604127	0.792766493	0.459626657
C	4.512047080	-0.334269651	0.061496986
C	2.862911267	-2.772711349	1.055333647
C	-1.853278889	2.394479620	1.473788326
C	-3.472489099	0.781188863	-0.634006313
C	-0.146484275	-1.521544533	-1.367432527
C	-0.789174031	-2.809111331	-1.847765762
C	-2.133892549	-2.509083121	-2.554388950
C	-1.057315369	-3.741035426	-0.646928057
C	0.127796401	-3.533333705	-2.862010079
C	1.173082197	1.519646333	-1.212890764
H	4.652651628	0.284228720	2.867577911
H	1.758458393	1.276460920	5.856617119
H	-0.048072776	0.478571745	4.396798640
H	-0.173160475	-2.259992730	3.856290306
H	-2.354353827	-3.161682494	4.556074074
H	-4.326399370	-0.725872130	1.642016717
C	5.765390454	-1.005635218	0.651325847
C	3.243435650	-3.578880545	-0.195503046
C	-1.794869166	3.637283025	0.570332356
C	-4.743664426	1.461410233	-0.098050529
H	-2.842408316	-2.043939474	-1.862336215
H	-2.589682680	-3.432807020	-2.934933321
H	-1.992160115	-1.829718773	-3.402532586
H	-0.121408192	-4.008301860	-0.144749969
H	-1.545900398	-4.669853669	-0.968720029
H	-1.704186781	-3.253358576	0.089800202
H	0.329678431	-2.897937252	-3.732189355
H	-0.341221318	-4.458200186	-3.222381822
H	1.087462492	-3.798578499	-2.409601536
C	4.555262464	-0.388113745	-1.477590062
H	4.519279834	0.722562271	0.359043683
C	3.652668433	-3.225046515	2.292055506
H	1.798348156	-2.951615038	1.252905593
C	4.457492494	1.376112663	5.345541111
C	-4.838185182	-2.591872035	3.559619935
C	-2.885417808	2.557887825	2.599707105
H	-0.868841951	2.278599223	1.946326907
C	-3.118330903	1.315900185	-2.033930045
H	-3.671073312	-0.293691245	-0.730740253
H	0.212181229	-0.866976143	-2.207566999
H	1.875510598	1.275187988	-2.022018087
H	0.280077755	1.933265592	-1.714703318
C	1.777646458	2.560280192	-0.259861327
H	-5.668198433	-2.104906540	3.038883371
H	-5.007104588	-2.474376466	4.636859271
H	-4.896380143	-3.665741531	3.342398201
H	4.089170230	1.624918009	6.345524078
H	4.909710371	2.284017268	4.926753744
H	5.263367315	0.641519427	5.462816795
H	5.487044787	0.062817715	-1.840403659
H	3.718904322	0.151855535	-1.926184828
H	4.524151552	-1.419452868	-1.843989849
H	6.659912047	-0.471178861	0.308414393
H	5.859999754	-2.041611852	0.312851398
H	5.781320056	-1.010752460	1.743134310
H	3.024014453	-4.641445141	-0.037089925
H	4.311958294	-3.499356530	-0.421282610
H	2.681265646	-3.246436076	-1.071782868
H	3.432428519	-4.279948580	2.498586656
H	3.386091676	-2.647162980	3.180582790
H	4.733090141	-3.141593851	2.144303033
H	-2.600816254	3.406231287	3.234610179
H	-2.940636801	1.669575704	3.234219369
H	-3.887541320	2.762485102	2.213097531
H	-1.531881629	4.519059784	1.166131995
H	-2.762163521	3.840331194	0.098811927
H	-1.046558884	3.538247958	-0.220883782
H	-3.973536289	1.193611975	-2.709641084
H	-2.267029552	0.779227552	-2.460106138
H	-2.870550687	2.382728863	-2.006451572
H	-5.581979952	1.251520542	-0.773610845
H	-4.629651623	2.548759791	-0.054725016
H	-5.028373268	1.117353499	0.898852047
H	1.130395765	2.723507491	0.613782158
H	2.731460248	2.204132713	0.148685879
C	2.032663376	3.931341325	-0.886362123
H	1.095123143	4.344349053	-1.300605434
H	2.743844975	3.843391453	-1.726985249
O	2.550062956	4.793768417	0.115205301
C	2.806307154	6.111210116	-0.326963208
H	3.544927735	6.108987744	-1.149596521
H	1.884413878	6.571593276	-0.727969259
C	3.330293881	6.922715908	0.853601741
H	4.232162485	6.430594286	1.237933875
H	2.585786663	6.879882216	1.658091848
C	3.633636973	8.378646022	0.487873964
H	4.008177604	8.933272655	1.354438870
H	4.393349594	8.445157472	-0.299992618
H	2.737255477	8.896879308	0.126823166

B-TS(^{n}Pr)			
Ti	0.419053048	-0.042596897	-0.191384476
P	2.726996923	-0.790362237	0.672911322
C	2.477176300	-0.048932332	2.333435353
C	3.450912993	0.518319303	3.160536153
C	3.150731525	1.001770334	4.440697162
C	1.825536118	0.883451816	4.878233699
C	0.829068872	0.351116770	4.065498687
C	1.121478400	-0.101515938	2.762052292
N	0.146672521	-0.527630404	1.852195972
C	-1.033074542	-1.119848629	2.328864653
C	-1.040862276	-2.153126691	3.286047811
C	-2.227019300	-2.785540814	3.641629636
C	-3.454282277	-2.428712208	3.063271142
C	-3.451730697	-1.381601965	2.135420813
C	-2.273290382	-0.716517413	1.775099603
P	-2.102895224	0.696166062	0.617047116
C	4.376109465	-0.149185269	0.018685176
C	2.852946646	-2.642298665	1.057072611
C	-2.060949336	2.195771380	1.779412399
C	-3.684937976	0.701398318	-0.420593410
C	-0.086940645	-1.430524003	-1.404133613
C	-0.279256862	-2.239509981	-2.683049202
C	-0.303792586	-3.745046430	-2.325487826
C	0.864479533	-1.994530679	-3.688575420
C	-1.626281470	-1.883660953	-3.358707622
C	1.344189442	1.787115616	-0.725919320
H	4.477655274	0.584876301	2.813214964
H	1.560202522	1.233732294	5.874172657
H	-0.192864613	0.299358783	4.428726146
H	-0.101264776	-2.465253658	3.732920812
H	-2.197668586	-3.589753346	4.374459139
H	-4.396877755	-1.084399025	1.690379568
C	5.662003018	-0.721464433	0.641267794
C	3.230677012	-3.452738110	-0.191632263
C	-2.002164517	3.516923818	0.994934464
C	-4.963475310	1.252222288	0.234992004
H	0.625059728	-4.051175268	-1.833866788
H	-0.427548974	-4.358771182	-3.226635718
H	-1.132876010	-3.974132711	-1.645905294
H	0.902607984	-0.949747417	-4.007586597
H	0.730161478	-2.610676649	-4.586270459
H	1.833827963	-2.245974983	-3.246060743
H	-2.465210193	-2.052199319	-2.674209463
H	-1.792005696	-2.498047093	-4.253533485
H	-1.648159292	-0.832661529	-3.666812256
C	4.432054205	-0.278671087	-1.515907602
H	4.316516117	0.919684925	0.262866487
C	3.691439709	-3.047163576	2.278276001
H	1.801202867	-2.857533776	1.286466142
C	4.211690019	1.640475352	5.306835185
C	-4.727114695	-3.160346952	3.421317285
C	-3.105879641	2.245880107	2.904637156
H	-1.080131125	2.043621157	2.249499970
C	-3.447357315	1.389094488	-1.777460835
H	-3.829615472	-0.370115032	-0.613959125
H	-0.639985086	-1.911521350	-0.565661167
H	1.134731037	2.485959770	0.089634108
H	2.362730115	1.898270244	-1.093898542
C	0.290666555	1.597769234	-1.732692754
H	-5.612344526	-2.606929490	3.093139374
H	-4.812226194	-3.314553524	4.502905212
H	-4.768894557	-4.152052331	2.952514451
H	4.002095516	1.492022800	6.371369606
H	4.273953313	2.723800782	5.138847379
H	5.204034282	1.225541542	5.100807939
H	5.324433142	0.229291333	-1.901691853
H	3.556783471	0.164780034	-1.995739875
H	4.490047867	-1.326447627	-1.827758951
H	6.527581514	-0.149149963	0.285099419
H	5.818589460	-1.762341940	0.341897814
H	5.667759253	-0.686894771	1.732629851
H	3.065343214	-4.521567071	-0.010184455
H	4.287481996	-3.329121966	-0.452236059
H	2.627262283	-3.161719976	-1.056007145
H	3.514987319	-4.105450147	2.508708802
H	3.428310052	-2.463173531	3.163963119
H	4.763981725	-2.928357602	2.099813482
H	-2.816638612	3.008948751	3.638140860
H	-3.184286764	1.290488644	3.430675311
H	-4.099011616	2.512593314	2.533278145
H	-1.803279622	4.348867340	1.680894469
H	-2.950876322	3.733204982	0.491545455
H	-1.210673813	3.514892790	0.239494154
H	-4.335896386	1.281356480	-2.411508869
H	-2.598917445	0.953257304	-2.308748553
H	-3.258123662	2.461622189	-1.659183831
H	-5.824870706	1.048666230	-0.413329236
H	-4.906738324	2.337739943	0.363433599
H	-5.172049221	0.812584589	1.212723905
H	-0.297635330	0.091350861	-1.755573527

H	-0.621877048	2.174093127	-1.585578178
C	0.700009557	1.644855454	-3.188861423
H	-0.084577809	1.224517125	-3.843557522
H	1.616927600	1.054788330	-3.358865676
O	0.927069125	3.004598995	-3.542194871
C	1.258488012	3.192386302	-4.903658234
H	0.456712747	2.799743447	-5.556179482
H	2.179604692	2.637338617	-5.160238557
C	1.454926269	4.684747678	-5.149517042
H	0.534079446	5.205387360	-4.859781366
H	2.242122589	5.045161980	-4.476384704
C	1.810788049	5.005178191	-6.604384341
H	1.023155169	4.674814763	-7.291834804
H	1.944836369	6.081965348	-6.749332627
H	2.742136723	4.512573301	-6.907670474

