Supporting Information

Mechanistic Study of Hydroamination of Alkyne Through Tantalum-Based Silica-Supported Surface Species

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General Procedures

All experiments were carried out under controlled atmosphere using high vacuum lines (< 10^{-5} mbar) and glovebox systems. Pentane was collected from a Solvent Purification System following by a freeze-pump collected in secured bottle covered with sodium mirror from inside to monitor air leak. Elemental analyses were performed at KAUST's analytical core lab facilities. Aniline, 4-iodoaniline, 2-iodo-4-nitroaniline, 3,4,5-trifluoroaniline, 3-hexyne, 1-Decyne, 1-octyne, 1-hexyne, 2-Pentyne, 2-Pentyn-1ol and diphenylacetylene are from Sigma Aldrich. Also Tris(ethylmethylamido)(tert-butylimido)tantalum(V) from Sigma Aldrich.

Fourier Transformed Infrared Spectroscopy

FTIR spectra were recorded on a Nicolet 6700 FT-IR spectrometer equipped with a cell under controlled atmosphere. Typically, 32 scans were accumulated for each spectrum (resolution 4 cm^{-1}).

Gas Chromatography–Mass Spectrometry

GC measurements were performed with an Agilent 7890A Series (FID detection; column HP-5 with 30 m length×0.32 mm i.d. × 0.25 µm film thickness; flow rate = 1 mL/min (N_2); split ratio = 50/1; inlet temperature = 250°C, detector temperature = 250°C; temperature program = 40 °C (3 min), 40−250°C (12 °C/min), 250°C (3 min), 250−300°C (10 °C/min),300 °C (3 min)). GC-MS measurements for the gas samples were performed with an Agilent 7890A series coupled with Agilent 5975C Series instruments. GC/MS equipped with column HP-PLOT/Q (with 30 m length×0.32 mm i.d. × 20 µm film thickness; flow rate = 1 mL/min (N_2); split ratio = 5/1; inlet temperature =250°C, detector temperature = 250 °C; temperature program = 50 °C (10 min), 50−185 °C (20 °C/min), 185 °C (5 min) was used for molecular weight determination and identification that allowed the separation of organics according to their polarity differences.

Solid State Nuclear Magnetic Resonance Spectroscopy:

One dimensional ^{1}H MAS and ^{13}C CP-MAS solid state NMR spectra were recorded on a Bruker AVANCE III spectrometer operating at 400 and 100 MHz resonance frequencies for ^{1}H, and ^{13}C respectively, with a conventional double resonance 4 mm CPMAS probe. The samples were introduced under argon into zirconia rotors, which were then tightly closed. The spinning frequency was set to 17, and 10 KHz for ^{1}H and ^{13}C spectra, respectively. NMR chemical shifts are reported with respect to TMS as an external reference. For CP/MAS ^{13}CNMR, the following sequence was used: 90^{o} pulse on the proton (pulse length 2.4 s), then a cross-polarization step with a contact time typically 2 ms, and finally acquisition of the ^{13}C signal under high power proton decoupling. The delay between the scan was set to 5 s, to allow the complete relaxation of the ^{1}H nuclei and the number of scans was between 3,000-5,000 for carbon and 32 for proton. An apodization function (exponential) corresponding to a line broadening of 80 Hz was applied prior to Fourier transformation.

Dynamic nuclear polarization surface enhanced solid state NMR spectroscopy:

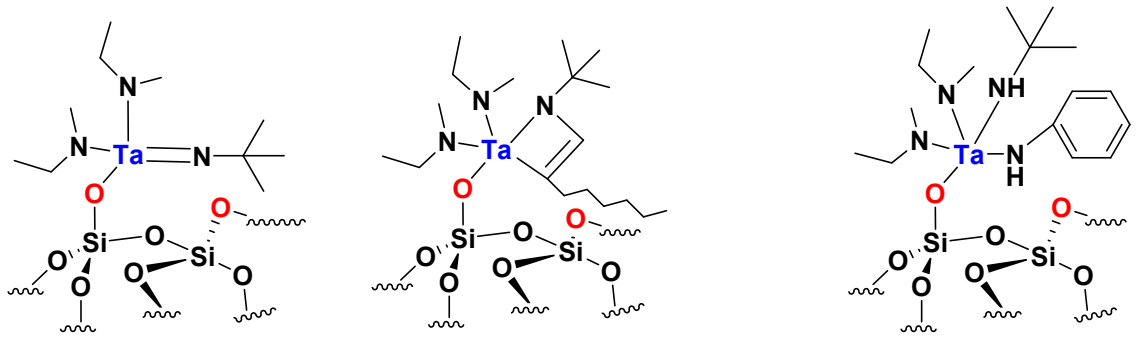
DNP-SENS-NMR experiments were performed on a 400 MHz (1H/electron Larmor frequencies) Bruker Avance III solid-state NMR spectrometer equipped with a 263 GHz gyrotron. The sweep coil of the main super conducting coil was set so that microwave irradiation occurred at the positive enhancement maximum of TEKPOL. At low temperature double resonance 3.2 mm probe configured for 29Si and after for ^{15}N CP/MAS. Sample temperature during DNP experiments were around 100 K. DNP enhancements were measured by comparing the intensity of spectra acquired with and without continuous wave irradiation. A 20 mg of powdered material was impregnated with 20 µL of 16 mM of TEKPOL tetrachloethane solution. Impregnated materials were then packed into sapphire rotors inside glovebox. The ^{15}N reference is glycine = 33.4 ppm correspond to NH_3 at 0 ppm.

Material Preparation

(1) **Preparation of [(≡Si-O-)Ta(NEtMe)$_2$(=NtBu)].** In a double schlenk, 1.000 g of $SiO_{2\text{-}700}$ (0.310 mmol silanols groups per gram) prepared at 700 °C was reacted at room temperature in pentane for 1 h with 0.0989 mL of [(TaNEtMe)$_3$(=NtBu)] in slight excess (1.1 equivalent, with respect to the amount of surface accessible silanols). After filtration and four washing cycles, all volatile compounds were evaporated and the solid was dried for 1 h under dynamic vacuum (< 10^{-5} mbar).

(2) **Preparation of [(≡Si-O-)Ta(η^{1}σ-NEtMe)$_2$(η^{2}N^{t}BuCH=C$_7$H$_{13}$)].** Under inert atmosphere inside the glovebox. 100 mg of **(1)** was reacted at 80 °C in toluene for 16 h with 46 uL of 1-Octyne, then washed several times with toluene followed by pentane.

(3) **Preparation of [(≡Si-O-)Ta(η^{1}σ-NEtMe)$_2$(-NH^{t}Bu)(NHC$_6$H$_5$)].** Under inert atmosphere inside the glovebox. 100 mg of **(1)** was reacted at 80 °C in toluene for 16 h with 24 uL of Aniline, then washed several times with toluene followed by pentane.



(1) **(2)** **(3)**

Figure S1. Prepared materials.

Table S1. Elemental analysis.

Material	M	%M	M/Silanol	%C	%N	C/N	N/M	C/M
(1)	Ta	5.24	1	4.2	1.3	3.5	3.0	10.9
(2)	Ta	5.21	1	5.2	1.3	4.7	3.1	14.9
(3)	Ta	5.18	1	6.2	1.5	4.8	3.7	17.9

Catalysis

Materials loaded with the catalyst in the glovebox (under inert atmosphere) to an ampule tube: Ta catalyst (0.03mmol, 10 mg), primary amine (e.g. Aniline = 0.03 mmol, 2.8uL) and alkyne (e.g. 1-0ctyne = 0.03 mmol, 4.6 uL) then degassed toluene (1 mL) added, after sealing the tube placed in an oil bath at 80 °C, for 16 h.

Conversion = $\text{conversion } \% = \frac{((\text{area of the blank alkyne} - \text{area of actual alkyne}))}{\text{area of the blank alkyne}} \times 100$

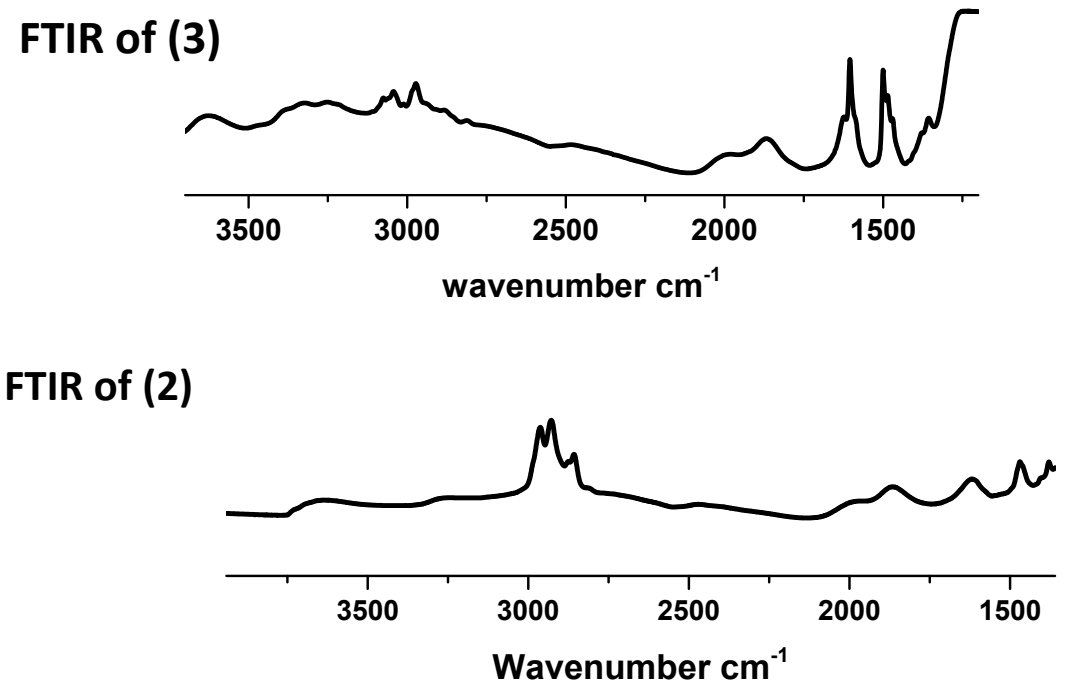


Figure S2. FTIR spectra of exchange products with 1-octyne (**2**) and aniline (**3**).

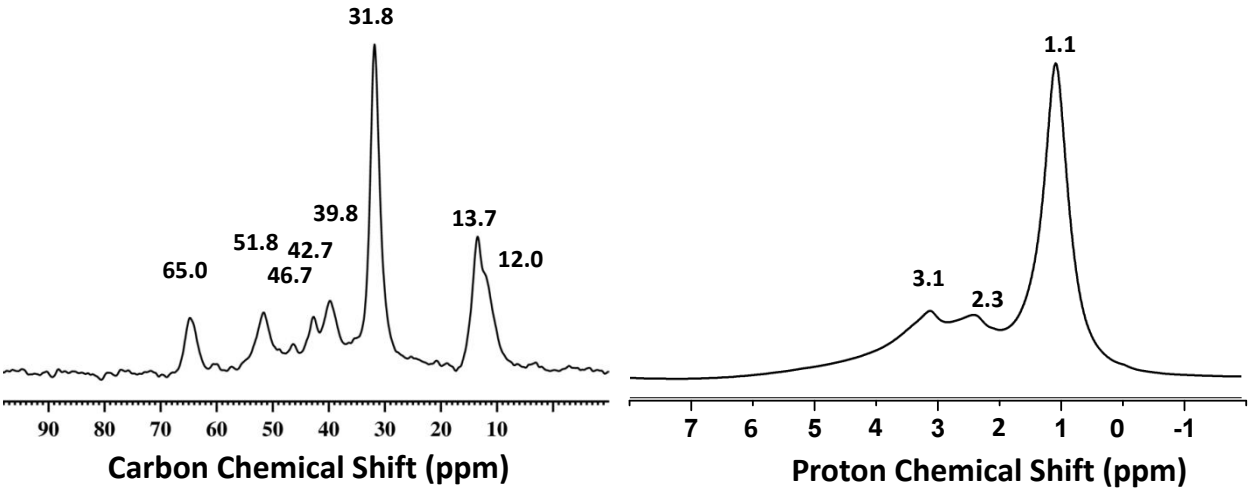


Figure S3. 1D ^{1}H and ^{13}C MAS NMR for (**1**) [(≡Si-O-)Ta($\eta^1\sigma$-NEtMe)$_2$(=N^{t}Bu)].

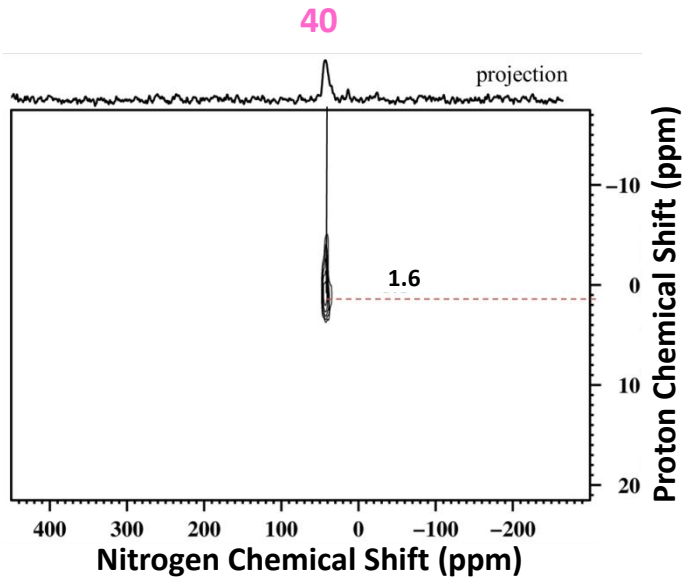


Figure S4. ^{1}H-^{15}N HETCOR DNP NMR spectra of (**1**).

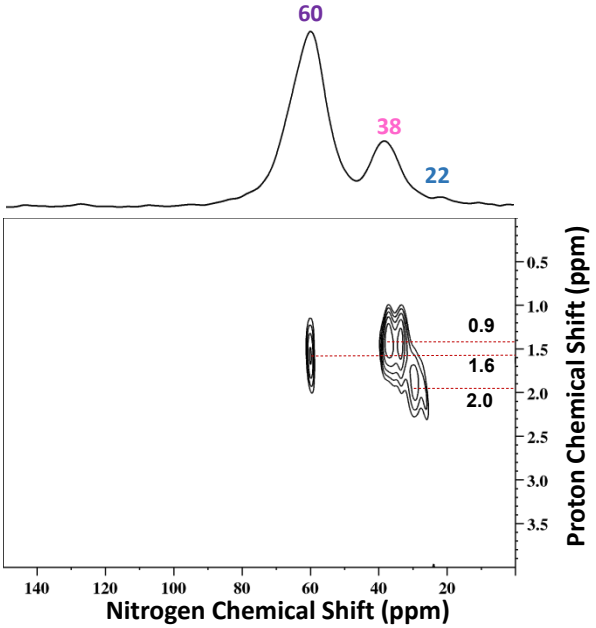


Figure S5. ^{1}H-^{15}N HETCOR DNP NMR spectra of (**2**).

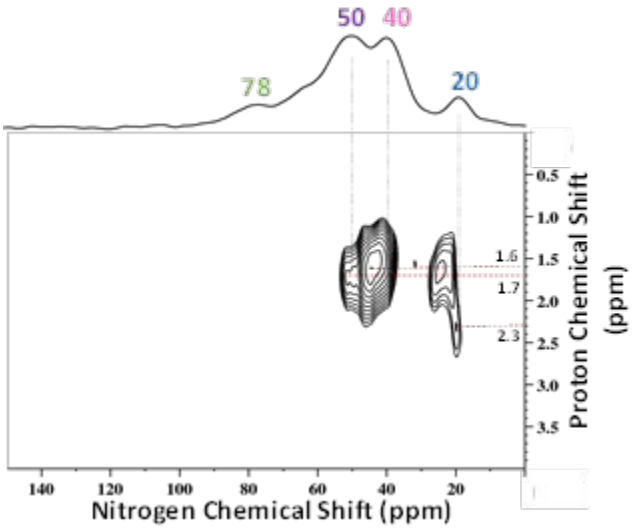


Figure S6. ^{1}H-^{15}N HETCOR DNP NMR spectra of (**3**).

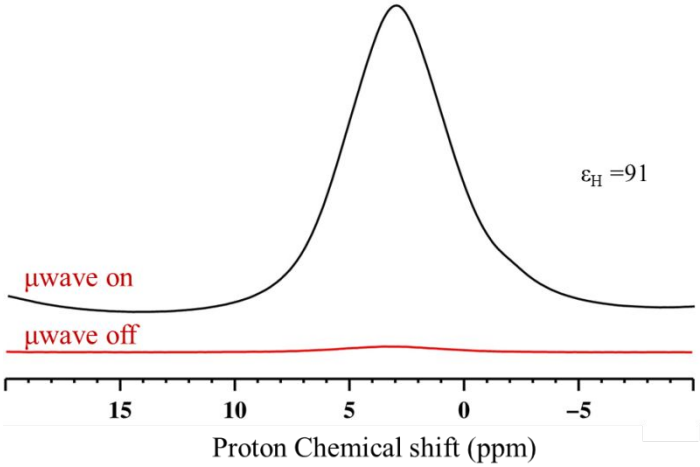


Figure S7. DNP SENS ^{1}H spectra for (**1**) [(≡Si-O-)Ta(NEtMe)$_2$(=N^{t}Bu)].

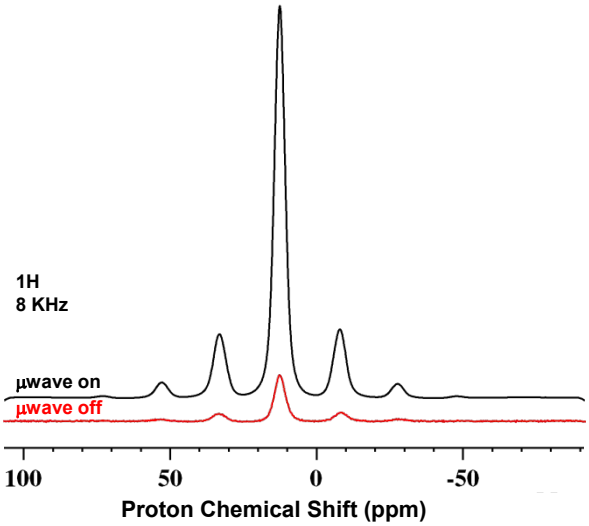


Figure S8. DNP SENS ^{1}H spectra for (**2**) exchange with 1-octyne.