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Ti	-2.171196947	-1.925515292	0.032920966
P	-0.585508410	-2.311119012	2.254050809
C	-2.009063729	-2.770289966	3.320615828
C	-2.145436667	-2.572951059	4.696477866
C	-3.274155135	-3.010786155	5.405495127
C	-4.266333135	-3.682492710	4.684600853
C	-4.170748912	-3.869110784	3.306852535
C	-3.058029915	-3.391072042	2.590305423
N	-2.963569520	-3.448069078	1.187862515
C	-3.610848156	-4.507261290	0.514363121
C	-3.388437454	-5.856257059	0.851518413
C	-3.975412885	-6.879840782	0.119190111
C	-4.796532448	-6.608842290	-0.987086055
C	-5.027426110	-5.270011516	-1.312563102
C	-4.468750821	-4.216778873	-0.572800595
P	-4.719532779	-2.417777763	-0.877712700
C	0.412013640	-1.034896209	3.230424208
C	0.398642522	-3.931413250	2.138663060
C	-6.007280052	-1.949228722	0.442545493
C	-5.495901918	-2.339088807	-2.607156872
C	-2.399511657	0.123080768	0.609752592
H	-1.356583287	-2.070701802	5.248096433
H	-5.145782607	-4.054976269	5.206271668
H	-4.969847588	-4.375825618	2.775069862
H	-2.741168734	-6.086863851	1.692868521
H	-3.781914737	-7.913142191	0.400364968
H	-5.670695968	-5.053197802	-2.159710872
C	1.240083404	-1.521868548	4.433624981
C	1.791518577	-3.719503683	1.521105899
C	-6.492675929	-0.500455431	0.275726230
C	-6.994627734	-2.663274626	-2.730372009
C	1.300843909	-0.214996716	2.275735492
H	-0.377893281	-0.368923743	3.604238396
C	0.476572064	-4.782151935	3.415260099
H	-0.208457518	-4.481559012	1.408044915
C	-3.407871255	-2.753331768	6.888441638
C	-5.402702912	-7.731635967	-1.796582379
C	-7.180334801	-2.916159648	0.667366497
H	-5.381253513	-1.985875854	1.343467291
C	-5.178480424	-0.999175439	-3.292168783
H	-4.936063019	-3.115536132	-3.143131812
H	-3.435235728	0.027211388	0.995370014
H	-1.777254593	0.231289515	1.511458411
C	-2.281260934	1.443269481	-0.196343184
C	-2.729124313	2.630095524	0.689841605
C	-0.819482955	1.681906168	-0.623774875
C	-3.160632295	1.423462304	-1.458666156
H	-0.724707187	2.615176615	-1.192771743
H	-0.160060112	1.762118607	0.247738004
H	-0.448593364	0.866959886	-1.254169336
H	-3.098508263	2.378799689	-1.994706572
H	-2.846939946	0.633525709	-2.146863081
H	-4.213927018	1.253680018	-1.210033558
H	-2.636203413	3.586327415	0.157798948
H	-3.775833403	2.518780554	0.996957300
H	-2.121393774	2.692374479	1.600102937
H	-6.139946817	-7.356067582	-2.512439264
H	-5.904113778	-8.464886688	-1.154341025
H	-4.637791321	-8.274789600	-2.365649458
H	-4.150442091	-3.416687562	7.342363050
H	-3.723626285	-1.721923270	7.093232407
H	-2.458175065	-2.907502706	7.412908441
H	1.746831460	0.632033312	2.811360274
H	0.734482127	0.178761482	1.429445181
H	2.121973072	-0.818781573	1.876155456
H	1.622746108	-0.656252419	4.988765679
H	2.107436559	-2.104388673	4.108842167
H	0.671626130	-2.138367603	5.132755739
H	2.230368827	-4.689442664	1.258246618
H	2.476590504	-3.236916128	2.225636059
H	1.757098150	-3.114020812	0.612155284
H	0.912596741	-5.760592021	3.176929686
H	-0.509318409	-4.951735424	3.855113296
H	1.110926361	-4.320463112	4.177410055
H	-7.682486943	-2.665530650	1.610160768

H	-6.848014943	-3.955649370	0.732626707
H	-7.928898513	-2.848902162	-0.126016712
H	-7.095209865	-0.207382268	1.143657084
H	-7.122862472	-0.380027723	-0.611805475
H	-5.660793820	0.204881304	0.197864398
H	-5.546308559	-1.012032197	-4.325423207
H	-4.103945647	-0.805803157	-3.318601099
H	-5.659151836	-0.157710206	-2.782377959
H	-7.267705893	-2.723945704	-3.791223993
H	-7.612584346	-1.878325959	-2.284066950
H	-7.269190145	-3.610960540	-2.262337289
C	-0.390747002	-2.248415360	-1.060418758
H	0.111592377	-3.203412421	-0.905590830
H	0.283190170	-1.394449736	-0.983779416
C	-1.495443760	-2.224461112	-1.985952083
H	-1.661564634	-1.292407097	-2.534389999
C	-1.784199831	-3.456520414	-2.799153008
H	-1.798646311	-4.356043087	-2.158281671
H	-2.769751276	-3.396919854	-3.290962226
O	-0.775723717	-3.615654267	-3.802574685
C	-0.929672495	-4.785571403	-4.577243893
H	-0.934484895	-5.683106744	-3.930171959
H	-1.897579612	-4.778203566	-5.114150601
C	0.223256755	-4.863740840	-5.573186772
H	0.210457631	-3.956965033	-6.190133227
H	1.164645915	-4.843764784	-5.010714058
C	0.160611705	-6.111073096	-6.459604206
H	1.000498727	-6.140002856	-7.161480981
H	0.198321910	-7.029948009	-5.862249385
H	-0.763307475	-6.139095856	-7.049613143

A-O^{n}Pr$_2$

Ti	0.378866567	0.182969148	0.045006695
P	2.984143536	-0.009709370	-0.678300511
C	3.642311883	0.040548560	1.038624594
C	4.919473838	0.481474844	1.409330351
C	5.359033454	0.482898268	2.737126627
C	4.462748488	0.011712804	3.708541842
C	3.183989794	-0.414357170	3.374219918
C	2.723891772	-0.400382415	2.034571668
N	1.419962548	-0.731592375	1.672169501
C	0.702548034	-1.659306026	2.440731346
C	1.265426986	-2.858620243	2.924269763
C	0.490755665	-3.803787563	3.585420878
C	-0.882350857	-3.609559292	3.797416012
C	-1.441671602	-2.413126852	3.338758014
C	-0.677351660	-1.435165492	2.688329041
P	-1.311521644	0.176294298	2.071226597
C	4.053567333	1.225478534	-1.643704091
C	3.341731082	-1.772807072	-1.260763359
C	-0.923385988	1.351040145	3.522107077
C	-3.186026304	-0.010800477	1.907587142
C	-0.486313998	-1.027324311	-0.879564550
C	-1.138918453	-2.234994055	-1.523800085
C	-2.539966543	-2.483944190	-0.915998692
C	-0.286421897	-3.506672257	-1.292543062
C	-1.302869500	-2.011750598	-3.047396649
H	5.607257617	0.830904769	0.644599392
H	4.768646462	-0.007875582	4.753436860
H	2.510553873	-0.751263170	4.155967520
H	2.320235493	-3.050602201	2.750789925
H	0.959610455	-4.723482539	3.931631519
H	-2.502482593	-2.246673888	3.501504185
C	5.441143696	0.763103110	-2.121194860
C	2.992368521	-1.939256000	-2.747360753
C	-1.495901067	2.758987867	3.288124213
C	-4.043971043	0.062042834	3.182120574
H	-2.458110951	-2.705519957	0.152941251
H	-3.035266494	-3.336864354	-1.401346623
H	-3.183328365	-1.605570754	-1.039197769
H	0.700249266	-3.404682515	-1.754667502
H	-0.769016548	-4.394972570	-1.725089846
H	-0.140939005	-3.680634108	-0.221841306
H	-1.950623405	-1.149994027	-3.247149132
H	-1.749414362	-2.889812972	-3.535205531
H	-0.334293546	-1.817833026	-3.520539810
C	3.254627809	1.808588799	-2.822458544
H	4.202072348	2.030505891	-0.910987874
C	4.715107394	-2.363434182	-0.912700236
H	2.582650270	-2.313144280	-0.682126699
C	6.734919774	0.981544723	3.113911465
C	-1.721627853	-4.660540998	4.487031262
C	-1.224959813	0.852292638	4.943632106
H	0.169949404	1.412833032	3.429895414
C	-3.714271461	0.972894533	0.848029624
H	-3.274276412	-1.018927355	1.487091578
H	7.230020834	0.305669331	3.820951709
H	6.694088326	1.969072827	3.592404295
H	7.381405809	1.072346382	2.235083637
H	-2.710314317	-4.272393237	4.751510954
H	-1.245924035	-5.015217937	5.409102619
H	-1.874709432	-5.539612066	3.847669295