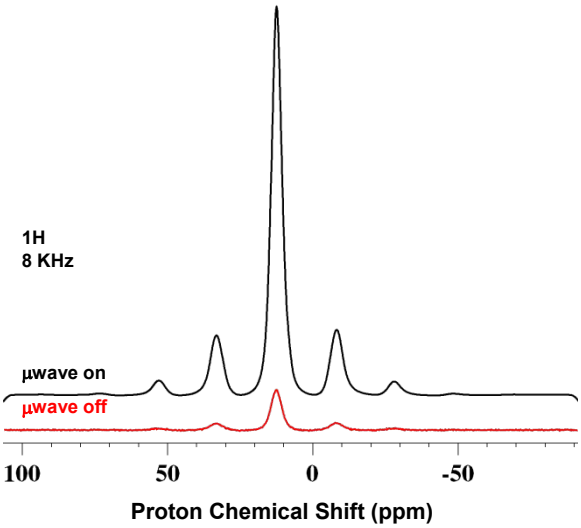
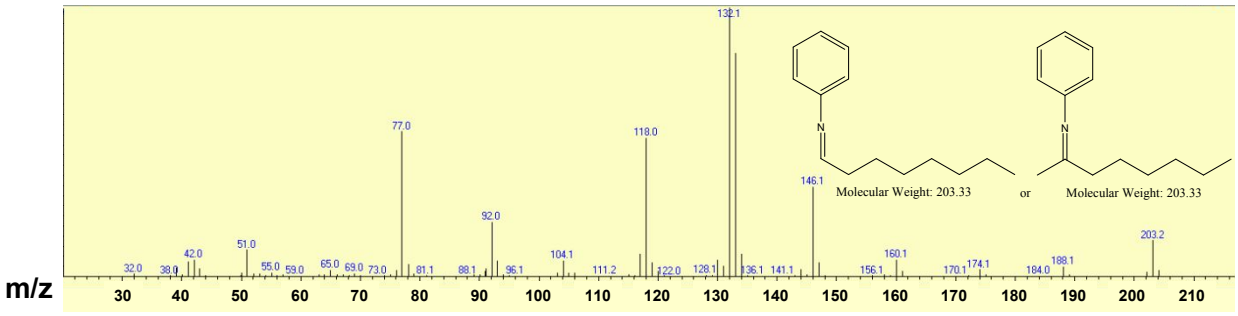


Figure S9. DNP SENS ^{1}H spectra for (**3**) exchange with aniline.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or
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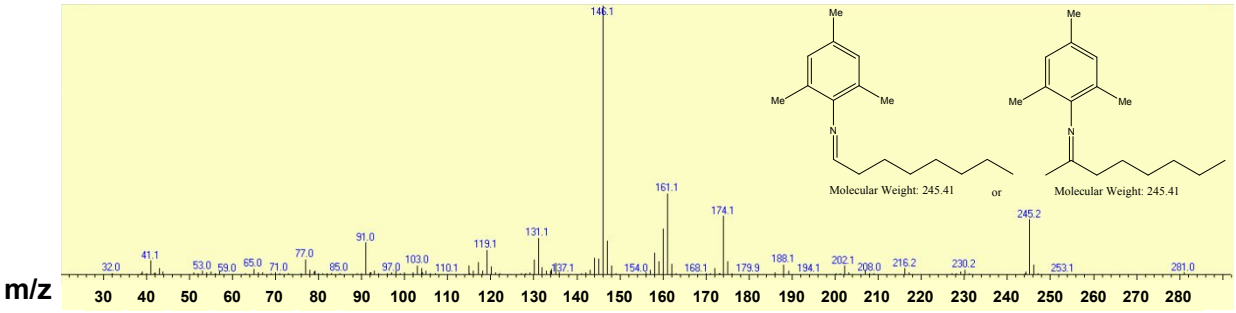
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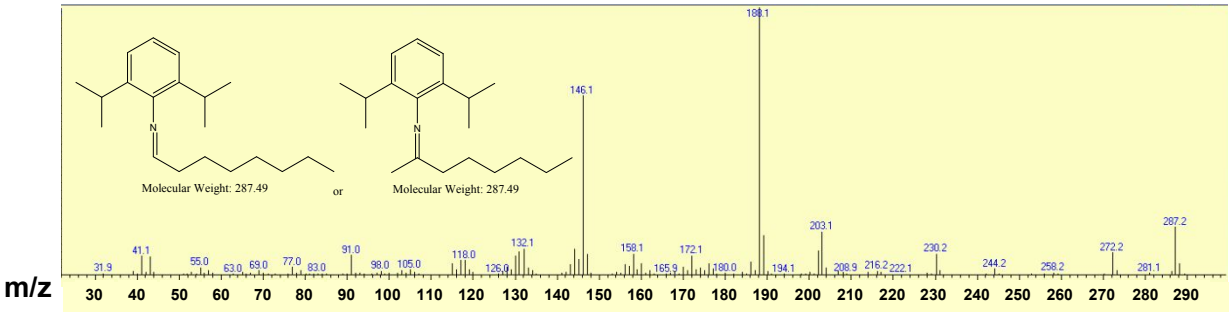
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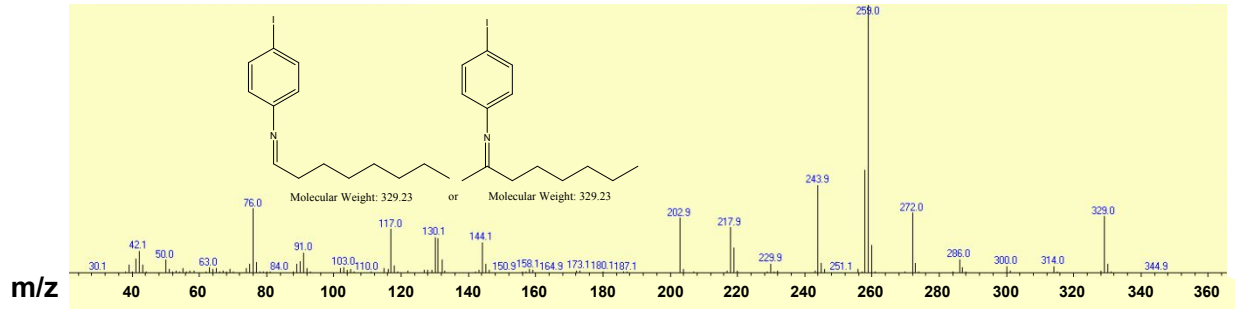
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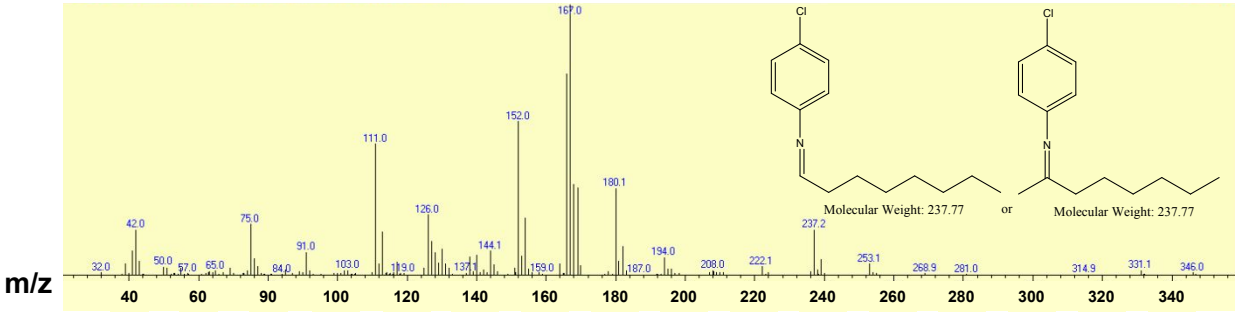
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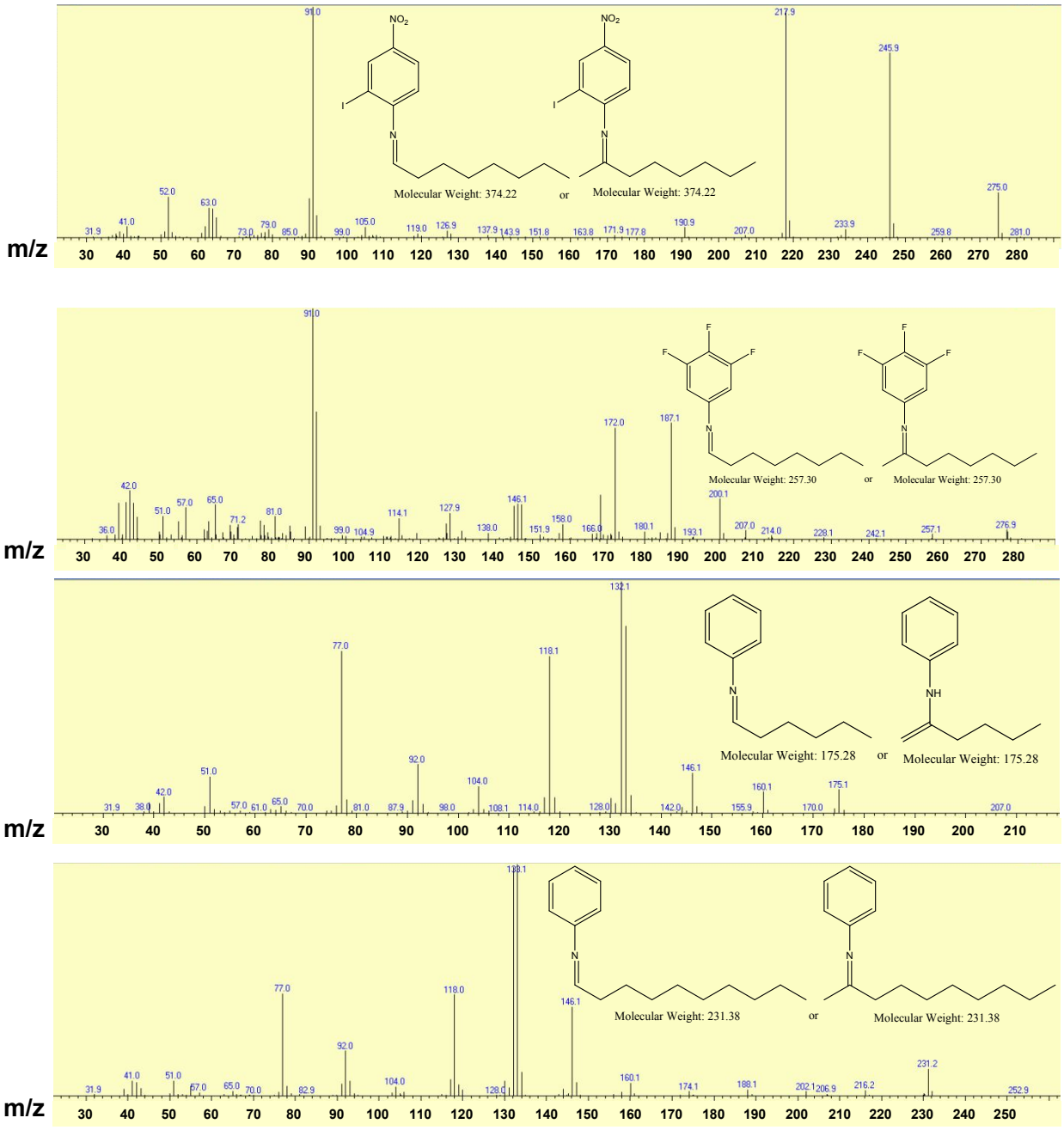

Figure S10. GC-MS of catalysis products.

EXAFS spectroscopy

Experimental Methods. X-ray absorption spectra were recorded at X-ray beamline BM30 at the European Synchrotron Radiation Facility (ESRF). A Si(220) monochromator was used. The sample was loaded into a transmission cell, which was sealed in an argon-filled glovebox with the concentrations of O_2 and of H_2O each being < 1 ppm. The samples were characterized by EXAFS spectroscopy without exposure to air or moisture; the data were collected at room temperature.

Extended X-ray Absorption Fine Structure (EXAFS) Data Analysis. Analysis of the EXAFS data was carried out with the software ATHENA and ARTEMIS of the IFEFFIT package.[1, 2] Three spectra were collected in transmission mode and merged after alignment. Values of the inner potential correction ΔE_0 were fixed for all absorber-backscatterer contributions, and the disorder terms (Debye-Waller factors) were fixed for shells that include the same elements and at similar distances. The number of free parameters used in the fitting is justified within limit according to Nyquist theorem.

Computational details

Geometries were optimized with Gaussian09 package[3] using the BP86 functional of Becke and Perdew.[4-6] The electronic configuration of the system was described with the split-valence SVP basis set for main group atoms (C, H, Si, N and O)[7] and the relativistic Stuttgart-Dresden effective core potential with the associated valence triple-ζ basis set for Ta.[8] All geometries were confirmed as minimum or transition state through frequency calculations. All the thermochemical analysis was corrected at pressure=1354atm, as recommend by Martin and coworkers.[9] The reported free energies were built through single point energy calculations on the BP86 geometries using the M06 functional and the triple- ζ TZVP basis set for main group atoms.[10, 11] Solvent effects were included with the PCM model using toluene as the solvent.[11] To this M06 /TZVP electronic energy in solvent, thermal corrections were added from the gas-phase frequency calculations at the BP86/SVP level.

The geometries for NMR calculations have been re-optimized with the B3PW91[12-13] functional, using the quasi-relativistic SDD effective core potential (ECP) for Ta and triple-ζ basis set for main group atoms. The NMR shieldings were calculated with the ADF package,[14] using the one-parameter hybrid B1PW91[15] functional and a triple-ξ basis set with two polarization functions on all atoms (TZ2P).[16] Relativistic effects were treated by the 2-component zeroth-order regular approximation (ZORA).[17]

The catalyst model[12] used in the calculations is reported in (Figure S11) The Tantalum complex is coordinated to the unsaturated oxygen of the silica cluster.

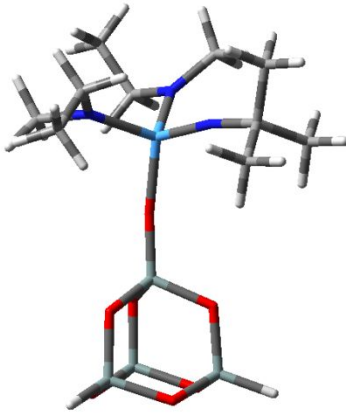

Figure S11. Catalyst model used in the calculations. The silicon atoms are shown in teal, the hydrogen in white, the carbon in grey, the nitrogen in blue, the tantalum in skyblue, and the oxygen atoms in red.

Initiation cycle.

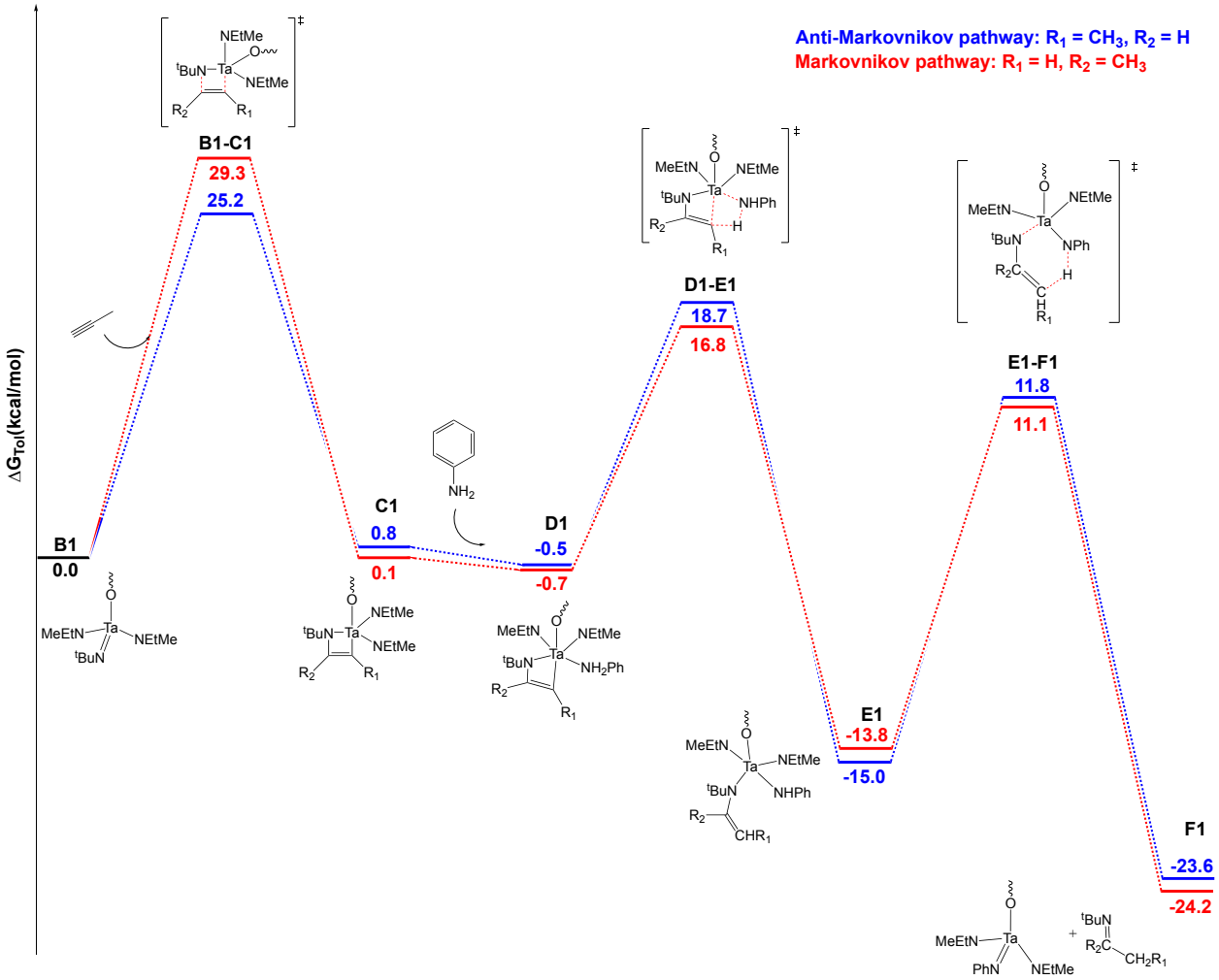

Figure S12. Initiation cycle. Free energies in toluene in kcal/mol.

The initiation cycle follows a similar pattern as the catalytic cycle reported in the main text (Scheme 3). The reaction starts from the *tert*-butyl amino ligand tantalum species **B1** with a {2+2} cycloaddition of the alkyne to the tantanium imido bond leading to the azametallacyclobutene intermediate **C1**. The following aniline coordination and proton transfer steps lead to the release of the *tert*-butyl imido product with the phenyl amino ligand remaining on Ta.

As for the catalytic cycle, the regioselective step is the cycloaddition but, in this case, a clear preference ($\Delta\Delta G^{\neq}$=4 kcal/mol) for the pathway leading to the anti-Markovnikov product (in blue in Figure S12) is observed.

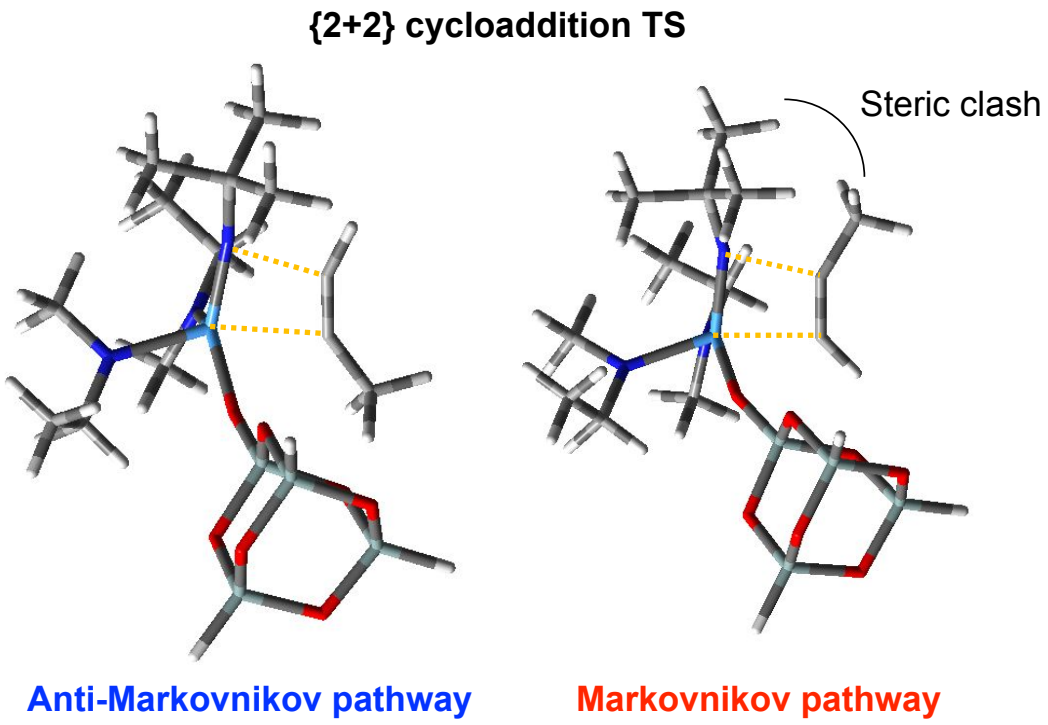

Figure S13. Optimized geometries for the cycloaddition transition state (**B1-C1**). The silicon atoms are shown in teal, the hydrogen in white, the carbon in grey, the nitrogen in blue, the tantalum in skyblue, and the oxygen atoms in red.

The unfavored steric clash between the hindered ^{t}Bu group and the substituent on the alkyne clearly disfavors the cycloaddition TS leading to the Markovnikov product, see (Figure S13).

Alternative reaction pathways investigated.

Alternative reaction pathways investigated are reported in (Figure S14). For each mechanism the preferred regioisomeric pathway is reported.

Both mechanisms start with the alkyne cycloaddition step leading to the azametallacyclobutene intermediate **C1**. In the following step, the "C=C bond" pathway consists in addition of the aniline N-H bond to the C=C bond; instead, the "C-N bond" pathway sees the same aniline N-H bond adding to the C-N^{t}Bu bond. The energies reported in (Figure S14) clearly show that these mechanisms can be ruled out for the high kinetic barriers involved after **C1** formation.

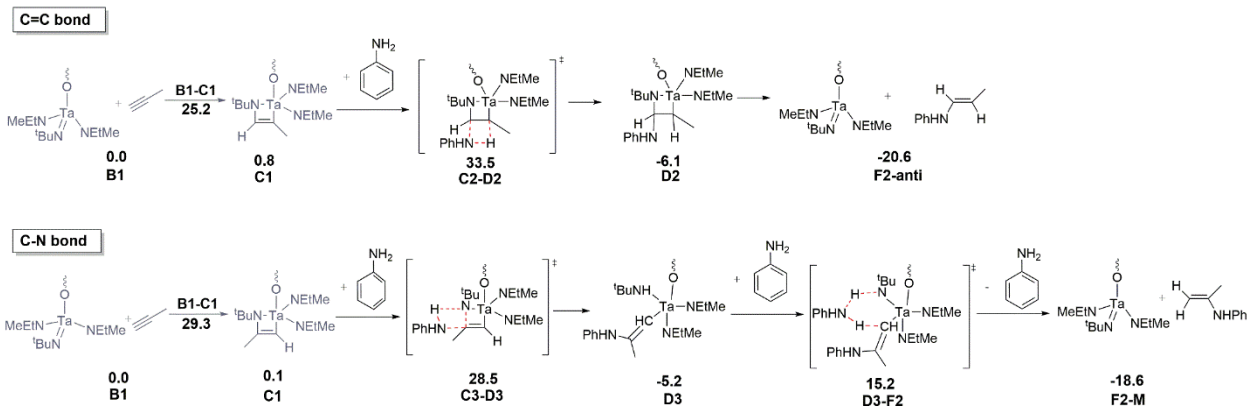

Figure S14. Alternative reaction mechanisms explored. Free energies in toluene in kcal/mol.

Aniline initiated pathway.

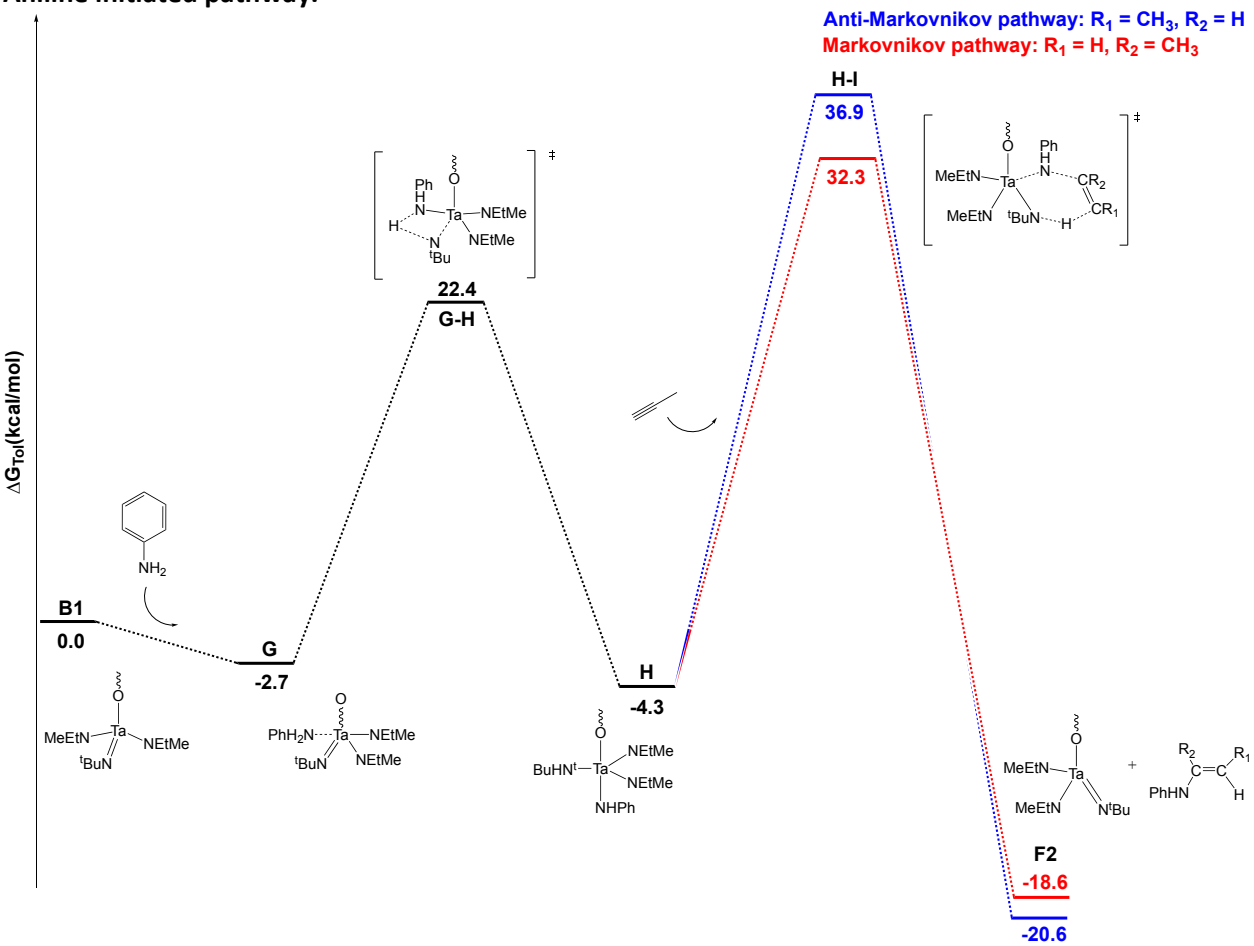

Figure S15. Aniline initiated reaction pathway. Free energies in toluene in kcal/mol.

As reported in (Figure S15), this alternative reaction pathway implies at first the coordination of aniline to Ta leading to the formation of **G**, located at -2.7 kcal/mol. The following amine N-H bond addition to the metal imido double bond occurring with an energy barrier of almost 25.0 kcal/mol is calculated to be slightly exergonic by 1.6 kcal/mol with respect to **G**. The accessible kinetic barrier and the overall energy

gain of almost 4.0 kcal/mol in the formation of **H** (isolated intermediate **3**) indicates that this intermediate is likely to form, in agreement with the experimental NMR results (see Figure 7) obtained for the catalyst-aniline mixture.
However, the high barrier involved for the following alkyne addition step makes this pathway unfeasible (36.6 kcal/mol for Markovnikov addition and 41.2 kcal/mol for Anti-Markovnikov addition).

DFT NMR calculations.

Table S2. Experimental ^{15}N DNP-SENS signals and theoretical magnetic shieldings (σ) for **1**

^{15}N DNP-SENS	N DFT σ
163	-121.8
43	78.6
14	79.2

Table S3. Experimental ^{15}N DNP-SENS signals and theoretical magnetic shieldings (σ) for **2** anti-Markovnikov and Markovnikov

^{15}N DNP-SENS	N DFT σ	
	Anti-Markovnikov	Markovnikov
60	27.6	26.9
38	36.9	30.8
22	46.3	58.9

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Cartesian coordinates and internal energies in gas phase (A.U.)

Propyne
E = -116.563283765 A.U.

C	0.000000	0.000000	1.437296
H	0.000000	0.000000	2.518510
C	0.000000	0.000000	0.214042
C	0.000000	0.000000	-1.246209
H	0.000000	1.035401	-1.649761
H	0.896684	-0.517701	-1.649761
H	-0.896684	-0.517701	-1.649761

NH_2Ph
E = -287.398207405 A.U.

C	0.223175	1.217308	-0.003169
C	-1.179242	1.210673	0.003011
C	-1.895788	-0.000079	0.005813
C	-1.179179	-1.210753	0.002937
C	0.223250	-1.217196	-0.003083
C	0.952456	0.000037	-0.007644
H	0.770017	2.175141	-0.008231
H	-1.720020	2.171139	0.007783
H	-2.996536	0.000056	0.011944
H	-1.719671	-2.171374	0.007717
H	0.770257	-2.174949	-0.008022
N	2.343732	0.000030	-0.070536
H	2.810911	0.850969	0.247960
H	2.810889	-0.851127	0.247416

B1
E = -2303.51668598 A.U.

O	2.541507	0.106538	1.498725
Si	4.209066	0.331777	1.614631
O	4.593546	1.608106	0.573873
Si	4.111624	1.397919	-1.033885
O	2.448785	1.111670	-1.000066
Si	1.928955	-0.190522	-0.051466
O	2.780802	-1.537366	-0.623002
Si	4.462985	-1.410276	-0.636495
O	4.832853	-0.040304	-1.557259
O	0.327814	-0.418221	-0.068115
O	4.926554	-1.048106	0.949868
H	4.473165	2.550471	-1.885501
H	5.120762	-2.629868	-1.150962
H	4.653963	0.583206	3.001548
Ta	-1.655962	-0.263347	-0.044655
N	-2.294495	1.384648	-0.396537
C	-2.567540	2.769296	-0.719828
C	-2.006771	3.085106	-2.129142
H	-2.208273	4.140984	-2.408796
H	-0.910521	2.918516	-2.158910
H	-2.475201	2.430283	-2.892680
C	-4.099191	3.000345	-0.701728
H	-4.516957	2.774263	0.300904

H	-4.344526	4.054243	-0.951381
H	-4.603125	2.341533	-1.438426
C	-1.887548	3.686360	0.326994
H	-2.275049	3.473179	1.344461
H	-0.790473	3.522164	0.333752
H	-2.078630	4.756718	0.100118
N	-2.346437	-0.724305	1.792901
N	-2.440442	-1.462953	-1.464073
C	-3.195901	0.067450	2.690604
H	-4.051672	-0.566036	3.035832
H	-3.634355	0.896350	2.100125
C	-2.466084	0.643492	3.914853
H	-3.170263	1.227525	4.544298
H	-2.031140	-0.149644	4.558039
H	-1.641800	1.317387	3.601249
C	-2.061872	-2.882537	-1.408088
H	-1.611856	-3.178846	-2.388610
H	-1.233297	-3.003002	-0.669239
C	-3.195162	-3.857523	-1.049019
H	-2.812853	-4.899228	-1.012596
H	-3.633657	-3.613210	-0.059217
H	-4.012624	-3.832087	-1.798336
C	-1.999898	-2.040663	2.328559
H	-1.402436	-1.974039	3.267471
H	-2.909088	-2.652694	2.547291
H	-1.379441	-2.617634	1.607522
C	-3.338203	-1.133329	-2.565200
H	-3.519400	-0.042783	-2.589109
H	-2.900007	-1.437717	-3.547166
H	-4.329078	-1.638500	-2.477092

B1-C1-anti

E = -2420.05671740 A.U.

O	-2.951577	-1.539647	-0.290478
Si	-4.619815	-1.338749	-0.398527
O	-4.883511	-0.063686	-1.479190
Si	-4.108025	1.385482	-1.081043
O	-2.467195	1.032020	-0.938439
Si	-2.035629	-0.184524	0.165397
O	-2.715176	0.309899	1.646812
Si	-4.372325	0.623522	1.658903
O	-4.647862	1.794502	0.469683
O	-0.461146	-0.482502	0.241274
O	-5.134085	-0.786054	1.115993
H	-4.377587	2.454141	-2.066758
H	-4.860122	1.048290	2.988714
H	-5.319939	-2.574295	-0.809681
Ta	1.576138	-0.279224	0.176468
N	3.085584	-1.251758	1.131047
N	1.441045	-1.623549	-1.369657
C	4.281817	-0.631331	1.710168
H	4.422658	-1.009845	2.753860
H	4.107909	0.461073	1.800309
C	5.569778	-0.874435	0.906914
H	6.441332	-0.410891	1.416132
H	5.790688	-1.956093	0.790686
H	5.487430	-0.432026	-0.107522
C	0.344048	-2.507739	-1.771632
H	0.735567	-3.551482	-1.878683
H	-0.409995	-2.531861	-0.961073
C	-0.356702	-2.098942	-3.079324
H	-1.163169	-2.820762	-3.327404
H	-0.816557	-1.094295	-2.978370
H	0.341831	-2.072493	-3.941949
C	2.982556	-2.679876	1.420373
H	3.877099	-3.245856	1.066253
H	2.884323	-2.876362	2.516251
H	2.098186	-3.120265	0.915168
C	2.642014	-1.826479	-2.176967
H	3.460522	-1.153213	-1.849710
H	3.020722	-2.876269	-2.091936
H	2.467935	-1.626428	-3.260894
N	2.327952	1.326945	-0.388476
C	1.652434	1.795940	1.545619
C	1.093737	0.823772	2.156760
H	2.018820	2.819994	1.486921
C	0.382324	0.366988	3.377072
H	0.831622	-0.566772	3.774481
H	-0.672963	0.138060	3.116659
C	2.686506	2.499333	-1.167963
C	1.485162	3.468095	-1.302187
H	1.168725	3.872291	-0.319218
H	1.748204	4.329570	-1.951192
H	0.615336	2.943608	-1.746826
C	3.906376	3.222036	-0.543089
H	4.227896	4.067376	-1.186442
H	3.676690	3.639336	0.459061
H	4.759008	2.521503	-0.433679
C	3.075806	1.981436	-2.576747
H	2.229638	1.430548	-3.034503
H	3.343402	2.832619	-3.237226
H	3.946352	1.297549	-2.517487
H	0.388679	1.135870	4.178078

C1-anti

E = -2420.10091390 A.U.