H	3.000998782	-3.001812137	-3.017925846
H	3.715895397	-1.434403181	-3.397225299
H	1.995153943	-1.545685604	-2.964359120
H	4.703397617	-3.444830740	-1.098224723
H	4.968884951	-2.207813538	0.139255811
H	5.517208696	-1.938559200	-1.522930850
H	3.827449625	2.604785974	-3.314643004
H	2.300237975	2.226289168	-2.494310254
H	3.038259493	1.043743033	-3.575979687
H	5.988382252	1.616952626	-2.540448086
H	5.360266900	0.011650974	-2.912192067
H	6.051243952	0.338078291	-1.321679552
H	-5.080791954	-0.203093938	2.939638105
H	-4.061279780	1.073293581	3.600833656
H	-3.705746277	-0.616346569	3.968345314
H	-4.779000957	0.788372417	0.657425095
H	-3.172833852	0.857938986	-0.094151828
H	-3.616509923	2.014054034	1.178090477
H	-0.747153130	1.514913038	5.676939153
H	-0.841198444	-0.157932300	5.105890320
H	-2.296645492	0.847465009	5.160371748
H	-1.074786119	3.466990693	4.012634479
H	-2.583833464	2.779293773	3.412103513
H	-1.271522738	3.136950137	2.285170150
C	0.225261974	3.409014515	-0.366117359
H	0.558889190	4.055605207	-1.187957965
H	-0.671443429	3.865789875	0.077873751
C	-1.145127367	2.194311069	-1.949378064
H	-1.889737907	2.948951590	-1.656370866
H	-1.602529330	1.204454188	-1.943964670
C	-0.548824503	2.502653819	-3.318145874
H	-0.001296442	3.453872068	-3.298514613
H	0.173658630	1.715970970	-3.560401608
C	1.327978461	3.268800888	0.673845521
H	2.217527132	2.836612728	0.204526427
H	1.007551837	2.568663120	1.455577409
O	-0.141156317	2.119864810	-0.898241434
C	-1.640717023	2.560281480	-4.393446880
H	-1.208689908	2.762555985	-5.378084288
H	-2.181866077	1.609745354	-4.457127632
H	-2.372868064	3.348661200	-4.182950068
C	1.680781455	4.617375691	1.313685926
H	0.818390649	5.053945252	1.829990215
H	2.481840591	4.495856090	2.048361792
H	2.023002893	5.339665703	0.563586261

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H	0.029213959	0.079866469	-0.295658472
C	-0.089167588	0.019230433	1.403966463
Ti	1.288292737	1.156856537	1.567331815
O	1.827210549	1.673866291	-0.266971209
C	2.832283872	2.605327446	-0.653882915
C	3.692040491	3.098428403	0.511164628
H	3.049876427	3.536550856	1.283035438
H	4.202563331	2.249920997	0.978275168
H	3.486437587	2.137656907	-1.407497388
H	2.353247675	3.468808579	-1.143855447
C	0.923188977	1.184536042	-1.868590504
C	0.045380177	0.102922592	-1.544699156
H	0.514340821	2.174588958	-2.048425409
H	-1.004131435	0.331738635	-1.756229698
H	1.846381003	0.978256030	-2.404826352
P	3.406329226	-0.378008492	2.196272204
C	4.851050896	-0.744066787	1.025424021
H	5.362209241	0.226773145	0.975966315
C	4.312191656	-1.063193902	-0.381118922
H	3.788769086	-2.025189068	-0.396401588
H	5.139726417	-1.126536827	-1.098814093
H	3.610851678	-0.298883557	-0.724150601
C	5.885598892	-1.800785216	1.449361636
H	5.452043126	-2.805243746	1.452133983
H	6.715286045	-1.808709268	0.731399142
H	6.307900403	-1.619191802	2.439784697
C	2.932941379	-1.933191724	3.160960647
C	2.461149206	-3.046718951	2.213705520
H	1.982074432	-3.849465845	2.786781767
H	3.297106766	-3.494859484	1.665294754
H	1.734759045	-2.668713925	1.48871022
H	2.051691104	-1.558380698	3.696444515
H	4.280205683	-1.641440132	4.864229600
C	3.934523084	-2.443557317	4.206928961
H	3.451015275	-3.204166245	4.832798177
H	4.811031915	-2.910301521	3.748914276
C	-1.261568693	-0.856808304	1.824429951
C	-1.448027305	-2.078336487	0.893126277
C	-2.578898966	-0.043180280	1.814370950
C	-1.034209844	-1.379449868	3.264852723
H	-0.157582129	-2.033352102	3.307983732
H	-1.901596479	-1.959126843	3.610711237
H	-0.874936944	-0.551812574	3.961772793
H	-2.539825619	0.753745278	2.562989546
H	-2.756301225	0.409982206	0.832961574

H	-3.438883927	-0.685001276	2.051702561
H	-0.525335435	-2.662287284	0.816329473
H	-2.235829588	-2.740445948	1.276840011
H	-1.739484058	-1.767742112	-0.114769121
C	-1.829739522	3.532886996	0.028278970
H	-1.422739981	2.564401193	-0.272760320
H	-2.847832015	3.618686353	-0.371326593
H	-1.226442276	4.320010860	-0.438863803
C	-2.542852809	4.973821173	1.982750836
H	-2.581718961	5.110246907	3.065885176
H	-2.048638505	5.851274768	1.554498125
H	-3.575428318	4.973371413	1.612066035
C	-1.849114422	3.667654964	1.562081523
H	-2.431873883	2.827072847	1.954246713
C	0.817955965	4.934843838	2.490255594
H	1.799580452	4.548458359	2.796807946
H	1.365211923	5.050616657	0.362407000
H	1.727517675	6.509178770	1.296498840
H	0.064735245	6.152114964	0.830076538
C	1.001804723	5.696954204	1.167233045
H	1.083807593	6.646178504	3.792211775
H	-0.603288679	6.367448264	3.357817679
H	0.184619775	5.324237341	4.551022284
C	0.333599205	5.865195982	3.613220088
N	1.801068643	1.598310753	3.585812239
C	4.083922422	0.746300565	3.481830800
P	-0.126154854	3.300525380	2.243534978
C	3.112018177	1.602295755	4.070301468
C	3.555535012	2.479005416	5.087804331
C	4.887192992	2.519505250	5.478885863
C	5.422955682	0.819972123	3.888356176
C	5.857235503	1.700485759	4.883703365
C	7.309285852	1.780646016	5.295282901
H	7.418950982	1.790354112	6.385969059
H	7.790177667	2.693298418	4.918975280
H	7.881128192	0.929458840	4.912656220
H	6.158565567	0.170626110	3.422741671
H	5.184268214	3.217064420	6.260484325
H	2.838954576	3.143976895	5.559711889
C	-0.339383107	2.704387216	3.966516400
C	0.749216421	1.933617005	4.453601677
C	-1.453216755	2.943426062	4.782519784
C	-1.525733943	2.472603732	6.096406320
C	-0.429278997	1.744769174	6.581875702
C	0.677239474	1.476012709	5.786367647
H	1.498136312	0.887268299	6.185045417
H	-0.450365753	1.365585000	7.602078954
H	-2.290052860	3.515971943	4.392962882
C	-2.741279455	2.720786020	6.959265015
H	-3.353715520	1.815894208	7.064379069
H	-2.459519292	3.035169758	7.970737850
H	-3.381015528	3.500499228	6.534374188
C	4.728838781	4.135752067	0.061453711
H	5.338615107	4.467365192	0.907536791
H	5.406619285	3.723219197	-0.695070957
H	4.248694720	5.021688427	-0.370222633
C	0.477873352	-1.278470441	-2.043801190
H	0.420467585	-1.358282432	-3.136539505
H	1.512729747	-1.485050322	-1.748303351
H	-0.143548674	-2.071427790	-1.620230531

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H	0.003608465	0.093316509	0.223472743
C	-0.046904609	-0.004333666	1.418425827
Ti	1.307509158	1.146351820	1.590140593
O	1.830058575	1.686348837	-0.285739069
C	2.836394743	2.627393715	-0.662709561
C	3.707044042	3.081708591	0.506813440
H	3.075877152	3.513311823	1.291072927
H	4.208065162	2.216162700	0.951645491
H	3.476493358	2.174401877	-1.436235191
H	2.352726551	3.502683620	-1.124968040
P	3.409691748	-0.380856947	2.207880061
C	4.837118964	-0.743234220	1.014852724
H	5.346555618	0.227943485	0.954957453
C	4.273653073	-1.066398134	-0.382187941
H	3.749117381	-2.027785719	-0.386287761
H	5.089021518	-1.132600914	-1.113492921
H	3.566542299	-0.303610819	-0.716873332
C	5.880713960	-1.797399181	1.422516320
H	5.449410735	-2.802687171	1.433618855
H	6.698216158	-1.804752846	0.690670517
H	6.318916272	-1.613138162	2.405582618
C	2.940960059	-1.946425179	3.156029699
C	2.477625145	-3.053334789	2.196901134
H	1.984229909	-3.855365812	2.758668074
H	3.319273865	-3.504607478	1.660097786
H	1.765352635	-2.668192825	1.462203666
H	2.056444171	-1.581701698	3.692591731
H	4.281726320	-1.664485554	4.865568824
C	3.944186267	-2.461203025	4.197680722
H	3.465619146	-3.233927379	4.812371008

H	4.825498294	-2.914559875	3.735078166
C	-1.212995826	-0.897028514	1.828544478
C	-1.329207030	-2.166297438	0.949609063
C	-2.548633939	-0.120233733	1.719006799
C	-1.041870859	-1.346009110	3.300585725
H	-0.151624795	-1.972421479	3.415403350
H	-1.909296176	-1.933608107	3.633511799
H	-0.936274295	-0.483484327	3.964309856
H	-2.562378324	0.714695360	2.425881777
H	-2.695601623	0.278335577	0.709187274
H	-3.402224355	-0.772010704	1.952276415
H	-0.395959018	-2.737880208	0.947948752
H	-2.125028246	-2.824467516	1.323952124
H	-1.569068465	-1.911390723	-0.086085403
C	-1.849191070	3.492820187	0.017329358
H	-1.443735285	2.522948891	-0.279238960
H	-2.870670847	3.572878082	-0.374793653
H	-1.251939967	4.277448843	-0.461823120
C	-2.554037951	4.950291164	1.959290085
H	-2.583753048	5.102626747	3.040454579
H	-2.068031372	5.823656826	1.513464381
H	-3.589864764	4.939665535	1.597736911
C	-1.857509634	3.641703464	1.549733399
H	-2.435455822	2.803097917	1.953942373
C	0.803931741	4.934994780	2.447457571
H	1.789401846	4.560279968	2.756042663
H	1.340989802	5.021875588	0.315619215
H	1.698857483	6.496711269	1.225198642
H	0.036302586	6.122224065	0.771634796
C	0.977541568	5.678157573	1.112130219
H	1.068284043	6.664361754	3.725369984
H	-0.618437806	6.377663154	3.295367266
H	0.170989693	5.351666053	4.502633742
C	0.318984367	5.880084487	3.557570084
N	1.809837362	1.601785252	3.603198550
C	4.088520092	0.738391273	3.499484322
P	-0.128203261	3.289660902	2.227715647
C	3.119799763	1.600006289	4.088449404
C	3.567134533	2.473926423	5.107503032
C	4.898579223	2.509149804	5.502033297
C	5.426795454	0.806953756	3.908403325
C	5.864465849	1.685021252	4.905239921
C	7.317801179	1.756477498	5.313549693
H	7.430479694	1.767664276	6.403878167
H	7.804223783	2.664630169	4.933335182
H	7.882285832	0.900109757	4.931210937
H	6.160078051	0.154057359	3.443351049
H	5.198258928	3.204784118	6.283997911
H	2.852362031	3.141983027	5.577636262
C	-0.335668434	2.710587852	3.957489770
C	0.753157021	1.948623519	4.460047645
C	-1.457543612	2.950051054	4.762355291
C	-1.540234303	2.489598350	6.079053656
C	-0.443650401	1.772223521	6.580230414
C	0.671372036	1.503605789	5.796520164
H	1.489935304	0.919657485	6.206516151
H	-0.472142303	1.399951686	7.602837185
H	-2.294612532	3.513327844	4.360110706
C	-2.767382466	2.735475998	6.925840211
H	-3.376328499	1.827726139	7.027161021
H	-2.500148016	3.056279534	7.939230830
H	-3.405731831	3.509668240	6.488738468
C	4.755709492	4.112832415	0.069625398
H	5.377073704	4.417167154	0.917340951
H	5.421250817	3.705608903	-0.700674081
H	4.285973317	5.014571908	-0.339985177