O	-2.500857	0.446455	-1.289680
Si	-4.177744	0.335477	-1.440861
O	-4.834719	1.367340	-0.273978
Si	-4.340003	1.068086	1.316273
O	-2.656844	1.138175	1.313240
Si	-1.845430	0.103838	0.241330

O	-2.414370	-1.450773	0.620760
Si	-4.084708	-1.679706	0.579846
O	-4.752236	-0.541388	1.637364
O	-0.245173	0.268450	0.307676
O	-4.593027	-1.235606	-0.971928
H	-4.949529	2.007459	2.281138
H	-4.477052	-3.063222	0.923621
H	-4.649288	0.657872	-2.804366
Ta	1.711136	-0.280058	0.040089
N	1.320905	-2.021812	-0.907929
N	2.387839	-0.837905	1.818477
C	1.163059	-2.114891	-2.365577
H	1.803028	-2.950554	-2.745196
H	1.576815	-1.183409	-2.811729
C	-0.278759	-2.316589	-2.860402
H	-0.293696	-2.356427	-3.969842
H	-0.720790	-3.265198	-2.492062
H	-0.936836	-1.483430	-2.538822
C	3.544188	-1.727332	2.011623
H	3.280203	-2.491559	2.784142
H	3.717407	-2.281939	1.064295
C	4.837397	-1.004042	2.412280
H	5.669146	-1.731905	2.515432
H	5.115081	-0.260030	1.637447
H	4.737274	-0.474654	3.382170
C	1.041990	-3.279626	-0.214353
H	-0.024179	-3.587906	-0.314391
H	1.671811	-4.108193	-0.621054
H	1.250093	-3.182857	0.869416
C	1.831487	-0.278023	3.052760
H	0.933162	0.332367	2.830188
H	1.528966	-1.091337	3.754154
H	2.559857	0.377499	3.581430
N	2.092062	1.842273	-0.297618
C	3.045265	1.488924	-1.219086
C	3.387111	0.133590	-1.178901
H	3.449235	2.239448	-1.942525
C	4.425817	-0.504098	-2.056727
H	4.079453	-1.473870	-2.475845
H	5.355404	-0.737245	-1.488175
C	1.400199	3.153491	-0.353448
C	2.443785	4.288882	-0.494582
H	2.985825	4.250785	-1.461781
H	1.936920	5.274463	-0.442294
H	3.191401	4.239024	0.324050
C	0.412782	3.202986	-1.545130
H	-0.114480	4.179613	-1.584652
H	0.947925	3.069145	-2.509301
H	-0.350173	2.403623	-1.458734
C	0.641220	3.351578	0.974117
H	1.347250	3.324063	1.830243
H	0.124668	4.333772	0.984600
H	-0.116404	2.558677	1.119112
H	4.727863	0.144192	-2.912966

D1-anti

E = -2707.50697935 A.U.

O	-2.593479	0.413733	-1.391026
Si	-4.257227	0.264437	-1.602579
O	-4.973754	0.788861	-0.161400
Si	-4.452992	-0.013388	1.233066
O	-2.775220	0.155118	1.284486
Si	-1.903071	-0.394551	-0.068674
O	-2.381585	-2.017134	-0.255613
Si	-4.034551	-2.316834	-0.401424
O	-4.762521	-1.655618	0.974529
O	-0.311126	-0.221411	0.049319
O	-4.578812	-1.393893	-1.709841
H	-5.111595	0.497390	2.454275
H	-4.340377	-3.754384	-0.562835
H	-4.755428	1.008730	-2.778640
Ta	1.715258	-0.236302	-0.246186
N	1.941952	-0.499882	2.028157
C	1.500880	-1.344992	3.164045
C	1.921886	-0.682518	4.499082
H	1.586990	-1.291609	5.364713
H	3.023965	-0.573699	4.575373
H	1.470682	0.327432	4.593640
C	-0.034384	-1.457471	3.120238
H	-0.369916	-1.972595	2.198340
H	-0.405792	-2.035319	3.992013
H	-0.511387	-0.457265	3.139467
C	2.113312	-2.764504	3.067994
H	1.838392	-3.235484	2.101879
H	3.221122	-2.736174	3.133250
H	1.743799	-3.414646	3.888910
N	1.691767	0.680644	-2.055581
N	2.092004	-2.117908	-0.833238
C	2.458683	0.225658	-3.223999
H	1.755501	0.099129	-4.086120
H	2.871600	-0.780705	-3.006206
C	3.603214	1.160552	-3.648359
H	4.136526	0.739949	-4.526881
H	3.234661	2.166762	-3.936396
H	4.337370	1.287519	-2.825975
C	0.993339	-3.055924	-1.149406
H	1.198091	-4.022982	-0.628053
H	0.049639	-2.666127	-0.718639
C	0.787233	-3.314273	-2.650219
H	-0.029881	-4.050646	-2.799219
H	0.503356	-2.380254	-3.177135
H	1.695754	-3.724648	-3.138169

C	0.895800	1.874879	-2.338287
H	1.506251	2.805373	-2.401751
H	0.364619	1.758744	-3.313119
H	0.124890	2.029604	-1.560231
C	3.410333	-2.735722	-0.970708
H	4.207443	-2.000651	-0.752602
H	3.522977	-3.589339	-0.259364
H	3.575790	-3.139955	-1.997006
C	3.262997	-0.279894	1.800536
C	3.596595	0.257839	0.543358
H	4.032295	-0.568447	2.563117
N	1.356434	2.128572	0.942678
H	2.331973	2.445019	0.925674
C	0.432846	3.200807	0.809657
C	-0.915365	3.049937	1.203696
C	0.847789	4.426502	0.240342
C	-1.822334	4.107707	1.026786
H	-1.258220	2.100989	1.642368
C	-0.066433	5.477363	0.067556
H	1.899676	4.554320	-0.065377
C	-1.408653	5.325430	0.458609
H	-2.870501	3.971315	1.337327
H	0.277737	6.426556	-0.373699
H	-2.125098	6.150571	0.323981
C	4.968454	0.776239	0.207933
H	5.722242	0.507071	0.985305
H	5.348987	0.396266	-0.766299
H	4.988491	1.888810	0.121381
H	1.223025	1.545235	1.787955

D1-E1-anti

E = -2707.48155521 A.U.

O	-2.573578	-0.361155	-1.297293
Si	-4.251611	-0.485394	-1.439272
O	-4.909943	0.516088	-0.247625
Si	-4.403957	0.201446	1.333548
O	-2.717479	0.290749	1.326277
Si	-1.920130	-0.711366	0.223361
O	-2.448897	-2.279452	0.581271
Si	-4.118169	-2.532769	0.549848
O	-4.789137	-1.418938	1.631674
O	-0.305145	-0.576826	0.276265
O	-4.643010	-2.069357	-0.990111
H	-5.015649	1.116831	2.319157
H	-4.486486	-3.926722	0.875131
H	-4.735702	-0.149910	-2.794332
Ta	1.609403	-0.238886	-0.082659
N	2.146167	1.057072	1.517248
C	1.808826	1.444675	2.915551
C	1.589264	2.977453	2.967477
H	1.280763	3.290812	3.986647
H	2.520296	3.525074	2.712131
H	0.805831	3.294528	2.251723
C	0.518590	0.712944	3.328072
H	0.654769	-0.387267	3.283252
H	0.239365	0.980682	4.367824
H	-0.331361	0.973650	2.667101
C	2.937788	1.076500	3.911820
H	3.067204	-0.020362	3.994331
H	3.911441	1.523970	3.623800
H	2.686367	1.462103	4.921684
N	1.842876	-1.122621	-1.922856
N	2.447926	-1.890633	0.779914
C	3.052110	-1.774640	-2.436159
H	2.811275	-2.843773	-2.669261
H	3.803050	-1.790486	-1.619868
C	3.670992	-1.136155	-3.690354
H	4.615282	-1.656912	-3.953795
H	3.001773	-1.206827	-4.572314
H	3.906182	-0.066276	-3.520134
C	1.956097	-3.243204	0.453970
H	1.282355	-3.579629	1.282161
H	1.315437	-3.162888	-0.447368
C	3.023604	-4.326119	0.221823
H	2.529334	-5.263225	-0.109369
H	3.746420	-4.028462	-0.565336
H	3.596594	-4.568907	1.139968
C	0.762503	-1.096648	-2.910297
H	0.962510	-0.407665	-3.767876
H	0.619605	-2.114516	-3.348054
H	-0.198436	-0.789318	-2.455051
C	3.396395	-1.902974	1.889165
H	3.698074	-0.874927	2.150923
H	2.958740	-2.382840	2.800221
H	4.323959	-2.466441	1.637804
C	3.279538	1.560486	0.892276
C	3.298826	1.362238	-0.474464
H	4.107891	2.001678	1.497337
N	0.830784	1.618299	-1.381176
H	1.036585	1.441292	-2.373668
C	-0.189458	2.586107	-1.282732
C	-0.797785	2.892795	-0.041090
C	-0.639068	3.288302	-2.432789
C	-1.805868	3.865180	0.045263
H	-0.479516	2.343059	0.854902
C	-1.649735	4.256378	-2.340729
H	-0.181253	3.063328	-3.411388
C	-2.240732	4.557058	-1.099609
H	-2.262883	4.079216	1.025102
H	-1.977768	4.783631	-3.251455
H	-3.032483	5.318752	-1.027050
C	4.531557	1.586689	-1.315042

H	5.235101	2.300914	-0.826685
H	5.105017	0.649747	-1.496817
H	4.289328	2.005295	-2.316270
H	2.021267	1.798525	-0.984275

E1-anti

E = -2707.52831386 A.U.

O	-2.847944	-0.054414	-1.290689
Si	-4.516454	-0.227620	-1.464669
O	-5.229779	0.759310	-0.291538
Si	-4.746526	0.462472	1.301066
O	-3.065068	0.601098	1.325325
Si	-2.205948	-0.377305	0.242907
O	-2.705744	-1.958837	0.600117
Si	-4.365679	-2.261711	0.534046
O	-5.093136	-1.166793	1.598046
O	-0.610021	-0.151477	0.326554
O	-4.873002	-1.820899	-1.017887
H	-5.404649	1.364121	2.269599
H	-4.697427	-3.665658	0.856917
H	-4.984717	0.090143	-2.829920
Ta	1.345049	-0.209362	-0.059521
N	2.936500	0.273829	1.134368
C	2.878851	1.204333	2.318553
C	3.421993	2.583551	1.881002
H	3.413191	3.298752	2.730376
H	4.467176	2.495046	1.518032
H	2.797979	3.003483	1.067076
C	1.411778	1.336234	2.773536
H	0.995694	0.357283	3.092834
H	1.334912	2.030460	3.634947
H	0.773037	1.756474	1.969996
C	3.720370	0.672687	3.501088
H	3.398756	-0.343316	3.811853
H	4.803126	0.639471	3.264851
H	3.593379	1.346644	4.372800
N	1.710974	-0.793741	-1.944478
N	1.393616	-2.151837	0.670945
C	2.630971	-1.853444	-2.379596
H	2.033795	-2.739062	-2.714172
H	3.215942	-2.180542	-1.497844
C	3.583939	-1.449161	-3.514682
H	4.277450	-2.286475	-3.738324
H	3.044243	-1.211144	-4.453940
H	4.193356	-0.563801	-3.238746
C	0.523368	-3.157127	0.035418
H	-0.416996	-3.259463	0.631435
H	0.204918	-2.765368	-0.954318
C	1.144802	-4.550491	-0.164190
H	0.444846	-5.192487	-0.738785
H	2.098751	-4.494271	-0.729159
H	1.347106	-5.067960	0.795841
C	0.848601	-0.293037	-3.023791
H	1.409151	0.342524	-3.747878
H	0.402886	-1.143813	-3.591934
H	0.019267	0.318024	-2.620845
C	1.840510	-2.593527	1.986600
H	2.414904	-1.793956	2.489172
H	0.975648	-2.858573	2.645666
H	2.492300	-3.496720	1.934529
C	4.179157	-0.333578	0.857607
C	4.869815	-0.211511	-0.305236
H	4.611676	-0.975672	1.653981
N	1.112850	1.812296	-0.684865
H	1.972072	2.034737	-1.214333
C	0.291370	2.936631	-0.722112
C	-0.884787	3.049684	0.072521
C	0.613106	4.040972	-1.566779
C	-1.693436	4.193796	0.003149
H	-1.160116	2.235279	0.755029
C	-0.199940	5.180368	-1.625952
H	1.523665	3.985124	-2.188870
C	-1.366905	5.268564	-0.843858
H	-2.597379	4.243744	0.632072
H	0.082617	6.010801	-2.293800
H	-2.007320	6.162992	-0.890367
C	6.149466	-0.935665	-0.611147
H	6.487935	-1.552853	0.246478
H	6.043848	-1.609981	-1.490375
H	6.964990	-0.223602	-0.866708
H	4.467680	0.467922	-1.079024

E1-F1-anti

E = -2707.49484896 A.U.

O	-2.786629	1.576893	0.928024
Si	-4.445859	1.886929	0.893546
O	-5.161727	0.785170	1.957091
Si	-4.825018	-0.842928	1.643533
O	-3.146226	-0.989711	1.630709
Si	-2.293269	-0.001977	0.553597
O	-2.968090	-0.319465	-0.978110
Si	-4.640304	-0.130856	-1.118653
O	-5.337528	-1.125752	0.055425
O	-0.698829	-0.258568	0.591513
O	-4.976421	1.460053	-0.655914
H	-5.470902	-1.750091	2.614865
H	-5.132686	-0.436498	-2.478868
H	-4.767120	3.289443	1.231486
Ta	1.026860	0.012007	-0.454091
N	1.419360	-2.301764	-0.029368
C	0.902796	-3.129889	1.124986
C	0.924417	-2.362887	2.467032

H	0.500163	-2.999162	3.272192
H	1.955216	-2.083936	2.763820
H	0.315435	-1.441070	2.403484
C	-0.550882	-3.506302	0.758563
H	-0.574128	-4.080305	-0.190799
H	-0.998850	-4.134783	1.555975
H	-1.179298	-2.607254	0.641581
C	1.683317	-4.460152	1.262987
H	1.743232	-4.983524	0.285979
H	2.713511	-4.333084	1.644711
H	1.147081	-5.123519	1.972251
N	1.331119	-0.277656	-2.407681
N	0.602075	1.989067	-0.651302
C	0.160008	-0.804402	-3.132931
H	-0.084016	-0.115767	-3.979454
H	-0.726194	-0.763473	-2.454510
C	0.317235	-2.242758	-3.646901
H	-0.616453	-2.571187	-4.148602
H	1.139761	-2.334532	-4.385875
H	0.521359	-2.933030	-2.802884
C	0.424145	2.780481	-1.871618
H	1.032613	3.716557	-1.791282
H	0.837921	2.203866	-2.723417
C	-1.034135	3.159362	-2.182499
H	-1.087266	3.741422	-3.126844
H	-1.663656	2.252557	-2.295479
H	-1.482349	3.782740	-1.382222
C	2.511822	-0.047112	-3.230641
H	2.887740	-0.984035	-3.704159
H	2.289093	0.668485	-4.059107
H	3.331934	0.378626	-2.620589
C	0.385215	2.772255	0.569289
H	0.664542	2.187625	1.469759
H	1.013829	3.693343	0.567125
H	-0.680768	3.068817	0.689722
C	2.709031	-2.351018	-0.367781
C	3.853028	-2.253523	0.486683
H	2.915888	-2.018159	-1.409575
N	2.695709	0.252864	0.487782
H	3.421401	-0.967765	0.601427
C	3.500209	1.278487	0.998948
C	4.075649	1.154541	2.294082
C	3.811130	2.444778	0.246770
C	4.917190	2.151912	2.810775
H	3.837793	0.260627	2.892204
C	4.650458	3.438782	0.771767
H	3.377724	2.552499	-0.759439
C	5.210870	3.302047	2.056068
H	5.346390	2.029549	3.818794
H	4.876355	4.331716	0.165723
H	5.871853	4.083460	2.462657
C	5.255086	-2.350673	-0.087499
H	5.290371	-1.975218	-1.132569
H	5.975202	-1.750254	0.505975
H	5.632768	-3.396908	-0.098861
H	3.752254	-2.600750	1.530741

F1-anti

E = -330.269069042 A.U.

C	1.004221	0.786078	0.000016
H	0.649492	1.847911	0.000124
C	2.506587	0.620849	0.000007
C	3.000860	-0.826259	-0.000023
H	2.627778	-1.372928	-0.889307
H	4.109339	-0.868432	0.000005
H	2.627816	-1.372968	0.889271
H	2.906425	1.179612	0.879608
N	0.212335	-0.216593	-0.000040
H	2.906434	1.179548	-0.879644
C	-1.256316	-0.068796	0.000009
C	-1.755199	-0.809708	1.262857
H	-1.406655	-0.296251	2.183214
H	-2.864305	-0.849978	1.286485
H	-1.360754	-1.845654	1.280489
C	-1.755259	-0.809445	-1.262987
H	-2.864377	-0.849303	-1.286650
H	-1.406467	-0.295985	-2.183248
H	-1.361135	-1.845509	-1.280703
C	-1.786057	1.380787	0.000143
H	-1.453672	1.942292	-0.898538
H	-2.895432	1.380742	-0.000017
H	-1.453844	1.942020	0.899061

B1-C1-M

E = -2420.05006016 A.U.

O	2.995031	-1.548965	0.152666
Si	4.665537	-1.416431	-0.004522
O	5.177926	-0.326583	1.183686
Si	4.426354	1.188616	1.138247
O	2.768146	0.909827	1.232800
Si	2.091338	-0.112684	0.059163
O	2.539654	0.576806	-1.431893
Si	4.184950	0.840593	-1.683696
O	4.720101	1.812987	-0.407714
O	0.514311	-0.357030	0.240200
O	4.949803	-0.654839	-1.489608
H	4.915857	2.087930	2.205044
H	4.466289	1.445688	-3.003809
H	5.355816	-2.720043	0.096173
Ta	-1.476300	-0.285515	-0.224244
N	-2.729328	-1.073816	-1.616166
N	-1.569068	-1.921366	1.026973

C	-3.870377	-0.412812	-2.254489
H	-3.693343	-0.354793	-3.359017
H	-3.914951	0.633481	-1.889581
C	-5.227298	-1.090850	-1.999783
H	-6.036082	-0.548588	-2.533707
H	-5.244555	-2.141460	-2.356813
H	-5.472850	-1.093984	-0.917515
C	-0.495202	-2.720247	1.628523
H	-0.703525	-3.805097	1.446555
H	0.455240	-2.486166	1.112859
C	-0.305043	-2.492897	3.138349
H	0.504729	-3.144668	3.529889
H	-0.022596	-1.438825	3.340092
H	-1.222884	-2.721631	3.719973
C	-2.341748	-2.323163	-2.265876
H	-3.159368	-3.082053	-2.248817
H	-2.059928	-2.165056	-3.336219
H	-1.470003	-2.779057	-1.749974
C	-2.888191	-2.467346	1.344596
H	-3.691378	-1.886489	0.848574
H	-2.984104	-3.529394	1.004319
H	-3.101239	-2.456091	2.440065
N	-2.399117	1.187653	0.471006
C	-1.407018	2.064052	-1.243369
C	-0.692949	1.145597	-1.788093
C	-2.905303	1.975276	1.593824
C	-1.794883	2.857623	2.214357
H	-1.404202	3.604192	1.494854
H	-2.184318	3.410787	3.094716
H	-0.942308	2.230617	2.545153
C	-4.136186	2.826693	1.195671
H	-4.592776	3.281841	2.099108
H	-3.874613	3.652294	0.507421
H	-4.901505	2.192142	0.703815
C	-3.359995	0.943757	2.662237
H	-2.515376	0.287823	2.953460
H	-3.730676	1.471166	3.566213
H	-4.176688	0.305662	2.269430
C	-1.942942	3.437626	-1.327257
H	-1.740014	4.041722	-0.421815
H	-1.447399	3.932503	-2.190181
H	-3.036938	3.442446	-1.507584
H	0.006708	1.069619	-2.627477

C1-M

E = -2420.09950132 A.U.

O	2.518681	0.565894	1.310425
Si	4.202090	0.544881	1.419140
O	4.771915	1.622203	0.247277
Si	4.253688	1.312147	-1.333002
O	2.569021	1.290434	-1.286752
Si	1.847272	0.201955	-0.205730
O	2.487552	-1.315344	-0.619411
Si	4.168393	-1.452297	-0.621480
O	4.744188	-0.268663	-1.683325
O	0.236714	0.280853	-0.234723
O	4.690595	-0.996136	0.921701
H	4.785495	2.293411	-2.302063
H	4.627182	-2.808564	-0.990362
H	4.689683	0.879519	2.773907
Ta	-1.635280	-0.474044	0.020749
N	-1.076744	-2.222673	0.884525
N	-2.513275	-1.149388	-1.631883
C	-0.846532	-2.403950	2.324269
H	-1.434758	-3.290829	2.671937
H	-1.273961	-1.523342	2.849686
C	0.624224	-2.577839	2.737682
H	0.693610	-2.702896	3.838812
H	1.091325	-3.471982	2.275468
H	1.228314	-1.691188	2.456185
C	-3.668957	-2.059763	-1.632287
H	-3.494751	-2.858679	-2.395377
H	-3.705459	-2.562418	-0.642578
C	-5.015066	-1.370773	-1.894452
H	-5.837832	-2.115864	-1.879112
H	-5.215465	-0.613084	-1.109053
H	-5.041978	-0.866266	-2.882590
C	-0.816036	-3.442175	0.117278
H	0.258826	-3.733472	0.151907
H	-1.409063	-4.302223	0.515124
H	-1.078096	-3.299401	-0.949076
C	-2.088701	-0.695263	-2.956331
H	-1.191593	-0.046254	-2.879867
H	-1.828239	-1.560489	-3.611510
H	-2.879604	-0.103263	-3.471346
N	-2.299097	1.624631	0.307404
C	-3.066072	1.239860	1.380112
C	-3.083822	-0.166737	1.477476
C	-1.819895	2.988918	-0.015926
C	-2.985529	4.010904	-0.077387
H	-3.389997	4.271906	0.918508
H	-2.626314	4.954138	-0.539625
H	-3.815611	3.620536	-0.702373
C	-0.749683	3.460207	1.000192
H	-0.366333	4.467826	0.733005
H	-1.162078	3.520567	2.028618
H	0.105711	2.756010	1.015462
C	-1.192103	2.931195	-1.427449
H	-1.948348	2.602961	-2.171235
H	-0.824236	3.933161	-1.730410
H	-0.337908	2.228870	-1.453239
C	-3.809195	2.159336	2.329625

H	-4.644770	2.674949	1.811692
H	-4.234658	1.566121	3.161612
H	-3.154705	2.945552	2.758283
H	-3.630450	-0.699131	2.271262

D1_M

E = -2707.50470521 A.U.

O	-2.693312	0.252822	-1.281471
Si	-4.352921	-0.018362	-1.374213
O	-5.005819	0.454904	0.113836
Si	-4.333155	-0.304199	1.466469
O	-2.674476	-0.012617	1.402051
Si	-1.858021	-0.495391	-0.009450
O	-2.226170	-2.151480	-0.164654
Si	-3.858226	-2.572476	-0.197884
O	-4.539252	-1.965480	1.226387
O	-0.276461	-0.207626	0.007724
O	-4.558172	-1.696102	-1.463154
H	-4.942378	0.159613	2.731436
H	-4.066347	-4.029377	-0.341794
H	-4.985918	0.682967	-2.511112
Ta	1.721178	-0.095121	-0.412838
N	2.207800	-0.034722	1.870339
C	1.840422	-0.782268	3.099075
C	2.167472	0.016193	4.387754
H	1.730210	-0.492724	5.272442
H	3.253671	0.115580	4.572949
H	1.729956	1.035206	4.334208
C	0.314647	-1.009552	3.071168
H	0.016647	-1.606171	2.187693
H	-0.010708	-1.553198	3.982106
H	-0.235983	-0.048956	3.029327
C	2.524610	-2.174037	3.139106
H	2.268044	-2.751984	2.227329
H	3.629490	-2.102725	3.195938
H	2.182979	-2.755111	4.021946
N	1.605677	0.554319	-2.329568
N	2.265040	-1.994067	-0.748320
C	2.355250	-0.027701	-3.453051
H	1.657267	-0.162152	-4.317405
H	2.694013	-1.041656	-3.159742
C	3.569310	0.799131	-3.906644
H	4.087209	0.294560	-4.749628
H	3.279172	1.811624	-4.256383
H	4.293796	0.918292	-3.074751
C	1.253487	-3.068593	-0.852119
H	1.516737	-3.872164	-0.120582
H	0.268033	-2.671522	-0.536854
C	1.109189	-3.683322	-2.253447
H	0.341978	-4.485015	-2.232814
H	0.783660	-2.922301	-2.992090
H	2.052887	-4.139158	-2.618061
C	0.819238	1.719245	-2.734168
H	1.451323	2.594645	-3.015393
H	0.190705	1.468137	-3.621816
H	0.134710	2.042377	-1.927913
C	3.634581	-2.502990	-0.838928
H	4.355966	-1.669323	-0.753910
H	3.838919	-3.230425	-0.016509
H	3.818396	-3.035386	-1.800884
C	3.471544	0.358726	1.522474
C	3.552433	0.717434	0.155517
N	1.169840	2.351942	0.517466
H	2.066991	2.796633	0.294621
C	0.066332	3.241471	0.428998
C	-1.143797	2.964309	1.102803
C	0.151569	4.402401	-0.373998
C	-2.238976	3.832908	0.971619
H	-1.232602	2.060586	1.723362
C	-0.948779	5.265278	-0.498542
H	1.093102	4.630220	-0.900722
C	-2.152400	4.986836	0.172892
H	-3.175916	3.597658	1.501072
H	-0.860182	6.166683	-1.126012
H	-3.015270	5.663623	0.074563
H	1.263739	1.870553	1.430082
C	4.676299	0.430838	2.447829
H	5.590865	0.625170	1.854902
H	4.558449	1.262629	3.175106
H	4.832267	-0.495163	3.035941
H	4.446833	1.222033	-0.247604

D1-E1-M

E = -2707.48271610 A.U.

O	2.723397	-0.548055	1.282117
Si	4.407125	-0.682325	1.254875
O	4.967997	0.520952	0.209421
Si	4.329152	0.486977	-1.355028
O	2.650160	0.553606	-1.190635
Si	1.943688	-0.631815	-0.216635
O	2.433263	-2.107738	-0.891073
Si	4.096557	-2.344030	-1.050149
O	4.679167	-1.050427	-1.970492
O	0.330028	-0.524088	-0.114238
O	4.752098	-2.155611	0.497314
H	4.861006	1.568525	-2.209770
H	4.429829	-3.654588	-1.647320
H	5.005946	-0.588892	2.602525
Ta	-1.597884	-0.280451	0.241068
N	-2.350363	1.029111	-1.285591
C	-2.028242	1.400222	-2.694334
C	-1.902736	2.941385	-2.806564

H	-1.548546	3.222712	-3.820311
H	-2.872131	3.452578	-2.640185
H	-1.182164	3.339229	-2.065498
C	-0.667953	0.761139	-3.045592
H	-0.715683	-0.344276	-2.962060
H	-0.386013	1.010963	-4.088924
H	0.141479	1.119440	-2.380124
C	-3.063219	0.901873	-3.736940
H	-3.131093	-0.203063	-3.743349
H	-4.075864	1.314494	-3.571312
H	-2.742673	1.221004	-4.750626
N	-1.824363	-1.223390	2.045826
N	-2.323942	-1.934030	-0.711810
C	-3.057477	-1.838637	2.542870
H	-2.826081	-2.881705	2.879834
H	-3.761484	-1.928943	1.689470
C	-3.751310	-1.098572	3.698911
H	-4.683720	-1.628680	3.985642
H	-3.112539	-1.046015	4.604860
H	-4.020530	-0.062966	3.407531
C	-1.633345	-3.224923	-0.543425
H	-1.133132	-3.482093	-1.511396
H	-0.813902	-3.088151	0.191226
C	-2.503491	-4.416004	-0.108328
H	-1.862070	-5.311041	0.032014
H	-3.021020	-4.214913	0.851364
H	-3.270400	-4.680644	-0.864719
C	-0.752569	-1.218934	3.040608
H	-0.942476	-0.525927	3.898435
H	-0.634028	-2.239597	3.478873
H	0.217022	-0.932706	2.589187
C	-3.421953	-2.008965	-1.665423
H	-3.864647	-1.010528	-1.831003
H	-3.084053	-2.408118	-2.654918
H	-4.240616	-2.677764	-1.310549
C	-3.473326	1.424202	-0.557994
C	-3.262584	1.192664	0.798378
N	-0.792871	1.568761	1.585944
H	-0.927577	1.329799	2.577657
C	0.210728	2.546263	1.468147
C	0.625098	3.026118	0.201017
C	0.839779	3.093216	2.619191
C	1.616584	4.012529	0.092044
H	0.158400	2.605819	-0.700731
C	1.832984	4.076645	2.503836
H	0.536380	2.733398	3.617353
C	2.230163	4.548309	1.238892
H	1.915821	4.364970	-0.908587
H	2.301691	4.480545	3.416157
H	3.007737	5.322696	1.149124
H	-2.013104	1.717980	1.252123
C	-4.783222	1.898744	-1.152238
H	-5.284945	1.092357	-1.728850
H	-5.463550	2.213843	-0.337954
H	-4.651157	2.756915	-1.842522
H	-4.107431	1.217057	1.508252

E1-M

E = -2707.52299293 A.U.

O	2.861639	0.069190	1.302315
Si	4.527400	-0.158310	1.436646
O	5.245645	0.814469	0.255167
Si	4.717224	0.546040	-1.328231
O	3.041289	0.738565	-1.311320
Si	2.175956	-0.221882	-0.219002
O	2.616132	-1.818828	-0.596872
Si	4.268493	-2.171995	-0.571534
O	5.003807	-1.091575	-1.644211
O	0.589622	0.071718	-0.273434
O	4.823115	-1.758550	0.971590
H	5.381962	1.433304	-2.305316
H	4.549889	-3.582717	-0.912007
H	5.035794	0.134535	2.793106
Ta	-1.334199	-0.221963	0.178723
N	-2.810165	-0.099313	-1.212866
C	-2.827214	0.807429	-2.423079
C	-3.545735	2.135399	-2.092033
H	-3.512026	2.818420	-2.966663
H	-4.612160	1.963339	-1.841832
H	-3.050419	2.642468	-1.239588
C	-1.369998	1.104098	-2.829101
H	-0.817957	0.173138	-3.073620
H	-1.351172	1.753281	-3.727968
H	-0.824420	1.644022	-2.029798
C	-3.542786	0.124010	-3.609305
H	-3.037556	-0.819796	-3.901054
H	-4.604711	-0.097161	-3.377660
H	-3.529501	0.800113	-4.488904
N	-1.879333	-0.595430	2.074024
N	-1.026056	-2.250749	-0.163855
C	-2.902614	-1.556420	2.505651
H	-2.411807	-2.368173	3.099220
H	-3.325175	-2.040197	1.602203
C	-4.038666	-0.943642	3.337227
H	-4.775494	-1.728007	3.608538
H	-3.670138	-0.495638	4.282646
H	-4.571932	-0.156618	2.764978
C	-0.382393	-3.149276	0.808716
H	0.688595	-3.295415	0.522530
H	-0.368595	-2.643890	1.796648
C	-1.051200	-4.526275	0.968602
H	-0.523235	-5.115020	1.748062

H	-2.112701	-4.425697	1.277231
H	-1.023008	-5.124852	0.034885
C	-1.117353	-0.007030	3.179517
H	-1.734027	0.696989	3.785732
H	-0.740046	-0.802384	3.865611
H	-0.245977	0.562869	2.803016
C	-0.858482	-2.749561	-1.529707
H	-1.388089	-2.094572	-2.248708
H	0.220972	-2.777248	-1.818040
H	-1.259231	-3.782272	-1.659750
C	-4.045920	-0.751850	-0.853104
C	-4.960516	-0.117865	-0.075014
N	-1.312206	1.856717	0.639157
H	-2.188209	2.031600	1.157896
C	-0.589517	3.050070	0.625049
C	0.597353	3.221565	-0.143061
C	-1.038575	4.171579	1.384136
C	1.289454	4.441734	-0.135130
H	0.972258	2.389873	-0.752547
C	-0.341670	5.387229	1.381940
H	-1.958806	4.070486	1.986149
C	0.834690	5.535603	0.623937
H	2.204696	4.536264	-0.742309
H	-0.723297	6.229381	1.982438
H	1.384549	6.489550	0.621792
H	-4.784857	0.902170	0.297807
C	-4.267638	-2.171713	-1.333704
H	-5.276398	-2.537664	-1.057334
H	-4.151075	-2.254387	-2.432587
H	-3.509947	-2.843550	-0.878761
H	-5.910216	-0.606196	0.196519

E1-F1-M

E = -2707.49021659 A.U.

O	-2.682104	-1.661492	-0.841492
Si	-4.326664	-2.043262	-0.819979
O	-5.079149	-0.989986	-1.906680
Si	-4.817867	0.655655	-1.613597
O	-3.147336	0.876433	-1.586630
Si	-2.264272	-0.056637	-0.485423
O	-2.967841	0.252857	1.033819
Si	-4.631630	-0.008058	1.160312
O	-5.359584	0.938134	-0.035158
O	-0.683761	0.271223	-0.508287
O	-4.892316	-1.618695	0.717451
H	-5.493039	1.519398	-2.604413
H	-5.151114	0.294577	2.511076
H	-4.581798	-3.463298	-1.140603
Ta	1.116135	0.065722	0.412136
N	1.438649	2.405107	-0.100596
C	0.694595	3.136488	-1.210551
C	0.545973	2.340671	-2.528355
H	-0.052227	2.928566	-3.256225
H	1.528918	2.132878	-2.996377
H	0.026515	1.379802	-2.361269
C	-0.698020	3.462976	-0.621319
H	-0.591765	4.116842	0.268712
H	-1.322320	3.992439	-1.370743
H	-1.232165	2.547508	-0.317313
C	1.360015	4.503890	-1.513056
H	1.523008	5.076083	-0.575773
H	2.331414	4.419117	-2.035087
H	0.684801	5.100431	-2.160688
N	1.418098	0.267120	2.377054
N	0.800102	-1.936586	0.554421
C	0.213421	0.688001	3.119241
H	-0.025808	-0.088425	3.887295
H	-0.656816	0.687046	2.419677
C	0.305203	2.070846	3.780650
H	-0.637418	2.294876	4.321632
H	1.131451	2.125048	4.519064
H	0.461588	2.860517	3.018229
C	0.638748	-2.773384	1.746086
H	1.256454	-3.698647	1.626855
H	1.051674	-2.227665	2.617865
C	-0.813740	-3.178378	2.053105
H	-0.853235	-3.801579	2.971632
H	-1.450329	-2.283403	2.211400
H	-1.264234	-3.768768	1.229725
C	2.572138	-0.040625	3.209667
H	2.926155	0.842845	3.789809
H	2.327445	-0.840155	3.950358
H	3.417488	-0.394739	2.588383
C	0.619041	-2.690544	-0.689328
H	0.857807	-2.061824	-1.571232
H	1.296661	-3.575553	-0.721343
H	-0.430383	-3.042073	-0.810889
C	2.774640	2.571420	-0.010416
C	3.666639	2.379519	-1.111609
N	2.746401	-0.138453	-0.608122
H	3.352655	1.069359	-0.978047
C	3.596880	-1.161818	-1.044330
C	4.092770	-1.157226	-2.377608
C	4.027538	-2.208926	-0.183463
C	4.967181	-2.158067	-2.828295
H	3.765948	-0.355529	-3.058581
C	4.898867	-3.208231	-0.642342
H	3.661590	-2.222194	0.854629
C	5.375797	-3.192436	-1.966721
H	5.331601	-2.130741	-3.868325
H	5.216673	-4.007782	0.047112
H	6.062547	-3.976751	-2.321825

H	3.321368	2.567698	-2.139853
C	3.409555	2.639234	1.363855
H	4.259589	1.935903	1.480991
H	3.821607	3.666400	1.483154
H	2.665375	2.472891	2.160434
H	4.741047	2.574882	-0.948539

F1-M

E = -330.265077637 A.U.