A-PrOPrβ

Ti	0.487109293	0.681656034	0.965481441
P	3.162775450	0.746136827	1.100235785
C	3.167652142	2.269295275	2.134266617
C	4.172133786	3.243546706	2.140258747
C	4.110470492	4.384151379	2.950644822
C	2.993901336	4.511210379	3.786359371
C	1.966814845	3.573763091	3.789089451
C	2.003046649	2.439709323	2.945099140
N	0.949989107	1.536518117	2.818678206
C	-0.021235532	1.429101961	3.831458396
C	0.298883028	1.189119024	5.180480889
C	-0.698450959	0.982834307	6.128921047
C	-2.057313883	1.001693375	5.776945233
C	-2.378635891	1.263764017	4.440431595
C	-1.392877495	1.495785131	3.471858025
P	-1.699996731	1.876310526	1.696148404
C	4.494248853	1.013103431	-0.218492407
C	3.678655800	-0.624838949	2.297302005
C	-1.624127062	3.775293882	1.652828609
C	-3.444079353	1.280205435	1.291561563
C	-0.114737620	-0.949873322	1.140355525
C	-0.593910235	-2.332159144	1.522598841
C	-2.124513091	-2.331169673	1.749092390

C	0.095003559	-2.798171301	2.827835456
C	-0.264304191	-3.333719596	0.389593814
C	0.305546200	1.101815222	-1.780906311
H	5.040802267	3.120362016	1.500027222
H	2.915167304	5.376811639	4.442128404
H	1.106060020	3.724148157	4.432537959
H	1.345073164	1.144283529	5.469662058
H	-0.417208958	0.787443136	7.161783473
H	-3.427410474	1.290471284	4.158188025
C	5.961822179	0.853779733	0.218182441
C	3.866001157	-1.960141210	1.561812181
C	-1.920108152	4.326451525	0.247832244
C	-4.627561375	2.161109389	1.724212079
H	-2.390671047	-1.658028880	2.570882503
H	-2.486718982	-3.337128233	2.003392899
H	-2.651679677	-2.000253816	0.847631353
H	1.181378912	-2.842963019	2.699085362
H	-0.251909560	-3.797976334	3.124738860
H	-0.118855709	-2.102869547	3.645925495
H	-0.755322593	-3.036803559	-0.543573798
H	-0.599523000	-4.348542591	0.645503121
H	0.814338124	-3.368687603	0.202590147
C	4.216336345	0.143089171	-1.458947443
H	4.333539861	2.061681198	-0.504135623
C	4.840429538	-0.311838884	3.250486860
H	2.761871899	-0.702524714	2.894246272
C	5.190294759	5.440969048	2.908162576
C	-3.133568036	0.738308822	6.804402026
C	-2.402244556	4.537889260	2.735958377
H	-0.554631580	3.928430218	1.853541043
C	-3.535827957	0.946028010	-0.209038033
H	-3.492972158	0.332600106	1.841117746
H	1.054577223	0.448728867	-1.299270202
H	-0.507210329	1.317327751	-1.065326533
H	5.326187766	5.914431100	3.886521989
H	4.951073468	6.242038094	2.195063999
H	6.154943708	5.019278184	2.606147887
H	-4.121816883	1.020987822	6.428684184
H	-2.954659903	1.299705851	7.728502467
H	-3.178002666	-0.323752755	7.077438394
H	3.958336666	-2.775666816	2.288760579
H	4.775722751	-1.967432554	0.950838100
H	3.010443159	-2.181662757	0.916999163
H	4.883747728	-1.078879239	4.033633314
H	4.713880382	0.657991754	3.739153102
H	5.807906799	-0.312995047	2.740648901
H	4.940252514	0.375120465	-2.249643433
H	3.214869654	0.310852847	-1.863134863
H	4.306332240	-0.923835555	-1.231869613
H	6.624142130	1.191592692	-0.588610570
H	6.203496264	-0.194535477	0.417336916
H	6.208250815	1.427217870	1.114069559
H	-5.567528089	1.626496826	1.539440603
H	-4.667973726	3.090876864	1.148058678
H	-4.600762501	2.426758534	2.783683656
H	-4.507664056	0.489763124	-0.434458686
H	-2.751982239	0.242177236	-0.502014564
H	-3.443357806	1.844207346	-0.830605300
H	-2.085663229	5.588686443	2.744500599
H	-2.220012423	4.126338767	3.732194270
H	-3.480350042	4.525483846	2.554128459
H	-1.686275005	5.397970231	0.212918882
H	-2.979402071	4.221744890	-0.011843541
H	-1.334657370	3.835127344	-0.535812348
C	0.967372909	2.420686538	-2.176916749
H	1.444358453	2.898625377	-1.302938117
H	1.761790327	2.235688141	-2.921730921
C	-0.690059879	5.307432610	-3.779232977
H	-1.437658254	5.450848915	-2.989912738
H	-1.170744774	4.708578731	-4.562129884
C	-0.299749795	0.340951618	-2.965880351
H	-1.052796787	0.953213468	-3.468818635
H	0.473866804	0.085715903	-3.699862744
H	-0.766533174	-0.586567996	-2.625114179
C	0.472289745	4.504807644	-3.206020469
H	1.236950916	4.325935081	-3.982277653
H	0.962106409	5.064144210	-2.390018040
C	-0.248385399	6.662423215	-4.341353842
H	0.480552516	6.543086054	-5.151383601
H	-1.101777972	7.216305616	-4.744815478
H	0.214401980	7.286829570	-3.568243652
O	-0.027962565	3.267674920	-2.719987009

A-PrOPr$_\beta$-TS

Ti	0.110547243	-0.203142593	-0.134395213
P	2.538473053	-1.028579200	0.616157267
C	2.509359872	-0.126758945	2.216679989
C	3.596842570	0.441944395	2.886588281
C	3.457858345	1.081216746	4.125672608
C	2.176672214	1.109996208	4.691003907
C	1.071455976	0.573905642	4.037733094

C	1.198447400	-0.028717039	2.767245347
N	0.118206018	-0.458240967	1.996403642
C	-1.061410382	-0.893319860	2.613332689
C	-1.081645907	-1.797360299	3.695156835
C	-2.280967397	-2.297626261	4.187274499
C	-3.516172516	-1.932572024	3.629740743
C	-3.503022411	-1.011046382	2.578792395
C	-2.309227066	-0.472481731	2.081827851
P	-2.159969190	0.797123137	0.766182243
C	4.229975812	-0.698157676	-0.156222915
C	2.406804787	-2.843571924	1.144697043
C	-1.900726864	2.395589657	1.762232821
C	-3.809148214	0.849601338	-0.146946437
C	-0.421310063	-1.396081078	-1.323391289
C	-0.874194543	-2.405596065	-2.351646139
C	-2.159142954	-1.918002812	-3.063951965
C	-1.187958600	-3.744347329	-1.641362946
C	0.222787660	-2.639933373	-3.417982692
C	0.571170817	1.366562462	-1.724469566
H	4.587557311	0.390442638	2.444104721
H	2.034272825	1.581699377	5.661771002
H	0.090103702	0.638643425	4.497729956
H	-0.139244596	-2.119768633	4.128964584
H	-2.258981866	-3.004240447	5.015003684
H	-4.452301515	-0.706837822	2.147447106
C	5.447112882	-1.396902236	0.476158975
C	2.627613130	-3.798591203	-0.036876983
C	-1.833559659	3.637448068	0.858404147
C	-4.990543184	1.547563061	0.548255652
H	-2.962533381	-1.747376368	-2.340294466
H	-2.508961890	-2.659227643	-3.794793034
H	-1.980890539	-0.978083737	-3.598321588
H	-0.300627354	-4.140918880	-1.138476946
H	-1.538325674	-4.495858116	-2.361004667
H	-1.965592608	-3.604632325	-0.883473721
H	0.453100885	-1.712300186	-3.954138301
H	-0.100744915	-3.384746856	-4.157099207
H	1.149696977	-2.998802872	-2.959462246
C	4.193803920	-0.967022548	-1.672927448
H	4.342431946	0.384827963	-0.011614951
C	3.224114257	-3.256302255	2.377458022
H	1.344540378	-2.887698865	1.413593527
C	4.636640468	1.728736866	4.815071412
C	-4.808294320	-2.522607025	4.144418847
C	-2.825569224	2.623698939	2.967709679
H	-0.891950816	2.213857924	2.156485162
C	-3.604832947	1.419796768	-1.562696981
H	-4.044195080	-0.218360131	-0.249714687
H	0.279198777	0.002465074	-1.862038610
H	-0.331289028	1.843042041	-1.302233437
H	4.583005842	1.606721303	5.902505792
H	4.683390451	2.808049674	4.616064184
H	5.585117514	1.297428231	4.478511671
H	-5.675836455	-1.962483856	3.781958522
H	-4.843908328	-2.520325758	5.239869735
H	-4.933105900	-3.564439844	3.822032610
H	2.327331393	-4.814655605	0.245909724
H	3.680811029	-3.844153885	-0.334857770
H	2.034018204	-3.503500856	-0.905961507
H	2.911449082	-4.256685185	2.701971562
H	3.073735725	-2.570133297	3.214772349
H	4.296245340	-3.303036587	2.165675329
H	5.125485703	-0.621497510	-2.137364463
H	3.359648461	-0.457982826	-2.162049598
H	4.096970822	-2.035888608	-1.886476553
H	6.370120660	-0.992216075	0.042434190
H	5.438070593	-2.471476584	0.270184224
H	5.502968996	-1.267304164	1.558948988
H	-5.909757523	1.370834336	-0.023954264
H	-4.841942464	2.631172938	0.591539812
H	-5.160530763	1.194398834	1.567873211
H	-4.533830712	1.334839630	-2.139777241
H	-2.821215486	0.880039228	-2.099131987
H	-3.332152100	2.480611633	-1.534576662
H	-2.424181532	3.434752765	3.588274897
H	-2.904278213	1.731303932	3.594049729
H	-3.834105577	2.916272798	2.663185442
H	-1.501684154	4.505083347	1.441123745
H	-2.813301144	3.887202161	0.437104086
H	-1.133090489	3.512680041	0.026755722
C	0.488534294	1.606448694	-3.229930544
H	1.386683926	1.203200248	-3.732190836
H	-0.387032504	1.090672384	-3.658669420
O	0.388864050	3.005607634	-3.459582750
C	0.374667456	3.369701313	-4.827559763
H	-0.474870381	2.890780556	-5.346717344
H	1.295621203	3.020728876	-5.328510888
C	0.264556656	4.888261133	-4.918647657
H	-0.650260999	5.200533058	-4.400328730
H	1.103156866	5.328449319	-4.365364027
C	1.819469588	2.050737718	-1.136361401
H	1.836673520	3.110091020	-1.418422895

H	1.864520810	2.002917055	-0.040517707
H	2.737321962	1.595147112	-1.521178429
C	0.256184344	5.397324221	-6.363383822
H	-0.589412624	4.987967622	-6.928446088
H	0.176404998	6.488647443	-6.394956473
H	1.174636222	5.117764893	-6.892765156

B_β

Ti	0.313713692	-0.091814366	-0.163879955
P	2.753288836	-0.820318360	0.698435709
C	2.549756019	-0.059318467	2.364518089
C	3.551553005	0.441931242	3.199981077
C	3.273799100	0.960863377	4.474347466
C	1.940032058	0.951225235	4.894687328
C	0.916373887	0.481700716	4.073773153
C	1.191920739	-0.013914171	2.786628893
N	0.193066705	-0.401723996	1.879082768
C	-1.001390734	-0.969685640	2.356135712
C	-1.028334932	-1.956641187	3.362864974
C	-2.216862240	-2.576965592	3.723532055
C	-3.432051585	-2.260583537	3.094639741
C	-3.410069758	-1.268924174	2.110864925
C	-2.229451186	-0.602092202	1.750492031
P	-2.095250437	0.766780005	0.527802411
C	4.430644746	-0.254097924	0.034098821
C	2.797498100	-2.674275225	1.089697791
C	-2.114449347	2.318547491	1.626513800
C	-3.670144350	0.680710797	-0.511850157
C	-0.180685900	-1.395591394	-1.387253667
C	-0.775021231	-2.680453451	-1.931451740
C	-2.125237189	-2.394097885	-2.633211914
C	-1.016280388	-3.677949497	-0.778625319
C	0.173074221	-3.320938936	-2.973676688
C	1.155176343	1.645092897	-1.152397708
H	4.584320694	0.431816535	2.865767225
H	1.689115086	1.335025241	5.881657990
H	-0.111227338	0.511226405	4.422787174
H	-0.098198873	-2.241530067	3.845557323
H	-2.201028088	-3.340313455	4.499217945
H	-4.344825623	-1.008910599	1.624270429
C	5.695174386	-0.858336873	0.672453572
C	3.173050935	-3.502011161	-0.148506889
C	-2.236871869	3.610469970	0.801775216
C	-4.967480115	1.232213980	0.104793751
H	-2.854719394	-1.988709335	-1.925758239
H	-2.544576525	-3.314096260	-3.061529814
H	-2.002854352	-1.669757224	-3.446322154
H	-0.074540687	-3.936739388	-0.283052527
H	-1.470275387	-4.606341544	-1.148546344
H	-1.684199377	-3.249075626	-0.024187990
H	0.349811262	-2.639699145	-3.814080452
H	-0.257067523	-4.247275241	-3.376128549
H	1.142848332	-3.566152716	-2.531282367
C	4.494924545	-0.422336064	-1.496889736
H	4.410310318	0.822838766	0.249644785
C	3.602600554	-3.101386630	2.325660470
H	1.735879615	-2.855307696	1.300624167
C	4.379524527	1.506939985	5.348055230
C	-4.710857751	-2.970751906	3.474449775
C	-3.092234821	2.312915237	2.811400315
H	-1.097943352	2.281543160	2.040346904
C	-3.429570456	1.295604958	-1.901790727
H	-3.786850203	-0.401945135	-0.647186843
H	0.151402038	-0.690618964	-2.196600485
H	2.082290186	1.252436357	-1.595763970
C	1.571491406	2.683810216	-0.123393638
H	-5.578200827	-2.527413598	2.976083868
H	-4.889877092	-2.926954847	4.555413683
H	-4.678944169	-4.032298339	3.198719065
H	4.027596211	1.685307721	6.368679466
H	4.767495916	2.458941420	4.963767775
H	5.228491365	0.815643043	5.406100098
H	5.411222956	0.041889610	-1.880383457
H	3.646814132	0.045482742	-2.000489405
H	4.515863104	-1.478222530	-1.783856004
H	6.579082931	-0.319243849	0.309879591
H	5.818946747	-1.907534475	0.387346209
H	5.702249264	-0.809773328	1.762892355
H	2.954113836	-4.561470016	0.029774504
H	4.241158497	-3.426328918	-0.377970885
H	2.608929073	-3.186261840	-1.029569923
H	3.399284669	-4.157042352	2.544970307
H	3.335375942	-2.517894225	3.210192399
H	4.680529468	-3.003727203	2.168070424
H	-2.866546753	3.157615208	3.474297226
H	-3.015309588	1.395517811	3.400243132
H	-4.130955486	2.421811080	2.487464106
H	-2.038330633	4.478845512	1.441166849
H	-3.244028668	3.735235594	0.391418734
H	-1.527548096	3.643230949	-0.029396994
H	-4.299373839	1.115247290	-2.545212616

H	-2.551600046	0.861052716	-2.384869059
H	-3.283893290	2.379552004	-1.842863636
H	-5.814709785	0.978349808	-0.544046330
H	-4.941518758	2.322779556	0.186945532
H	-5.179196609	0.829686224	1.097736059
H	0.686928744	3.203526208	0.286235976
H	2.090828518	2.223401839	0.736077767
C	3.698305102	5.690503680	-0.555685980
H	4.580124765	5.149019530	-0.919508575
H	3.166729961	6.053975793	-1.443516909
C	0.326551117	2.268231302	-2.289423178
H	0.144137058	1.551370195	-3.098325432
H	-0.655730002	2.612350067	-1.942394530
H	0.836630355	3.137973717	-2.726030300
C	2.793226441	4.703944191	0.175822507
H	3.309475431	4.302430247	1.068187343
H	1.887106383	5.222035440	0.542188119
C	4.124572210	6.867753937	0.327045850
H	4.678644632	6.527105755	1.209884878
H	4.771285822	7.560395585	-0.221335666
H	3.257132847	7.436923669	0.681997031
O	2.443496304	3.661072262	-0.709889760

C_β

Ti	0.026434567	-0.208678097	-0.194867212
O	0.848433686	1.223567268	2.893662356
C	1.372419835	1.738987531	4.110810675
C	-0.325243034	0.419326469	3.053267727
C	-0.623790108	-0.444334389	1.835632576
H	0.112287761	-1.284466293	1.839468047
H	-0.194490619	-0.207399557	3.957910127
H	-1.195249396	1.065083416	3.253722055
H	1.478075916	0.924802463	4.848718626
H	2.381114208	2.096105692	3.870857863
C	0.555697217	2.882767886	4.726186211
H	-0.464106765	2.538336282	4.937630497
H	0.469112044	3.691383878	3.989479856
P	-0.317871304	2.448117760	-0.299426670
C	1.042788696	3.623727867	-0.863975587
C	2.100369021	3.805887386	0.234950925
C	1.676467272	3.128179360	-2.171763979
H	0.933488757	3.029262414	-2.968673650
H	2.157205470	2.155446751	-2.029838915
H	2.547035805	2.844250582	0.501194210
H	2.440147016	3.839693803	-2.509169016
H	2.900826574	4.467068638	-0.118859383
H	1.688036978	4.243236382	1.148972654
H	0.552949008	4.586577127	-1.060762179
C	-1.158074769	3.350758994	1.138827539
C	-1.173290256	4.888791221	1.114877225
C	-2.580464627	2.810614811	1.358044472
H	-0.182437438	5.329127648	0.982418932
H	-1.567306936	5.256441941	2.070846813
H	-1.826219671	5.284947623	0.331557013
H	-2.976004971	3.177222259	2.313009331
H	-3.258346440	3.140595208	0.565020015
H	-2.603180396	1.719183160	1.383199323
C	1.866815774	-0.504963925	-0.400628392
H	1.861314460	-0.420564435	-1.509855042
C	3.264898735	-0.805131090	0.120693456
C	3.825930953	-2.080735750	-0.555369663
C	4.218487667	0.364602291	-0.224774670
C	3.261636591	-1.005041241	1.649593522
H	2.821953673	-0.138927593	2.150809033
H	2.670277085	-1.884216417	1.930250816
H	4.280911838	-1.156485955	2.027929456
H	3.216482062	-2.955918298	-0.311876987
H	4.851089396	-2.282585150	-0.217337036
H	3.846535662	-1.973510164	-1.646203755
H	3.915099951	1.282201534	0.285973683
H	4.227914463	0.563502867	-1.302642618
H	5.246347032	0.131492332	0.083163302
C	0.491742188	-4.142196337	-0.831277371
C	0.091660000	-5.499983065	-1.437457369
C	0.746123059	-4.291912107	0.679696287
H	1.427908712	-3.815170819	-1.298099914
H	0.917649787	-6.209877219	-1.308849776
H	1.495664823	-5.072029761	0.861531722
H	-0.163873125	-4.580756354	1.217664047
H	1.113563837	-3.360359212	1.116025874
H	-0.780071646	-5.929376275	-0.935258279
H	-0.135848962	-5.454570904	-2.504755120
C	-2.367852623	-3.432478223	-1.413500174
C	-3.370374501	-2.382525370	-1.914154109
C	-2.923042263	-4.153379196	-0.173676222
H	-3.038979820	-1.915098312	-2.843735426
H	-3.524949977	-1.589593763	-1.174785960
H	-4.341494665	-2.856522874	-2.103107791
H	-3.142639722	-3.453376743	0.637453083
H	-3.863592175	-4.654327320	-0.433597481
H	-2.245696601	-4.914487752	0.220928655