C	-1.726577	-1.341928	0.002448
H	-2.404314	-1.569684	0.853625
C	-1.383165	0.144620	0.001008
C	-2.608755	1.044590	-0.002763
H	-3.256370	0.832493	-0.881965
H	-3.233561	0.868004	0.900519
H	-2.293341	2.104188	-0.026960
H	-0.854446	-2.014488	0.063882
N	-0.237613	0.725969	-0.001538
H	-2.295132	-1.594045	-0.919442
C	1.089045	0.068403	0.000067
C	2.112603	1.229563	-0.032041
H	1.970131	1.888974	0.848162
H	3.157092	0.852365	-0.029917
H	1.959819	1.848238	-0.939742
C	1.304142	-0.800676	-1.262637
H	0.657617	-1.700077	-1.282689
H	1.091753	-0.207337	-2.176336
H	2.358325	-1.144847	-1.319227
C	1.319584	-0.745105	1.296696
H	2.372282	-1.093954	1.351734
H	1.124929	-0.110499	2.186207
H	0.667241	-1.637931	1.366249

B

E = -2377.27557241 A.U.

O	3.125599	-1.592710	0.258175
Si	4.753790	-1.150056	0.208263
O	4.936732	0.112703	1.318461
Si	3.931089	1.449312	1.068540
O	2.348355	0.860099	1.067698
Si	2.007924	-0.363089	-0.051523
O	2.430577	0.271814	-1.561299
Si	4.016330	0.828375	-1.721161
O	4.240282	1.983593	-0.505538
O	0.474130	-0.888271	0.016283
O	5.018423	-0.474431	-1.319672
H	4.141928	2.509308	2.076263
H	4.300019	1.363396	-3.069070
H	5.658428	-2.284566	0.488449
Ta	-1.503346	-0.687170	0.006167
N	-2.209381	-1.350324	-1.756416
N	-2.292210	-1.671554	1.572512
C	-3.022540	-0.620519	-2.739144
H	-2.543591	-0.722225	-3.744580
H	-2.987865	0.456763	-2.479720
C	-4.487835	-1.075753	-2.826328
H	-5.030213	-0.476131	-3.587196
H	-4.582534	-2.142040	-3.119913
H	-5.002741	-0.940762	-1.852282
C	-2.021300	-3.112736	1.686792
H	-2.989970	-3.672403	1.713683
H	-1.508238	-3.455811	0.757062
C	-1.155816	-3.513485	2.891777
H	-0.979887	-4.609511	2.892263
H	-0.170638	-3.004086	2.859121
H	-1.644381	-3.256776	3.853894
C	-1.902190	-2.726622	-2.146370
H	-2.803310	-3.381814	-2.192702
H	-1.406109	-2.757428	-3.145927
H	-1.193573	-3.198374	-1.429340
C	-3.188212	-1.151687	2.603053
H	-3.396711	-0.080821	2.419891
H	-4.160682	-1.702440	2.605463
H	-2.753917	-1.243196	3.625400
N	-2.098958	1.020892	0.159334
C	-2.339111	2.373300	0.283762
C	-1.283835	3.284969	0.568622
C	-3.655491	2.890186	0.129279
C	-1.542796	4.657469	0.688885
H	-0.264040	2.887959	0.692387
C	-3.900667	4.266003	0.251425
H	-4.475011	2.187350	-0.087520
C	-2.849206	5.158303	0.530698
H	-0.711768	5.347320	0.908780
H	-4.927682	4.646351	0.126992
H	-3.046066	6.237733	0.625155

B-C-anti

E = -2493.81665262 A.U.

O	3.260779	-1.109852	0.794856
Si	4.904641	-0.740725	0.823323
O	5.031136	0.835116	1.425047
Si	4.149282	2.002887	0.576622
O	2.546483	1.480929	0.560735
Si	2.247815	-0.063244	-0.077415
O	2.919190	-0.024647	-1.640615
Si	4.544006	0.412117	-1.761868
O	4.691142	1.926340	-1.024389
O	0.704168	-0.504457	-0.042945
O	5.406949	-0.670558	-0.790890
H	4.304103	3.353506	1.157118
H	5.025665	0.418694	-3.159738

H	5.693992	-1.708493	1.614424
Ta	-1.331705	-0.646832	-0.057213
N	-2.305659	-2.371463	-0.442793
N	-1.080062	-0.920571	1.953454
C	-3.521896	-2.513329	-1.251397
H	-3.350808	-3.301044	-2.027378
H	-3.691032	-1.566428	-1.804582
C	-4.783677	-2.863072	-0.446327
H	-5.657491	-2.968617	-1.123306
H	-4.675956	-3.819504	0.106231
H	-5.014121	-2.067258	0.291962
C	0.090076	-1.160086	2.798857
H	-0.118931	-2.032100	3.468445
H	0.939756	-1.456190	2.152655
C	0.512228	0.045201	3.656827
H	1.381370	-0.221138	4.294710
H	0.808427	0.898884	3.013429
H	-0.301141	0.386195	4.330955
C	-1.750699	-3.642174	0.020064
H	-2.463361	-4.202841	0.669953
H	-1.486059	-4.307942	-0.836668
H	-0.829093	-3.475601	0.614607
C	-2.333188	-0.935182	2.710107
H	-3.200187	-0.730852	2.046858
H	-2.506768	-1.925989	3.198271
H	-2.352896	-0.157114	3.508469
N	-2.597195	0.737290	-0.298175
C	-1.832487	0.643262	-2.118202
C	-0.946316	-0.272744	-2.294638
H	-2.439036	1.467160	-2.511089
C	-0.025335	-0.860000	-3.303217
H	-0.185857	-1.955770	-3.384489
H	1.025462	-0.715373	-2.973835
H	-0.148484	-0.406343	-4.309316
C	-3.365360	1.882715	-0.157047
C	-2.801013	3.181425	-0.285174
C	-4.753449	1.770620	0.125870
C	-3.599441	4.322940	-0.119593
H	-1.725045	3.275138	-0.500803
C	-5.539649	2.918747	0.302845
H	-5.193284	0.765015	0.209547
C	-4.969233	4.199250	0.179020
H	-3.144293	5.321871	-0.215758
H	-6.611986	2.812703	0.533253
H	-5.590608	5.098471	0.313595

C-anti

E = -2493.86227231 A.U.

O	2.459948	0.284578	1.157138
Si	4.144428	0.288079	1.202584
O	4.668805	0.901429	-0.284207
Si	4.089433	0.090262	-1.648583
O	2.405944	0.106432	-1.542587
Si	1.736008	-0.540147	-0.127757
O	2.352361	-2.120049	-0.033512
Si	4.032673	-2.275697	-0.051673
O	4.564058	-1.524054	-1.471240
O	0.122455	-0.502678	-0.123697
O	4.618284	-1.338051	1.227740
H	4.582784	0.683213	-2.909822
H	4.472663	-3.684547	0.035574
H	4.687109	1.046706	2.348628
Ta	-1.866326	-0.322077	-0.025295
N	-2.231168	-2.253460	0.442502
N	-2.903973	-0.152169	-1.706678
C	-1.724367	-2.769384	1.724817
H	-2.573775	-3.214318	2.300968
H	-1.371372	-1.903882	2.331912
C	-0.584878	-3.793382	1.603589
H	-0.251208	-4.107900	2.614605
H	-0.904367	-4.709147	1.064513
H	0.286390	-3.361814	1.070432
C	-4.374951	-0.163957	-1.766550
H	-4.692971	-0.833552	-2.603639
H	-4.754952	-0.625859	-0.829844
C	-5.006782	1.224572	-1.934507
H	-6.112806	1.140476	-1.971843
H	-4.734104	1.878104	-1.080643
H	-4.678551	1.721050	-2.870572
C	-2.984924	-3.243634	-0.319236
H	-2.357280	-4.122989	-0.594805
H	-3.853969	-3.632338	0.266255
H	-3.366908	-2.804278	-1.260986
C	-2.237189	0.078024	-2.989688
H	-1.133846	0.054518	-2.868857
H	-2.514672	-0.708872	-3.729977
H	-2.502198	1.067862	-3.424970
N	-1.444633	1.794494	0.535883
C	-2.401013	1.697840	1.513693
C	-3.046153	0.461042	1.538505
H	-2.621842	2.566080	2.181835
C	-4.146728	0.072804	2.483664
H	-3.883198	-0.831596	3.075526
H	-5.095609	-0.173847	1.955965
H	-4.379028	0.884379	3.210750
C	-0.469176	2.785629	0.478556
C	0.229879	2.996872	-0.741237
C	-0.134604	3.609915	1.589246
C	1.207139	3.994903	-0.848078
H	-0.022118	2.369962	-1.610345
C	0.833737	4.617290	1.466282

H	-0.619591	3.439730	2.562647
C	1.513465	4.819797	0.251215
H	1.731921	4.136945	-1.806721
H	1.074196	5.242645	2.341760
H	2.278361	5.607051	0.163579

D-anti

E = -2781.26979521 A.U.

O	2.619355	-1.288267	-0.930311
Si	4.285982	-1.232462	-1.176555
O	4.969691	-0.687052	0.273647
Si	4.383931	0.798102	0.831039
O	2.710386	0.620590	0.968957
Si	1.869221	0.147694	-0.432497
O	2.298191	1.297038	-1.607480
Si	3.944869	1.511602	-1.899101
O	4.646614	1.911414	-0.412965
O	0.278486	0.037118	-0.214856
O	4.560447	-0.008176	-2.311921
H	5.017609	1.211577	2.100906
H	4.211533	2.528328	-2.938351
H	4.844306	-2.531992	-1.605652
Ta	-1.741450	-0.161958	-0.368993
N	-1.944226	1.274236	1.418458
N	-1.853031	-1.846796	-1.488079
N	-2.224751	1.198121	-1.742864
C	-2.550111	-1.969418	-2.778394
H	-1.825473	-2.358328	-3.537308
H	-2.842464	-0.955216	-3.115663
C	-3.790700	-2.877146	-2.761193
H	-4.268022	-2.888859	-3.763587
H	-3.540669	-3.927120	-2.504164
H	-4.539081	-2.515075	-2.026240
C	-1.202355	2.050176	-2.391413
H	-1.488293	3.117997	-2.236091
H	-0.234854	1.906740	-1.872024
C	-1.006587	1.774989	-3.889921
H	-0.240822	2.465477	-4.300044
H	-0.653845	0.737443	-4.061967
H	-1.936243	1.927355	-4.476626
C	-1.203577	-3.097992	-1.091952
H	-1.931410	-3.888509	-0.795144
H	-0.600184	-3.503044	-1.938833
H	-0.512247	-2.941458	-0.243014
C	-3.590350	1.579740	-2.106876
H	-4.323922	0.870108	-1.680751
H	-3.829883	2.596109	-1.713214
H	-3.727700	1.606999	-3.212056
C	-3.254339	0.882854	1.493794
C	-3.582056	-0.215404	0.694118
H	-3.974715	1.432768	2.148734
N	-1.206683	-1.505263	1.879424
H	-2.159245	-1.804731	2.117102
C	-0.225775	-2.465805	2.260583
C	1.118970	-2.084705	2.460834
C	-0.583916	-3.825170	2.405245
C	2.081091	-3.051100	2.796271
H	1.414510	-1.030072	2.353994
C	0.385008	-4.783690	2.742401
H	-1.633149	-4.130594	2.257270
C	1.724450	-4.403711	2.938277
H	3.126132	-2.736307	2.945516
H	0.085586	-5.837848	2.856526
H	2.483540	-5.155899	3.203134
C	-4.906030	-0.926513	0.765950
H	-5.622505	-0.421065	1.454827
H	-5.404777	-1.004898	-0.226231
H	-4.800258	-1.976834	1.125733
H	-1.058887	-0.571463	2.296952
C	-1.477492	2.508437	1.883831
C	-0.079169	2.699801	2.057885
C	-2.339811	3.597277	2.195599
C	0.426306	3.916334	2.536697
H	0.607052	1.875143	1.816438
C	-1.822137	4.806681	2.684794
H	-3.424290	3.503047	2.032279
C	-0.437534	4.979697	2.861143
H	1.515199	4.032547	2.662320
H	-2.514255	5.632881	2.917390
H	-0.036354	5.933199	3.238702

D-E-anti

E = -2781.24695962 A.U.

O	2.664783	-0.577631	-1.419084
Si	4.338570	-0.733659	-1.595176
O	4.801678	-2.009158	-0.585926
Si	4.374822	-1.837563	1.042020
O	2.699705	-1.619638	1.070081
Si	2.102645	-0.323081	0.159019
O	2.915703	1.044474	0.714832
Si	4.601780	0.989971	0.671975
O	5.054991	-0.379236	1.558016
O	0.485955	-0.221232	0.244001
O	5.022405	0.662809	-0.935089
H	4.808891	-2.987194	1.863116
H	5.228905	2.226600	1.180654
H	4.741046	-0.951328	-3.000510
Ta	-1.441978	-0.572254	-0.005314
N	-2.038220	1.100982	-1.164061
N	-1.891326	-2.170878	1.172315
N	-1.373555	-1.767940	-1.666384
C	-3.012969	-3.106673	1.074751

H	-2.607016	-4.134261	0.893001
H	-3.599957	-2.837696	0.172695
C	-3.941264	-3.160881	2.298506
H	-4.790016	-3.847129	2.097761
H	-3.421544	-3.539197	3.202614
H	-4.360005	-2.161272	2.533160
C	-0.886832	-3.162591	-1.626422
H	0.104835	-3.199655	-2.143049
H	-0.695971	-3.431090	-0.569062
C	-1.809898	-4.217103	-2.260902
H	-1.389660	-5.229933	-2.087519
H	-2.825728	-4.188951	-1.815166
H	-1.914919	-4.091841	-3.357699
C	-1.013786	-2.430293	2.318441
H	-1.495780	-2.192530	3.297423
H	-0.723423	-3.507745	2.348630
H	-0.080526	-1.837253	2.252854
C	-1.581800	-1.344336	-3.055275
H	-1.822223	-0.269770	-3.118593
H	-0.668822	-1.531070	-3.670357
H	-2.418551	-1.903272	-3.532406
C	-3.406239	0.994806	-0.911194
C	-3.696777	0.249836	0.207427
H	-4.136452	1.406187	-1.645096
N	-1.724815	0.694348	1.959641
H	-1.954053	0.090186	2.759771
C	-1.169536	1.907336	2.417249
C	-0.832169	2.948809	1.516759
C	-0.943779	2.123275	3.802113
C	-0.289947	4.153091	1.990299
H	-0.997098	2.804401	0.439623
C	-0.398478	3.329413	4.266465
H	-1.201763	1.325039	4.519482
C	-0.066961	4.356467	3.364398
H	-0.036125	4.945132	1.267302
H	-0.232306	3.466788	5.347489
H	0.359493	5.304155	3.728481
C	-5.100508	-0.184094	0.546990
H	-5.860840	0.402756	-0.018280
H	-5.285769	-1.255939	0.311899
H	-5.327652	-0.058389	1.628029
H	-2.819756	0.645774	1.260830
C	-1.489648	2.035463	-2.058245
C	-2.219838	3.177425	-2.483921
C	-0.163925	1.866768	-2.538702
C	-1.645101	4.101198	-3.370801
H	-3.233220	3.357236	-2.095233
C	0.399920	2.799455	-3.419738
H	0.422439	0.993735	-2.215170
C	-0.335508	3.920476	-3.848651
H	-2.229587	4.982091	-3.682132
H	1.430594	2.644924	-3.777062
H	0.111418	4.649913	-4.541805

E-anti

E = -2781.29041490 A.U.

O	-3.185825	-0.288943	-1.397393
Si	-4.867243	-0.328172	-1.265504
O	-5.295318	0.928905	-0.217901
Si	-4.563372	0.888439	1.305265
O	-2.896031	0.862418	1.032510
Si	-2.310746	-0.384124	0.045344
O	-2.839959	-1.813519	0.788793
Si	-4.501896	-1.956553	1.053815
O	-4.953207	-0.614292	1.977550
O	-0.710366	-0.312580	-0.171802
O	-5.244160	-1.763801	-0.451937
H	-4.979920	2.016273	2.164317
H	-4.862856	-3.234858	1.702254
H	-5.545084	-0.228589	-2.574483
Ta	1.270095	-0.451264	-0.245126
N	2.915342	0.311142	0.816852
N	1.732758	-1.583172	-1.829329
N	1.228107	-1.954625	1.167978
C	2.467514	-2.859910	-1.809257
H	1.737566	-3.702639	-1.904041
H	2.942269	-2.957917	-0.813042
C	3.532763	-3.010532	-2.905636
H	4.083730	-3.962339	-2.757909
H	3.093108	-3.041040	-3.923165
H	4.270010	-2.181904	-2.876622
C	0.322280	-3.091316	0.906645
H	-0.618846	-2.954751	1.492838
H	0.010353	-3.055054	-0.159483
C	0.904690	-4.483040	1.203685
H	0.183826	-5.263921	0.883443
H	1.857169	-4.654416	0.660302
H	1.096670	-4.639047	2.284688
C	1.089722	-1.295303	-3.119745
H	1.836630	-1.073173	-3.915469
H	0.478478	-2.165852	-3.456415
H	0.420849	-0.418371	-3.035441
C	1.682288	-1.934088	2.554268
H	2.227453	-0.998648	2.775839
H	0.822271	-2.006401	3.264727
H	2.364207	-2.785088	2.784732
C	4.173500	-0.319110	0.866002
C	4.847955	-0.829500	-0.195230
H	4.626430	-0.392814	1.877277
N	1.245957	1.385660	-1.261652
H	2.197645	1.511861	-1.645194
C	0.510276	2.532456	-1.572806

C	-0.728975	2.839821	-0.949086
C	0.994427	3.444565	-2.554610
C	-1.452003	3.984134	-1.316282
H	-1.113136	2.191667	-0.151261
C	0.265882	4.586757	-2.912536
H	1.961395	3.235265	-3.044314
C	-0.969942	4.866168	-2.300657
H	-2.409348	4.193212	-0.811494
H	0.670999	5.267760	-3.678859
H	-1.542999	5.764171	-2.579262
C	6.142957	-1.583249	-0.090559
H	6.510160	-1.624304	0.955783
H	6.043659	-2.632687	-0.449710
H	6.937769	-1.118148	-0.714932
H	4.418619	-0.684106	-1.203150
C	2.741264	1.450001	1.634316
C	3.827643	2.286899	1.998944
C	1.444938	1.798884	2.096835
C	3.615604	3.427373	2.789367
H	4.837472	2.049962	1.630668
C	1.237508	2.953425	2.864544
H	0.579753	1.145855	1.877493
C	2.323145	3.773825	3.221862
H	4.474523	4.063800	3.057452
H	0.218594	3.202338	3.200533
H	2.162415	4.673786	3.835308

E-F-anti

E = -2781.25832640 A.U.

O	-3.110930	1.349660	0.025954
Si	-4.793280	1.290262	0.024087
O	-5.225832	0.013006	1.049699
Si	-4.548461	-1.483299	0.653120
O	-2.874511	-1.259826	0.625599
Si	-2.288907	-0.055908	-0.432444
O	-2.905794	-0.463506	-1.955655
Si	-4.578812	-0.634510	-2.075499
O	-5.016180	-1.809392	-0.937950
O	-0.681850	0.068246	-0.397422
O	-5.255947	0.816614	-1.532917
H	-4.959346	-2.551937	1.589313
H	-5.018745	-0.985044	-3.442450
H	-5.414903	2.567999	0.430282
Ta	1.077766	-0.470360	0.435448
N	1.008199	1.785187	1.116415
N	1.343139	-1.120240	2.300453
N	1.004260	-2.290086	-0.454393
C	0.097448	-1.329679	3.064239
H	0.093091	-2.372143	3.467126
H	-0.765325	-1.283483	2.356934
C	-0.135986	-0.319999	4.197331
H	-1.099966	-0.532199	4.704219
H	0.660321	-0.366151	4.968621
H	-0.176946	0.712828	3.794395
C	1.051481	-3.623216	0.152153
H	1.848944	-4.227648	-0.350007
H	1.360349	-3.510196	1.211638
C	-0.275159	-4.401156	0.093881
H	-0.172622	-5.373318	0.620623
H	-1.093390	-3.825581	0.573920
H	-0.584811	-4.622952	-0.948181
C	2.571347	-1.432300	3.022545
H	2.691920	-0.811786	3.940908
H	2.580741	-2.500629	3.347131
H	3.450474	-1.260769	2.371868
C	0.851749	-2.322983	-1.910166
H	0.929970	-1.303562	-2.340981
H	1.648847	-2.944010	-2.382709
H	-0.137704	-2.730928	-2.221134
C	2.210478	1.967334	1.675623
C	3.335474	2.516920	0.985751
H	2.438232	1.300577	2.533082
N	2.775010	0.104966	-0.292500
H	3.240075	1.384015	0.263266
C	3.769339	-0.357884	-1.162821
C	4.354647	0.523175	-2.114471
C	4.258335	-1.693265	-1.111098
C	5.373616	0.085693	-2.974903
H	3.984405	1.559127	-2.171459
C	5.275808	-2.122834	-1.976029
H	3.820090	-2.385763	-0.375940
C	5.841801	-1.239386	-2.914763
H	5.806131	0.790292	-3.704092
H	5.637577	-3.162369	-1.911757
H	6.642281	-1.580340	-3.589881
C	4.674626	2.687070	1.679567
H	4.839325	1.902843	2.448814
H	5.511001	2.619839	0.953833
H	4.759315	3.673884	2.184934
H	3.101168	3.273279	0.212333
C	0.539397	2.838604	0.260613
C	0.481925	2.741496	-1.147524
C	0.090731	4.031447	0.876714
C	-0.013440	3.810425	-1.913137
H	0.842988	1.831485	-1.646209
C	-0.401027	5.096460	0.106521
H	0.125324	4.103064	1.975111
C	-0.458926	4.991386	-1.294443
H	-0.045534	3.716203	-3.010610
H	-0.747225	6.014479	0.608287
H	-0.848405	5.824514	-1.900382

F-anti

SCF Done: -404.024333111 A.U.

C	1.721308	-0.568212	-0.477469
H	1.310307	-1.390752	-1.118572
C	3.221357	-0.493029	-0.380554
C	3.759930	0.634271	0.501314
H	3.389754	0.536941	1.541754
H	4.868650	0.626956	0.521197
H	3.421620	1.622974	0.131569
H	3.622297	-0.418555	-1.419743
N	0.948534	0.262027	0.123324
C	-0.449729	0.119923	0.068322
C	-1.100277	-1.126063	0.251984
C	-1.238673	1.280564	-0.124366
C	-2.501981	-1.206111	0.219939
H	-0.496660	-2.025673	0.452337
C	-2.636604	1.188530	-0.175685
H	-0.725723	2.247646	-0.241273
C	-3.276410	-0.053861	-0.002521
H	-2.994153	-2.179742	0.376447
H	-3.235879	2.098397	-0.340856
H	-4.375508	-0.120174	-0.026268
H	3.582046	-1.488282	-0.025643

B-C-M

E = -2493.81870057 A.U.

O	3.462969	-1.252478	0.539603
Si	5.108023	-1.101257	0.213430
O	5.631445	0.305988	0.993695
Si	4.786315	1.712288	0.580959
O	3.160221	1.401549	0.887096
Si	2.466367	0.056454	0.119080
O	2.766986	0.308721	-1.542806
Si	4.374169	0.552710	-1.994591
O	4.933095	1.872675	-1.098075
O	0.921554	-0.175763	0.489693
O	5.239446	-0.791501	-1.445515
H	5.289072	2.900718	1.302580
H	4.525711	0.760577	-3.451100
H	5.884637	-2.290614	0.623416
Ta	-1.110070	-0.386272	0.126650
N	-1.209228	-2.387277	-0.002395
N	-1.269286	0.143523	2.093471
C	-2.256949	-3.158507	-0.683853
H	-1.762932	-3.956048	-1.292212
H	-2.770878	-2.487907	-1.401701
C	-3.298170	-3.803033	0.245321
H	-4.037460	-4.383183	-0.346504
H	-2.834363	-4.502813	0.970549
H	-3.849175	-3.029623	0.820003
C	-0.313507	0.797062	2.991025
H	-0.321634	0.264450	3.974547
H	0.700057	0.672682	2.564029
C	-0.583013	2.293100	3.226537
H	0.166023	2.715795	3.929016
H	-0.512074	2.858900	2.273716
H	-1.587693	2.479043	3.661441
C	-0.240431	-3.219505	0.718994
H	-0.698739	-3.757858	1.581238
H	0.197765	-3.986031	0.036325
H	0.590513	-2.600575	1.108558
C	-2.555505	-0.121255	2.741946
H	-3.235244	-0.680578	2.067017
H	-2.414594	-0.732867	3.666100
H	-3.090456	0.812291	3.036701
N	-2.845299	0.156226	-0.456543
C	-1.691769	0.574922	-2.196074
C	-0.466055	0.318291	-1.908278
C	-4.072576	0.786485	-0.501555
C	-4.211695	2.167446	-0.178734
C	-5.247382	0.055561	-0.836716
C	-5.472717	2.780211	-0.181152
H	-3.307325	2.738334	0.085048
C	-6.504861	0.677493	-0.834313
H	-5.147935	-1.012699	-1.084167
C	-6.625935	2.041211	-0.508802
H	-5.558794	3.847456	0.080020
H	-7.402073	0.090223	-1.088588
H	-7.614590	2.526280	-0.507865
C	-2.733046	1.029168	-3.130053
H	-3.253831	1.936678	-2.762657
H	-2.244208	1.266723	-4.098484
H	-3.506128	0.251487	-3.296248
H	0.525830	0.361536	-2.377539

C-M

E = -2493.86459600 A.U.

O	-2.163204	-0.147937	1.458339
Si	-3.803744	-0.071845	1.850796
O	-4.505987	-1.481485	1.234856
Si	-4.287135	-1.730453	-0.424873
O	-2.621052	-1.707849	-0.690107
Si	-1.792524	-0.312112	-0.192496
O	-2.576215	0.964813	-0.969551
Si	-4.234800	1.111341	-0.714741
O	-4.918266	-0.362615	-1.191094
O	-0.203400	-0.380985	-0.464442
O	-4.455480	1.207953	0.960839
H	-4.919526	-2.981908	-0.893170
H	-4.828418	2.261123	-1.427869
H	-4.029837	0.079316	3.304183
Ta	1.746543	-0.646937	-0.090503

N	1.804943	-2.601805	-0.592581
N	2.479859	-0.743297	1.753941
C	1.376629	-2.974597	-1.951370
H	2.224163	-3.487788	-2.470894
H	1.196026	-2.039462	-2.528337
C	0.116271	-3.851536	-2.007511
H	-0.141072	-4.076051	-3.063808
H	0.261823	-4.823270	-1.491400
H	-0.748343	-3.333962	-1.544632
C	3.898885	-0.887959	2.115834
H	3.981555	-1.634920	2.943595
H	4.434862	-1.314668	1.242023
C	4.576186	0.426894	2.526184
H	5.638874	0.245225	2.790058
H	4.544174	1.153875	1.689321
H	4.088528	0.891785	3.407807
C	2.351810	-3.720427	0.166868
H	1.595131	-4.522662	0.331426
H	3.215253	-4.189556	-0.365564
H	2.700297	-3.382220	1.161566
C	1.567911	-0.607821	2.892496
H	0.514729	-0.508190	2.551073
H	1.622427	-1.502949	3.556154
H	1.801196	0.289247	3.510133
N	1.917231	1.558350	-0.533044
C	3.002322	1.310716	-1.332194
C	3.268713	-0.073023	-1.378982
C	1.191035	2.734623	-0.378335
C	0.514344	2.952191	0.855033
C	1.039099	3.720663	-1.393861
C	-0.253339	4.104021	1.070090
H	0.615285	2.196349	1.649658
C	0.277440	4.876792	-1.164817
H	1.491212	3.561169	-2.382594
C	-0.371248	5.083476	0.065814
H	-0.761796	4.242442	2.038143
H	0.176279	5.621168	-1.971634
H	-0.970768	5.991132	0.236698
C	3.835045	2.382226	-2.001666
H	3.454057	2.600681	-3.022411
H	3.824668	3.332603	-1.431044
H	4.879119	2.027916	-2.111893
H	4.085344	-0.512352	-1.971886

D-M

E = -2781.27072032 A.U.

O	2.521718	-1.210920	-1.358801
Si	4.194045	-1.203483	-1.565654
O	4.868235	-1.220157	-0.012216
Si	4.368772	0.037423	1.000197
O	2.682392	-0.046236	1.063604
Si	1.856180	0.038026	-0.422528
O	2.403671	1.467603	-1.154276
Si	4.069315	1.642440	-1.344629
O	4.746339	1.474741	0.196700
O	0.254241	-0.035846	-0.289733
O	4.591253	0.300309	-2.231586
H	4.986962	-0.039050	2.340936
H	4.441920	2.920450	-1.986721
H	4.673006	-2.329247	-2.395202
Ta	-1.773953	-0.026452	-0.421323
N	-1.751900	1.319986	1.455654
N	-2.081254	-1.662372	-1.573256
N	-2.123981	1.416978	-1.759033
C	-2.983798	-1.690469	-2.734248
H	-2.435104	-2.132681	-3.603638
H	-3.228973	-0.646102	-3.015240
C	-4.289703	-2.470210	-2.509480
H	-4.920441	-2.435948	-3.422854
H	-4.104711	-3.539251	-2.276387
H	-4.869503	-2.031381	-1.671066
C	-1.017362	2.043586	-2.517036
H	-1.130997	3.151971	-2.448754
H	-0.056709	1.803025	-2.020778
C	-0.943815	1.615457	-3.990847
H	-0.105100	2.138506	-4.495960
H	-0.766164	0.523653	-4.076960
H	-1.870793	1.859722	-4.550361
C	-1.443125	-2.955543	-1.328646
H	-2.148981	-3.724574	-0.938381
H	-1.008839	-3.352176	-2.277312
H	-0.615404	-2.861436	-0.600761
C	-3.420659	2.024196	-2.061779
H	-4.224290	1.514340	-1.498168
H	-3.423607	3.103232	-1.775110
H	-3.658189	1.971757	-3.149868
C	-3.105547	1.122394	1.572247
C	-3.550944	0.115609	0.690400
N	-1.369918	-1.589367	1.717904
H	-2.370348	-1.661303	1.941118
C	-0.649948	-2.783551	2.001840
C	0.754849	-2.762233	2.147891
C	-1.332793	-4.016981	2.101808
C	1.454674	-3.956150	2.388438
H	1.302047	-1.809898	2.070876
C	-0.623612	-5.204888	2.339425
H	-2.430157	-4.040700	1.996331
C	0.775012	-5.183328	2.483770
H	2.550208	-3.921931	2.500090
H	-1.173749	-6.156306	2.418330
H	1.329881	-6.115438	2.672183
H	-1.002315	-0.754468	2.198004

C	-1.037422	2.447292	1.884456
C	0.314381	2.290624	2.294722
C	-1.577092	3.763732	1.883170
C	1.077813	3.392255	2.706126
H	0.763633	1.286494	2.283398
C	-0.807471	4.860060	2.303680
H	-2.601360	3.931096	1.519197
C	0.523462	4.685689	2.722219
H	2.122901	3.235861	3.018869
H	-1.253256	5.868340	2.289742
H	1.124960	5.548929	3.047330
C	-3.986700	1.875083	2.550244
H	-4.522889	2.711767	2.053677
H	-4.762466	1.188788	2.946881
H	-3.407355	2.301978	3.393196
H	-4.576224	-0.287004	0.757747

D-E-M

E = -2781.25093619 A.U.

O	2.683124	-1.242843	0.814887
Si	4.371383	-1.314915	0.795560
O	4.921934	0.267918	0.589345
Si	4.330236	1.076235	-0.773098
O	2.646854	1.020313	-0.671959
Si	1.955506	-0.509029	-0.525712
O	2.511877	-1.386589	-1.863874
Si	4.187425	-1.476922	-2.051188
O	4.751375	0.116234	-2.102755
O	0.333511	-0.506217	-0.439689
O	4.790034	-2.145060	-0.618266
H	4.851425	2.453721	-0.886932
H	4.583149	-2.254213	-3.244576
H	4.923934	-1.956232	2.006986
Ta	-1.556833	-0.586849	0.119723
N	-2.279880	1.385618	-0.218942
N	-1.818386	-2.415629	0.969736
N	-2.408836	-1.228451	-1.630285
C	-3.083544	-3.132606	1.149046
H	-2.981484	-4.152995	0.699503
H	-3.857402	-2.598821	0.559595
C	-3.559810	-3.279376	2.603380
H	-4.543373	-3.793089	2.630058
H	-2.859181	-3.882618	3.217003
H	-3.676179	-2.288254	3.087464
C	-2.056870	-2.545821	-2.196863
H	-1.397799	-2.382707	-3.086470
H	-1.441074	-3.087818	-1.451460
C	-3.238015	-3.438376	-2.615437
H	-2.857347	-4.430268	-2.937266
H	-3.942376	-3.600772	-1.773596
H	-3.811776	-3.017994	-3.466254
C	-0.671327	-3.094422	1.576161
H	-0.725056	-3.125118	2.691787
H	-0.616588	-4.152810	1.224128
H	0.282720	-2.599813	1.306747
C	-3.238960	-0.460871	-2.558722
H	-3.391959	0.569977	-2.194700
H	-2.769968	-0.402097	-3.571440
H	-4.244470	-0.921626	-2.693605
C	-3.424500	1.270614	0.583646
C	-3.244635	0.243307	1.495597
N	-0.708995	0.085495	2.240697
H	-0.693952	-0.710313	2.892318
C	0.223621	1.059487	2.648969
C	0.364073	2.283038	1.946503
C	1.045304	0.847570	3.787721
C	1.288705	3.249026	2.372336
H	-0.258589	2.471410	1.060162
C	1.968316	1.817426	4.204928
H	0.952388	-0.099220	4.346939
C	2.098509	3.028758	3.501167
H	1.375952	4.190335	1.805937
H	2.593102	1.623148	5.092081
H	2.821765	3.791319	3.829704
H	-1.973044	0.323419	2.136290
C	-1.924106	2.473394	-1.035003
C	-2.279597	3.810089	-0.711251
C	-1.120748	2.254270	-2.185956
C	-1.869457	4.876417	-1.527204
H	-2.850267	4.016820	0.204897
C	-0.712000	3.327363	-2.989417
H	-0.814793	1.228002	-2.439976
C	-1.089264	4.645864	-2.673330
H	-2.155296	5.904350	-1.251363
H	-0.088891	3.128846	-3.876147
H	-0.767890	5.485983	-3.308287
C	-4.686874	2.066059	0.338919
H	-5.568672	1.455725	0.617249
H	-4.713052	2.979257	0.971293
H	-4.784959	2.392164	-0.716206
H	-4.103749	-0.159446	2.059419

E-M

E = -2781.29082007 A.U.