H	-2.224169537	-4.174284392	-2.209907990
C	-0.422560806	-0.694338218	-3.097152943
P	-0.646887240	-2.661675108	-1.153114920
C	-0.237200292	-2.080934381	-2.853174727
C	0.248685103	-2.907077231	-3.877864046
C	0.550693325	-2.425660874	-5.152826012
C	0.360940489	-1.054730758	-5.385014089
C	-0.103927878	-0.210376268	-4.386562942
H	0.399824158	-3.963736508	-3.684302895
C	1.084829920	-3.336026532	-6.233753573
H	0.933022248	-4.389748960	-5.980135581
H	2.161180921	-3.188298109	-6.390685521
H	0.593109027	-3.150517034	-7.195381426
H	0.595138364	-0.639075457	-6.363080895
H	-0.221842061	0.848147275	-4.593459923
N	-0.835191178	0.157649349	-2.053718875
C	-1.522840973	2.474367355	-1.680208503
C	-1.652238667	1.253278497	-2.385740038
C	-2.633670892	1.191188251	-3.402692411
H	-2.772730318	0.262603410	-3.946102347
C	-3.410722056	2.294255707	-3.728653480
C	-3.256517717	3.523236177	-3.067213156
C	-2.306169560	3.580168430	-2.045925944
H	-2.167735603	4.522186829	-1.524072629
C	-4.093587779	4.724127106	-3.442854216
H	-4.155636545	2.200443800	-4.516676596
H	-3.978884319	4.981990504	-4.502824479
H	-5.162220229	4.540974143	-3.273447400
H	-3.813995181	5.604933988	-2.856714136
H	-0.538717405	3.028596155	1.981419422
C	-2.023508434	-1.053428538	2.014352757
H	-2.285683982	-1.721306862	1.191810176
H	-2.121041603	-1.637816229	2.945349988
H	-2.798739005	-0.277885072	2.051150235
C	1.191739821	3.418321936	6.013664848
H	2.205410419	3.795044522	5.832006055
H	0.604023556	4.240590583	6.434729756
H	1.262313099	2.636536760	6.779105441

C_β-TS

C	0.311599579	-0.293117249	-0.202687419
O	0.110756352	0.087996368	1.488418946
C	1.663253692	-0.002496145	-0.519829684
Ti	2.110162300	0.083845076	1.996944366
H	2.273703612	-0.887753524	-0.648102700
H	-0.012660928	-1.334098396	-0.127825135
H	-0.469266497	0.352230141	-0.609658660
C	-1.124315719	-0.178745507	2.125626035
H	-1.499068503	-1.164547281	1.797360246
H	-0.939181688	-0.238823327	3.204310818
H	-1.783671992	1.865945899	2.158696614
C	-2.177143764	0.895286247	1.832148200
H	-2.333633407	0.969244358	0.748548650
C	1.884136723	-0.469408867	3.768808207
H	2.876203400	0.058723825	3.833319671
C	1.533406737	-1.039684270	5.139922204
C	0.473519658	-2.158208294	5.053821712
H	-0.430045044	-1.816808802	4.539892517
H	0.182270894	-2.483865195	6.060307098
H	0.852168684	-3.032479952	4.519931782
C	2.793709269	-1.601621972	5.843327946
H	2.543833691	-2.006939392	6.832473348
H	3.547562320	-0.818467762	5.982287416
H	3.258837937	-2.401351547	5.258752827
H	1.692685789	0.883776450	6.185919157
H	0.680122357	-0.303996170	7.020401211
H	0.064962023	0.530918597	5.578736112
C	2.745660959	3.615222947	3.894595250
H	3.070629413	4.620081528	3.594131884
C	1.588252233	3.741562222	4.896980897
H	1.164506900	2.762108787	5.133836785
H	1.951710301	4.182687253	5.832991078
H	0.778479272	4.378715994	4.530500701
C	3.950159289	2.907928284	4.528662797
H	4.792431673	2.840832368	3.836152907
H	3.696855061	1.893863411	4.851364144
H	4.284182465	3.466491223	5.411717410
C	0.981479130	5.442141428	1.871736981
C	0.788330420	3.920351318	1.735079989
H	0.002654418	3.623683149	2.443834508
H	0.041910896	2.518004486	0.244358318
C	0.286447499	3.576717512	0.328450051
H	1.038696789	3.817955527	-0.428399336
H	-0.615538295	4.158628994	0.101924629
H	0.009498588	5.936232038	1.750965451
H	1.635405322	5.839911707	1.090750325
H	1.384542058	5.749780580	2.838952085
P	2.196759310	2.776499319	2.286651879
C	3.667803450	2.985410309	1.211908488
C	4.028170715	4.160652771	0.538737184
H	3.407076618	5.043780280	0.644307360
C	5.167740736	4.245879125	-0.264869420

C	5.536025152	5.520230182	-0.988600431
H	5.644944885	5.354115872	-2.067304831
H	4.774054964	6.293221900	-0.849165541
H	6.489732919	5.928557741	-0.630938437
C	5.961474485	3.094546763	-0.371762706
H	6.851680084	3.115598108	-0.998016011
C	5.635378970	1.918519412	0.291487267
H	6.269073866	1.045376927	0.175871455
C	4.484158157	1.825667273	1.104227783
N	4.112893861	0.639779598	1.757339071
C	5.108031150	-0.195224228	2.288415169
C	6.306628890	0.305150870	2.848295457
H	6.497980827	1.372510963	2.813641159
C	7.234110873	-0.534146996	3.450611809
H	8.137916886	-0.102960124	3.876923747
C	7.023700966	-1.918999747	3.535332581
C	8.022580526	-2.822433882	4.219860020
H	7.801257362	-3.877593928	4.031583179
H	8.020156804	-2.676261698	5.307752861
H	9.044904239	-2.630047128	3.874136290
C	5.850821652	-2.422928948	2.969119753
H	5.682395123	-3.494442565	3.012126190
C	4.899577117	-1.602822448	2.346200341
P	3.390975192	-2.208299579	1.483133445
C	2.756487622	-3.756814759	2.364723163
H	2.823456969	-3.473862371	3.420737673
C	3.516524450	-5.078236465	2.161719625
H	3.450006757	-5.433649606	1.128875363
H	3.071978539	-5.853802424	2.797550086
H	4.575526996	-5.013638346	2.421185786
H	0.828125237	-4.735352001	2.644552148
H	1.126473778	-4.244231584	0.976180683
H	0.695437532	-3.028460894	2.188106543
H	2.377704615	-2.783973604	-1.413782506
H	3.625649827	-3.902606713	-1.971066597
C	3.117721626	-3.517288937	-1.078127176
H	2.579424760	-4.354199385	-0.625701452
H	4.834336493	-3.683457533	0.209964155
C	4.152589481	-2.891006285	-0.126560987
C	4.998259426	-1.834068007	-0.855175415
H	5.449553549	-2.279956788	-1.750532350
H	5.808485322	-1.463760180	-0.222491751
H	4.399539020	-0.976885272	-1.175280177
C	1.264773392	-3.945731609	2.020580809
C	0.957368606	0.088074625	6.032927791
C	2.008068330	1.087261305	-1.526410265
H	2.958038787	1.588467431	-1.306606586
H	2.096863812	0.687602918	-2.550390962
H	1.240077173	1.865329308	-1.566177572
C	-3.512085532	0.608972832	2.528715101
H	-4.247229247	1.392006044	2.316250818
H	-3.939818709	-0.344584292	2.197065048
H	-3.390336870	0.555169290	3.617104171

MeOEt

C	-0.207666515	-1.534598989	0.014423384
H	0.194637573	-2.548984215	0.088039973
H	0.151547411	-1.075320480	-0.920837203
H	-1.307547998	-1.589289428	-0.029835265
O	0.235158812	-0.822364801	1.150361107
C	-0.224287979	0.519503074	1.169792274
H	-1.328110164	0.544273882	1.155493410
H	0.123395984	1.054044301	0.268353949
C	0.307055884	1.192829331	2.426121219
H	1.401244859	1.179109256	2.433179562
H	-0.029359449	2.234274840	2.474184811
H	-0.048566417	0.669903185	3.319184283

A-MeOEt

Ti	0.482706318	0.937785997	0.981847725
P	3.156643884	0.978273969	1.129057318
C	3.182594045	2.280288805	2.430191553
C	4.229144631	3.184237484	2.639746980
C	4.197248146	4.154772162	3.649514057
C	3.061689544	4.184062222	4.467371539
C	1.993169342	3.315087452	4.272106433
C	2.006719166	2.351949475	3.237897527
N	0.922087859	1.529409826	2.937814417
C	-0.062836872	1.276948201	3.908068517
C	0.230772178	0.821337562	5.207027649
C	-0.785739823	0.486576103	6.095170907
C	-2.138730766	0.586067088	5.735147238
C	-2.433709015	1.057157057	4.451671517
C	-1.427391658	1.418613090	3.545633783
P	-1.698757544	2.059378658	1.842651751
C	4.474985515	1.489085451	-0.129615017
C	3.681151033	-0.590398369	2.047598291
C	-1.564932450	3.941051701	2.071425608
C	-3.458618387	1.578389015	1.358586816
C	-0.133111211	-0.699996235	0.963108170
C	-0.620313308	-2.118394552	1.150436037
C	-2.139668083	-2.133787364	1.442045678
C	0.114462898	-2.780773680	2.340956651

C	-0.354908610	-2.944423317	-0.131381128
C	0.319329435	1.416937423	-1.649477840
H	5.109229810	3.138520671	2.005029721
H	3.001852433	4.916720272	5.270489183
H	1.120665201	3.388635833	4.913012325
H	1.270456240	0.711700459	5.501690926
H	-0.523818915	0.124758671	7.087740451
H	-3.476939843	1.144639475	4.162052791
C	5.941753192	1.190271824	0.227356158
C	3.829164409	-1.772767962	1.078112124
C	-1.813022653	4.686839664	0.750228473
C	-4.614280970	2.432338415	1.904967245
H	-2.360227717	-1.576156987	2.358122338
H	-2.506564057	-3.161509744	1.571546949
H	-2.698621935	-1.677668649	0.617418431
H	1.193728371	-2.816297032	2.160353804
H	-0.235892166	-3.810233536	2.500333718
H	-0.054835595	-2.213369790	3.261642759
H	-0.879652118	-2.508261061	-0.988716176
H	-0.696548771	-3.982391029	-0.014061409
H	0.714480140	-2.962946797	-0.367689255
C	4.138309689	0.927004137	-1.523385599
H	4.345889587	2.578384625	-0.173619506
C	4.869607143	-0.473753988	3.012621219
H	2.777204543	-0.765133321	2.644078972
C	5.331974535	5.137018774	3.829139111
C	-3.232670073	0.192909106	6.700737930
C	-2.333154187	4.576679460	3.239929707
H	-0.494299906	4.024689405	2.303002068
C	-3.558687744	1.444223272	-0.171479513
H	-3.538532807	0.569054368	1.779010900
H	0.928615418	0.611996163	-1.202928577
H	-0.594067761	1.595911316	-1.050629430
H	5.367354055	5.522046147	4.853458577
H	5.232227093	6.004078018	3.161783165
H	6.302891164	4.677247370	3.613290945
H	-4.219855428	0.475892230	6.322632478
H	-3.100055693	0.672831890	7.677560256
H	-3.245416581	-0.890330077	6.875420199
H	3.938813468	-2.706534793	1.642300346
H	4.716061058	-1.672509666	0.442462933
H	2.949383526	-1.870724003	0.435202748
H	4.911875115	-1.368348685	3.646403297
H	4.776433222	0.396018190	3.668521817
H	5.825758468	-0.403584159	2.486831548
H	4.905026634	1.238769171	-2.243844279
H	3.175474641	1.299957038	-1.878465782
H	4.114654671	-0.167953989	-1.524807886
H	6.600663947	1.671456627	-0.506151397
H	6.149073381	0.116467263	0.191508248
H	6.227588826	1.550644352	1.217740763
H	-5.571009981	1.957037711	1.655523730
H	-4.623975997	3.430377129	1.455204578
H	-4.579063705	2.556761933	2.989721829
H	-4.548124472	1.064113572	-0.453608484
H	-2.805855660	0.748534926	-0.552454392
H	-3.425083814	2.410509335	-0.672475962
H	-1.976506373	5.602056869	3.400591768
H	-2.183169862	4.022169895	4.170104558
H	-3.407693020	4.633137965	3.046234412
H	-1.507221096	5.736067340	0.841758811
H	-2.872910867	4.680137744	0.472305851
H	-1.247035066	4.248216302	-0.078717453
H	-0.017907469	1.021841301	-2.619383150
O	1.110249068	2.578950456	-1.788748675
C	0.518111734	3.569673727	-2.625399456
H	0.335890731	3.145552832	-3.626519065
H	-0.458141582	3.875325016	-2.216057532
C	1.457771356	4.760254476	-2.705276956
H	1.032322206	5.536146530	-3.349875614
H	1.623224917	5.188294818	-1.711986585
H	2.425963401	4.460259000	-3.116983033

A-MeOEt-TS

Ti	-0.016633125	-0.133366619	-0.056263568
P	2.552641834	-0.491968354	0.483576869
C	2.445066341	0.073334016	2.230119253
C	3.474475567	0.652071256	2.979640705
C	3.309540053	1.024477931	4.319875870
C	2.058859324	0.779274850	4.900651834
C	1.008107085	0.224657951	4.177669127
C	1.159033923	-0.122065675	2.816146732
N	0.113563829	-0.567826590	2.010517798
C	-1.020539239	-1.168953702	2.575552560
C	-0.953000218	-2.217948315	3.514176639
C	-2.103583105	-2.858045090	3.956123812
C	-3.375168342	-2.496082138	3.483077646
C	-3.449384238	-1.443536272	2.567563004
C	-2.305830245	-0.763605287	2.126283405
P	-2.289093217	0.658021858	0.961590788
C	4.022471252	0.405002334	-0.293938915
C	2.903838385	-2.343814210	0.646664255

C	-2.100045900	2.151088590	2.117203341
C	-3.962780138	0.684587495	0.094395612
C	-0.459606172	-1.297786286	-1.307607663
C	-0.859769490	-2.262497968	-2.395783543
C	-2.291110561	-1.948997371	-2.893580518
C	-0.832355159	-3.704656967	-1.836172347
C	0.112369107	-2.156197400	-3.595456350
C	0.278831237	1.553554114	-1.636828969
H	4.442397989	0.821645325	2.517295457
H	1.895659790	1.043613479	5.944207402
H	0.046900726	0.074340219	4.658759075
H	0.020798450	-2.536592830	3.874636715
H	-2.014797355	-3.671332265	4.674005543
H	-4.427764085	-1.147840610	2.200124689
C	5.434098100	-0.082093963	0.080047455
C	3.178551510	-2.986204331	-0.720513114
C	-2.098532392	3.476623449	1.338624397
C	-5.167303648	1.234127990	0.876705314
H	-3.010372139	-2.007367945	-2.069942349
H	-2.601105696	-2.661843515	-3.669452404
H	-2.342479409	-0.942086263	-3.321603494
H	0.170281967	-3.968353408	-1.485191058
H	-1.126225299	-4.428960709	-2.607686037
H	-1.520461157	-3.804990659	-0.990499329
H	0.125938418	-1.136596997	-3.993727004
H	-0.184857277	-2.840390303	-4.401659707
H	1.134261204	-2.410694650	-3.296851987
C	3.874659807	0.455399644	-1.827501063
H	3.897152535	1.426525696	0.091995943
C	3.944050000	-2.753856408	1.698951483
H	1.921449213	-2.694830722	0.986998268
C	4.425160796	1.682007080	5.098783948
C	-4.613735816	-3.228737409	3.943476375
C	-3.024512501	2.210428555	3.342760030
H	-1.080257303	1.978721322	2.486439650
C	-3.832608359	1.392445934	-1.266990884
H	-4.129889873	-0.382333523	-0.103774164
H	-0.051245986	0.262636493	-1.762097405
H	-0.632763106	2.149838385	-1.465760160
H	4.417277479	1.373003194	6.149807518
H	4.340820230	2.777003911	5.086299310
H	5.407113084	1.429451653	4.685256011
H	-5.524297055	-2.692293530	3.659515128
H	-4.626039439	-3.353845424	5.032313671
H	-4.673723161	-4.232983024	3.504879478
H	3.168392080	-4.078667867	-0.627217695
H	4.161390657	-2.703669049	-1.113567102
H	2.417922639	-2.702794222	-1.452375219
H	3.908244939	-3.841140691	1.840834732
H	3.752130366	-2.283243618	2.666583905
H	4.962725780	-2.499376497	1.392625030
H	4.653226075	1.102156413	-2.251132475
H	2.902656295	0.834215699	-2.151718461
H	4.001677816	-0.538348876	-2.268974470
H	6.179552929	0.618195977	-0.316738705
H	5.643182509	-1.060555441	-0.362894613
H	5.595675736	-0.164321388	1.156732286
H	-6.088237846	1.047907500	0.310628819
H	-5.089570117	2.316938888	1.017747859
H	-5.284731399	0.777613948	1.862228996
H	-4.771296843	1.303969010	-1.827093379
H	-3.034816647	0.952217354	-1.869845469
H	-3.623316450	2.461615077	-1.146845028
H	-2.652589998	2.966232618	4.045847798
H	-3.059635150	1.253308269	3.869914665
H	-4.046888743	2.490302433	3.074993633
H	-1.805088145	4.300227072	2.000271393
H	-3.091365987	3.717099086	0.942957915
H	-1.396632742	3.461547725	0.498100188
O	0.687836271	1.643609120	-2.997679254
C	0.911127397	2.982637618	-3.416518844
H	1.693612065	3.446498560	-2.790993431
H	-0.007641656	3.577564935	-3.277786861
C	1.326959092	2.973991139	-4.878325195
H	1.503378589	3.996341549	-5.229145272
H	2.246474051	2.397022096	-5.015121936
H	0.544868880	2.524844037	-5.497791002
H	1.076410315	1.978516529	-0.995664332

B-MeOEt

Ti	0.396264010	-0.230430727	-0.224990449
P	2.828185894	-0.867199251	0.656278770
C	2.594543101	-0.115049837	2.317890978
C	3.586938944	0.401161531	3.152936822
C	3.299786752	0.921518977	4.424274887
C	1.965055957	0.901010185	4.839011515
C	0.949797651	0.414961445	4.017752214
C	1.234628965	-0.086553841	2.734003169
N	0.248706705	-0.497342468	1.826200856
C	-0.990736616	-0.956822449	2.311668983
C	-1.104266362	-1.916773114	3.336804453
C	-2.346994582	-2.398258771	3.729076860

C	-3.532750483	-1.962979787	3.114506421
C	-3.422750989	-1.005724590	2.102450600
C	-2.182923222	-0.483093413	1.708049890
P	-1.906020811	0.806299477	0.429441286
C	4.488337771	-0.246330566	0.005676870
C	2.926663249	-2.719278831	1.043175600
C	-1.745662238	2.398666293	1.442800589
C	-3.457145910	0.845453809	-0.640793565
C	-0.168169376	-1.591221321	-1.338137413
C	-0.801671459	-2.884805345	-1.805902274
C	-2.170457053	-2.603529763	-2.472210865
C	-1.020249467	-3.818639917	-0.596727768
C	0.102935682	-3.593478025	-2.841619554
C	1.181294255	1.451906345	-1.302155162
H	4.620594655	0.403461154	2.820510314
H	1.706045972	1.288408128	5.822650279
H	-0.078299707	0.438586412	4.364563323
H	-0.200993141	-2.286275298	3.813324096
H	-2.400281431	-3.142213856	4.521766825
H	-4.331880794	-0.655645485	1.622228655
C	5.767784087	-0.840998593	0.621670329
C	3.280651910	-3.535647254	-0.209064682
C	-1.656647395	3.635049935	0.534838528
C	-4.693037026	1.568246425	-0.079388876
H	-2.862465194	-2.148153676	-1.757027419
H	-2.625040833	-3.532972533	-2.839869497
H	-2.063270105	-1.921203351	-3.323034940
H	-0.065895138	-4.068452397	-0.121399041
H	-1.502040910	-4.755566026	-0.904485377
H	-1.653903922	-3.339796628	0.156659903
H	0.267261831	-2.958179325	-3.719817306
H	-0.353656681	-4.530877363	-3.184785794
H	1.080552839	-3.832843509	-2.412626806
C	4.544483824	-0.364900693	-1.529610400
H	4.438647626	0.820799246	0.257201606
C	3.772108647	-3.135829495	2.255601777
H	1.874813811	-2.921067085	1.282830884
C	4.396434136	1.482267390	5.300550795
C	-4.874695461	-2.512915627	3.539949651
C	-2.750570571	2.598866305	2.586817008
H	-0.754859418	2.245095035	1.888799372
C	-3.107089007	1.369427422	-2.046006731
H	-3.693430265	-0.222089347	-0.736337070
H	0.187772693	-0.930327918	-2.180721558
H	1.987124312	1.302339972	-2.035370059
H	-5.696566791	-2.000831297	3.030430377
H	-5.031441188	-2.400403940	4.619514369
H	-4.961810672	-3.583074908	3.314230252
H	4.034261778	1.674316458	6.315265521
H	4.786994358	2.429789061	4.907397030
H	5.246503584	0.793827043	5.377595266
H	5.449308759	0.126481811	-1.907961252
H	3.680145978	0.100814146	-2.006632507
H	4.581211177	-1.411166061	-1.849851941
H	6.639795655	-0.276770024	0.268055902
H	5.910249701	-1.880856927	0.311893578
H	5.779077773	-0.817490207	1.713041703
H	3.100555037	-4.601534660	-0.024963036
H	4.336948605	-3.428056274	-0.478399470
H	2.674066039	-3.235518297	-1.067837191
H	3.586218082	-4.192875918	2.483947355
H	3.523948217	-2.552350086	3.145691493
H	4.844121937	-3.028044533	2.067089407
H	-2.420104453	3.431402104	3.220579418
H	-2.831608447	1.710682736	3.218929003
H	-3.750400254	2.846630733	2.219323047
H	-1.366936735	4.511638155	1.126517161
H	-2.617990901	3.866099998	0.063477596
H	-0.910276286	3.504333804	-0.252377744
H	-3.977048351	1.279685453	-2.707868609
H	-2.282935662	0.802434853	-2.486678182
H	-2.819197004	2.426269214	-2.021950983
H	-5.551457086	1.393064870	-0.739465671
H	-4.537757649	2.650459465	-0.032411871
H	-4.969873894	1.228880303	0.921640670
H	0.368764042	1.996698642	-1.819105725
O	1.628203826	2.202035605	-0.162134027
C	1.992635928	3.559808632	-0.394764529
H	2.032193354	4.031643098	0.593876223
H	1.201046420	4.061223531	-0.975709617
C	3.334560906	3.718892104	-1.104889733
H	4.140588317	3.267189284	-0.517621518
H	3.322484468	3.249388586	-2.093042218
H	3.566266234	4.781382957	-1.241396386

E			
Ti	-0.173956079	-0.458772178	-2.303822919
P	2.003452131	-0.899081005	-0.949794141
C	1.224146819	-1.459546013	0.619693213
C	1.953345819	-1.772098748	1.776173294
C	1.349644093	-2.129507738	2.984844069
C	-0.051009644	-2.159379291	3.003094121

C	-0.807710874	-1.864021597	1.877489056
C	-0.205869690	-1.520392972	0.641614455
N	-0.928677647	-1.174815368	-0.494764290
C	-2.329572303	-1.297147594	-0.557524598
C	-3.036363413	-2.469866119	-0.216796647
C	-4.411655358	-2.560931782	-0.398757474
C	-5.151891374	-1.500977901	-0.945065720
C	-4.457229389	-0.339661308	-1.296251187
C	-3.073713065	-0.212986683	-1.107662079
P	-2.047069579	1.228822452	-1.626608578
C	3.271759401	0.426162064	-0.460904166
C	2.869741723	-2.421643647	-1.671234644
C	-1.697005180	2.161625128	-0.017581419
C	-3.123114380	2.256243375	-2.788968508
C	-1.134591579	-2.030180636	-5.088654579
C	-2.279910670	-1.018255178	-5.297344325
C	-1.683909659	-3.261337103	-4.338331758
C	-0.627926971	-2.487581596	-6.476349113
H	3.037831103	-1.733456297	1.741140148
H	-0.567212763	-2.416909064	3.926685763
H	-1.888922235	-1.885853272	1.951663065
H	-2.484918959	-3.318259348	0.176177164
H	-4.921574674	-3.482974119	-0.127044214
H	-5.018370802	0.485833598	-1.725564745
C	4.646148046	-0.024135356	0.060105897
C	3.665042920	-2.052746990	-2.934971325
C	-0.877312659	3.435627406	-0.276243569
C	-4.175485071	3.184699204	-2.161037573
H	-2.721340737	-0.720994262	-4.337986336
H	-3.084883146	-1.438401584	-5.914647379
H	-1.915912820	-0.111757608	-5.796996317
H	-0.892996202	-4.004633835	-4.177226698
H	-2.488762196	-3.750605146	-4.902696223
H	-2.084846654	-2.985679476	-3.355646379
H	-0.244866639	-1.636082967	-7.051840594
H	-1.421690084	-2.963260161	-7.069710134
H	0.190126791	-3.210326762	-6.371713927
C	3.440323113	1.429921528	-1.616557993
H	2.747054180	0.938297421	0.356616302
C	3.692985432	-3.294222880	-0.712719879
H	2.002630760	-3.015558546	-1.992177176
C	2.162292644	-2.429105793	4.223096002
C	-6.641594065	-1.623143800	-1.166248322
C	-2.896364629	2.419767181	0.906544286
H	-1.042687256	1.437122476	0.483085319
C	-2.224587842	3.031730679	-3.771445517
H	-3.645686611	1.482226027	-3.366067232
H	-7.090204166	-0.654858441	-1.408230562
H	-7.150075901	-2.013517160	-0.277322921
H	-6.871019607	-2.307100601	-1.993196937
H	1.708993696	-3.231878274	4.815212578
H	2.244011982	-1.553650498	4.881787019
H	3.181126567	-2.739649911	3.969559600
H	4.060204426	2.275978785	-1.295342863
H	2.474846845	1.822562073	-1.950997971
H	3.931084951	0.970614379	-2.481512160
H	5.224638727	0.854962201	0.370358462
H	5.225669840	-0.534047160	-0.715477402
H	4.578044115	-0.689332577	0.923211334
H	4.005501169	-2.964891177	-3.438834045
H	4.556306235	-1.463027508	-2.695293744
H	3.058590012	-1.486062206	-3.647548629
H	4.009146857	-4.206464898	-1.233915889
H	3.112120130	-3.595409637	0.161926393
H	4.598097116	-2.787118465	-0.366034009
H	-2.536016306	2.739953359	1.892119831
H	-3.498069644	1.517924955	1.049223230
H	-3.549040706	3.209707384	0.525388991
H	-0.524164066	3.852252550	0.674371548
H	-1.473122204	4.211810840	-0.768839996
H	0.000077732	3.234969659	-0.900372806
H	-2.840410677	3.545254817	-4.519523017
H	-1.537535100	2.364504325	-4.299973583
H	-1.626997068	3.792914698	-3.258051445
H	-4.812282775	3.605812110	-2.948616920
H	-3.706136178	4.026065769	-1.641551707
H	-4.824427504	2.671810469	-1.446914578
C	0.005255473	-1.385026146	-4.263249250
H	0.808522332	-2.140728452	-4.153984293
H	0.472839815	-0.580783206	-4.873956019

F

Ti	0.291108408	0.555055128	-1.830555631
P	2.041586330	-1.365818731	-1.057255122
C	1.489637346	-1.137718239	0.687921631
C	2.281797710	-1.265855493	1.835927844
C	1.752146389	-1.125793709	3.124969994
C	0.381898688	-0.852454103	3.241657733
C	-0.419900164	-0.683278856	2.117061680
C	0.118388273	-0.800719155	0.822067628
N	-0.634658974	-0.534459506	-0.338565320
C	-1.905809191	-1.122073941	-0.472342055

C	-2.206181605	-2.410273360	0.013380229
C	-3.439651351	-2.999817053	-0.244099168
C	-4.422796556	-2.345480503	-0.998394660
C	-4.136123483	-1.050655956	-1.448071648
C	-2.914442180	-0.421841796	-1.181102547
P	-2.402849591	1.278302621	-1.657135147
C	3.931658951	-1.308134808	-0.954814587
C	1.456037706	-3.128423058	-1.450691595
C	-2.731678247	2.275238741	-0.075993084
C	-3.616088131	1.814153646	-3.006574665
C	0.764164971	0.473536850	-5.171477467
C	2.226214574	0.001094725	-5.082659754
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