O	2.830499	0.511903	1.274470
Si	4.475613	0.633518	1.620568
O	5.173882	1.525021	0.365054
Si	4.916539	0.911334	-1.189252
O	3.248057	0.778525	-1.384668
Si	2.416297	-0.140598	-0.232159
O	3.168891	-1.666306	-0.266585
Si	4.836046	-1.685989	-0.007963

O	5.518167	-0.670813	-1.175714
O	0.828397	-0.240245	-0.515594
O	5.100906	-0.934012	1.483574
H	5.548606	1.742202	-2.235678
H	5.399070	-3.052746	-0.055126
H	4.738659	1.226813	2.948486
Ta	-1.108094	-0.512872	-0.005891
N	-3.182943	-0.304238	0.396695
N	-0.741267	-1.954709	1.312119
N	-1.406043	-1.283310	-1.878777
C	-0.338780	-3.320901	0.942795
H	0.711750	-3.482818	1.286995
H	-0.313546	-3.386840	-0.164363
C	-1.244140	-4.430930	1.495622
H	-0.878481	-5.420180	1.150397
H	-1.252086	-4.450905	2.604592
H	-2.289252	-4.306545	1.146698
C	-0.319651	-1.843851	-2.711810
H	-0.167980	-1.188403	-3.605561
H	0.622430	-1.804858	-2.134328
C	-0.560592	-3.286750	-3.184808
H	0.327694	-3.650180	-3.742275
H	-0.724384	-3.971426	-2.325606
H	-1.433966	-3.379276	-3.862253
C	-0.627233	-1.658765	2.737794
H	-1.401170	-2.194791	3.334229
H	0.379019	-1.949798	3.120087
H	-0.752382	-0.572915	2.922457
C	-2.634403	-1.132691	-2.664671
H	-3.435274	-0.653649	-2.076357
H	-2.456852	-0.512844	-3.577157
H	-3.019502	-2.118724	-3.012163
C	-3.856206	-1.367724	1.110206
C	-3.919503	-1.385409	2.461001
N	-1.009251	1.413560	0.737840
H	-1.758027	1.594196	1.421313
C	-0.312931	2.605263	0.481944
C	0.428050	2.811669	-0.710813
C	-0.351028	3.663693	1.430422
C	1.119785	4.014270	-0.924761
H	0.455271	2.021752	-1.474689
C	0.338681	4.862798	1.205439
H	-0.927955	3.527256	2.360709
C	1.086088	5.047966	0.027419
H	1.689478	4.143090	-1.859182
H	0.292455	5.662340	1.962682
H	1.628650	5.989805	-0.148484
H	-3.474715	-0.579322	3.064079
C	-4.015218	0.780793	0.012496
C	-5.306021	0.986695	0.574819
C	-3.573970	1.722424	-0.961011
C	-6.097537	2.081340	0.193467
H	-5.681160	0.285375	1.333712
C	-4.365473	2.820627	-1.324563
H	-2.591578	1.599242	-1.442366
C	-5.636447	3.011841	-0.753043
H	-7.091202	2.208443	0.653298
H	-3.981682	3.531267	-2.073906
H	-6.259108	3.871287	-1.046136
C	-4.506291	-2.418561	0.240329
H	-3.749163	-2.913204	-0.405014
H	-5.023125	-3.191149	0.842921
H	-5.249305	-1.949881	-0.441208
H	-4.430175	-2.203188	2.993466

E-F-M

SCF Done: -2781.25913465 A.U.

O	-3.121715	0.615018	-1.380051
Si	-4.787809	0.866145	-1.339506
O	-5.140501	1.511293	0.184181
Si	-4.624151	0.578436	1.496614
O	-2.968675	0.338966	1.298365
Si	-2.463498	-0.365711	-0.161256
O	-3.330924	-1.826017	-0.257767
Si	-5.009223	-1.720508	-0.151078
O	-5.351986	-0.937471	1.308978
O	-0.872714	-0.583124	-0.283382
O	-5.504756	-0.666632	-1.377485
H	-4.959264	1.202041	2.794888
H	-5.669278	-3.040422	-0.246023
H	-5.261571	1.732294	-2.439920
Ta	1.161710	-0.461110	0.002661
N	0.670294	1.409706	1.223763
N	1.243964	-2.183654	1.042264
N	1.486569	-0.820596	-1.959504
C	0.187384	-3.213091	0.926895
H	0.674575	-4.195937	0.716121
H	-0.453977	-2.983287	0.053774
C	-0.708247	-3.331485	2.169356
H	-1.455496	-4.139219	2.024720
H	-0.129564	-3.572837	3.085018
H	-1.263245	-2.387320	2.344734
C	0.666992	-1.805765	-2.687748
H	1.354693	-2.510554	-3.217628
H	0.102990	-2.420847	-1.956098
C	-0.329691	-1.201506	-3.689703
H	-0.899234	-2.010113	-4.194279
H	-1.056354	-0.541134	-3.174379
H	0.178215	-0.612930	-4.481492
C	2.346559	-2.635222	1.891530
H	2.001454	-2.841014	2.931972
H	2.790008	-3.583720	1.503797

H	3.143836	-1.872459	1.937446
C	2.472726	-0.166388	-2.817754
H	3.129619	0.498017	-2.226920
H	3.115983	-0.917925	-3.334620
H	1.990257	0.451947	-3.610340
C	1.426887	1.402481	2.345385
C	2.721628	2.016728	2.331673
N	2.993696	0.101823	0.351180
H	3.065534	1.116512	1.445690
C	4.330012	-0.099217	0.011898
C	5.303854	0.933280	0.139479
C	4.776472	-1.360707	-0.483086
C	6.647036	0.711641	-0.200791
H	4.984876	1.924925	0.495206
C	6.121119	-1.574286	-0.815950
H	4.035984	-2.166598	-0.603853
C	7.069262	-0.542643	-0.676879
H	7.373863	1.533599	-0.094225
H	6.434097	-2.562291	-1.192051
H	8.124570	-0.714042	-0.940727
H	2.850310	2.945478	1.751466
C	0.536874	2.600177	0.461287
C	0.451740	2.556874	-0.951541
C	0.357433	3.854378	1.101975
C	0.242407	3.727248	-1.697909
H	0.540916	1.598125	-1.494525
C	0.145767	5.018821	0.351336
H	0.367110	3.900834	2.201862
C	0.093306	4.967395	-1.054104
H	0.187080	3.661872	-2.795982
H	0.005392	5.978695	0.874026
H	-0.079669	5.883081	-1.640289
C	1.082432	0.410571	3.425027
H	0.309092	-0.306413	3.091489
H	1.973627	-0.134132	3.797640
H	0.666211	0.977019	4.288829
H	3.324868	1.969825	3.254665

F_M

SCF Done: -404.028486698 A.U.

C	1.992987	0.878293	1.230521
H	2.606776	0.461659	2.058013
C	2.077998	-0.027512	0.016325
C	3.470804	-0.367711	-0.464988
H	4.036011	0.555876	-0.717877
H	4.049020	-0.882117	0.333530
H	3.417282	-1.020531	-1.356099
H	0.953117	1.013644	1.583142
N	1.075876	-0.535640	-0.613969
C	-0.266439	-0.262587	-0.312454
C	-1.098001	-1.300890	0.178365
C	-0.848594	1.001006	-0.587189
C	-2.461156	-1.068787	0.412766
H	-0.651967	-2.289098	0.370231
C	-2.218444	1.217219	-0.365238
H	-0.215254	1.804054	-0.996341
C	-3.032583	0.188676	0.140705
H	-3.088497	-1.885441	0.805540
H	-2.652801	2.205019	-0.589992
H	-4.105862	0.362405	0.315258
H	2.421601	1.877762	0.999506

C2-D2-anti

SCF Done: -2707.45603733 A.U.

O	3.362724	1.502372	1.222413
Si	5.013884	1.847042	1.109011
O	5.340792	2.030260	-0.540907
Si	4.923559	0.718174	-1.519974
O	3.274190	0.439425	-1.256613
Si	2.813407	0.164111	0.351714
O	3.750498	-1.140359	0.877585
Si	5.427165	-0.960876	0.743791
O	5.731547	-0.623514	-0.885215
O	1.218102	-0.077194	0.501443
O	5.821635	0.443888	1.596544
H	5.236511	0.948996	-2.945252
H	6.164163	-2.146390	1.226504
H	5.402636	3.031987	1.900162
Ta	-0.606545	-0.607154	-0.066333
N	-0.474132	-2.568355	0.384138
N	-1.075575	-0.714100	-1.981838
C	0.030488	-2.948257	1.717057
H	-0.760383	-3.520638	2.259970
H	0.195648	-2.022526	2.312804
C	1.336452	-3.757076	1.689315
H	1.643530	-4.011930	2.725142
H	1.222161	-4.711678	1.135539
H	2.155133	-3.172528	1.223705
C	0.037032	-0.717217	-2.952839
H	-0.070545	0.177737	-3.612722
H	0.995285	-0.574322	-2.402414
C	0.135647	-1.983472	-3.814825
H	0.994701	-1.897930	-4.512120
H	0.292247	-2.886125	-3.189479
H	-0.775843	-2.138123	-4.427443
C	-1.033492	-3.696754	-0.355673
H	-0.266343	-4.479347	-0.557896
H	-1.859965	-4.184705	0.214863
H	-1.440041	-3.361909	-1.328467
C	-2.418633	-0.687138	-2.572944
H	-3.184056	-0.392104	-1.814939
H	-2.453238	0.056912	-3.403298

H	-2.700439	-1.678009	-2.996191
N	-1.295686	1.513122	0.331841
C	-2.148990	1.143469	1.266256
C	-2.311057	-0.328986	1.260701
H	-2.610552	1.842896	1.997971
C	-2.738506	-1.027949	2.541957
H	-2.882269	-2.114975	2.378028
H	-3.710085	-0.625056	2.906834
C	-0.939602	2.929166	0.042802
C	-0.125172	2.946949	-1.265473
H	-0.716346	2.518167	-2.100359
H	0.153261	3.985713	-1.537073
H	0.811766	2.362026	-1.164009
C	-2.215660	3.780082	-0.135259
H	-1.942369	4.831682	-0.360011
H	-2.833218	3.399578	-0.974569
H	-2.845480	3.784020	0.777125
C	-0.080993	3.478353	1.205750
H	0.833992	2.867224	1.343359
H	0.227890	4.524045	0.998166
H	-0.650332	3.476287	2.158487
H	-1.999936	-0.908013	3.364375
H	-3.132800	-0.404602	0.446831
N	-4.446216	0.681844	-0.308760
H	-4.256176	1.584740	-0.774227
C	-5.780353	0.585861	-0.049215
C	-6.314276	-0.618055	0.533071
C	-6.736183	1.630134	-0.312746
C	-7.673131	-0.752793	0.830055
H	-5.616633	-1.448049	0.734575
C	-8.094675	1.481696	-0.012545
H	-6.372865	2.570386	-0.764240
C	-8.584969	0.292004	0.564555
H	-8.036868	-1.694992	1.274714
H	-8.789568	2.310139	-0.233189
H	-9.655186	0.178636	0.797796

D2-anti

E = -2707.51793978 A.U.

O	-2.912035	1.270240	-1.341883
Si	-4.356452	2.143774	-1.416932
O	-4.294575	3.270165	-0.157341
Si	-4.049192	2.624969	1.386417
O	-2.622690	1.723232	1.300646
Si	-2.576063	0.505171	0.129513
O	-3.912884	-0.482181	0.447771
Si	-5.418599	0.284389	0.478558
O	-5.299345	1.512916	1.634124
O	-1.179598	-0.309439	0.104689
O	-5.588320	1.056235	-1.016525
H	-4.000225	3.664768	2.434786
H	-6.526441	-0.651846	0.760496
H	-4.568217	2.778182	-2.734353
Ta	0.501965	-1.325703	-0.102496
N	-0.199784	-2.535080	-1.611926
N	0.990576	-2.849556	1.115629
C	-1.112404	-2.017739	-2.646267
H	-0.652128	-2.139175	-3.658271
H	-1.250300	-0.924369	-2.506486
C	-2.495201	-2.690131	-2.623813
H	-3.132175	-2.292407	-3.441752
H	-2.423395	-3.789009	-2.761917
H	-3.010011	-2.496017	-1.660646
C	2.330477	-3.208295	1.599068
H	2.659699	-4.151839	1.093182
H	3.028129	-2.412516	1.265808
C	2.459890	-3.394931	3.119028
H	3.519441	-3.593149	3.383296
H	2.136196	-2.486888	3.668438
H	1.864047	-4.252938	3.492074
C	0.420461	-3.792815	-2.012954
H	-0.340918	-4.564393	-2.275512
H	1.075672	-3.669317	-2.911855
H	1.044622	-4.201019	-1.193167
C	-0.065337	-3.788774	1.499722
H	-1.019201	-3.521452	0.999312
H	0.188935	-4.833074	1.193897
H	-0.251820	-3.793931	2.597533
N	1.829046	0.085084	0.658504
C	2.573565	0.478393	-0.550929
C	2.083500	-0.633473	-1.499020
H	2.236422	1.473321	-0.920897
C	1.835130	-0.225213	-2.949062
H	1.556077	-1.092874	-3.580975
H	2.742209	0.235526	-3.404733
C	1.914307	0.866459	1.922510
C	3.262824	0.636097	2.653283
H	4.119611	1.022883	2.069366
H	3.259957	1.158008	3.633960
H	3.426879	-0.444281	2.846660
C	1.738657	2.376574	1.634308
H	1.713349	2.946362	2.586769
H	2.574073	2.785169	1.029855
H	0.784710	2.565436	1.099005
C	0.768256	0.401820	2.848717
H	0.830444	-0.689787	3.040103
H	0.825269	0.920625	3.828067
H	-0.223109	0.624469	2.405766
H	1.015660	0.521709	-3.036914
N	4.022961	0.563799	-0.420112
H	4.472880	-0.280648	-0.059838
C	4.857278	1.656393	-0.604552

C	4.418494	2.897794	-1.143543
C	6.232753	1.542836	-0.251574
C	5.317098	3.964178	-1.305661
H	3.372066	3.028652	-1.455936
C	7.118044	2.613611	-0.426480
H	6.600457	0.589469	0.164989
C	6.672015	3.840810	-0.952339
H	4.943192	4.911788	-1.727016
H	8.175429	2.485660	-0.142295
H	7.368337	4.682382	-1.087373
H	2.822184	-1.474060	-1.466179

F2-anti

E = -404.024892978 A.U.

C	-1.906380	0.074074	0.000174
H	-1.724770	1.160688	0.000439
C	-3.178126	-0.400959	-0.000312
C	-4.403279	0.468630	-0.000307
H	-5.046478	0.281967	0.889499
H	-4.139795	1.546857	0.000182
H	-5.046015	0.282803	-0.890674
H	-3.336567	-1.496491	-0.000269
N	-0.757998	-0.706890	0.000653
H	-0.899532	-1.719448	0.000460
C	0.571467	-0.287953	0.000191
C	1.595458	-1.272735	-0.000064
C	0.955156	1.078227	0.000264
C	2.946760	-0.905367	-0.000270
H	1.315417	-2.340002	-0.000034
C	2.313646	1.430574	-0.000018
H	0.195579	1.873237	0.000561
C	3.322221	0.451087	-0.000292
H	3.717288	-1.693154	-0.000443
H	2.584929	2.498799	0.000025
H	4.384393	0.739505	-0.000522

C3-D3-M

E = -2707.46267864 A.U.

O	-2.640329	0.353307	1.401506
Si	-4.316332	0.506130	1.356950
O	-4.937042	-1.067671	1.312670
Si	-4.364902	-2.031858	0.046995
O	-2.683560	-2.034159	0.161439
Si	-1.908504	-0.523843	0.147888
O	-2.451900	0.228691	-1.283907
Si	-4.122532	0.362420	-1.488978
O	-4.744674	-1.204540	-1.380470
O	-0.310067	-0.601695	0.249315
O	-4.699565	1.200331	-0.139878
H	-4.939608	-3.393721	0.074084
H	-4.486204	1.024185	-2.760510
H	-4.853043	1.289169	2.489739
Ta	1.727189	-0.681604	0.398531
N	1.534075	0.612745	-1.641925
C	1.606399	0.131868	-3.077528
C	2.942573	-0.553738	-3.400819
H	2.917438	-0.905049	-4.453638
H	3.807539	0.129075	-3.288422
H	3.116735	-1.424269	-2.742758
C	0.451577	-0.877431	-3.248657
H	-0.521041	-0.433718	-2.951690
H	0.377232	-1.201205	-4.307380
H	0.621993	-1.775390	-2.621100
C	1.375272	1.324106	-4.037997
H	0.419670	1.842989	-3.809937
H	2.193101	2.069131	-3.987482
H	1.315826	0.964378	-5.086234
N	1.950585	-0.809061	2.401160
N	2.098234	-2.616809	-0.008356
C	1.141615	0.006210	3.318932
H	0.621101	-0.681052	4.033126
H	0.341043	0.504701	2.733418
C	1.916587	1.062669	4.122572
H	1.220899	1.633338	4.772374
H	2.687348	0.608148	4.778581
H	2.423199	1.786425	3.451275
C	1.135120	-3.631205	0.466155
H	1.676121	-4.353694	1.127144
H	0.379536	-3.128236	1.105934
C	0.405814	-4.400311	-0.645382
H	-0.291134	-5.140448	-0.200278
H	-0.192651	-3.710396	-1.274485
H	1.105784	-4.956441	-1.302661
C	2.935824	-1.650869	3.071685
H	3.778368	-1.065185	3.509447
H	2.465471	-2.228597	3.904985
H	3.374853	-2.372640	2.354230
C	3.283771	-3.203829	-0.627976
H	4.008376	-2.406075	-0.877647
H	3.776828	-3.927567	0.066851
H	3.042248	-3.766245	-1.560407
C	2.681872	1.271139	-0.963770
C	3.434983	0.213498	-0.319227
H	4.453944	0.431595	0.054773
C	3.298939	2.526050	-1.558130
H	3.878614	2.276560	-2.471728
H	2.538023	3.289763	-1.820292
H	4.009438	2.974533	-0.834180
C	-0.416439	2.985070	-0.206838
C	-1.201491	4.143937	-0.309562
C	-0.749086	5.370110	0.210597
C	0.509186	5.422038	0.839060

C	1.305406	4.271490	0.931034
C	0.863170	3.023552	0.409357
H	-0.819303	2.032920	-0.583088
H	-2.194364	4.077861	-0.783090
H	-1.374531	6.273337	0.137029
H	0.877303	6.371503	1.260923
H	2.292564	4.324448	1.421196
N	1.682550	1.876850	0.473067
H	2.488466	2.074412	1.082266
H	0.702252	1.222380	-1.587165

D3-M

E = -2707.52393773 A.U.

O	3.067784	0.103739	0.291994
Si	4.549212	-0.701482	0.300978
O	4.675118	-1.489332	-1.190053
Si	3.396940	-2.535076	-1.556354
O	1.984156	-1.623348	-1.458587
Si	1.671433	-0.828911	0.011236
O	1.734408	-2.055242	1.189047
Si	3.135924	-2.991715	1.250413
O	3.333681	-3.658042	-0.291512
O	0.332091	0.064853	0.018630
O	4.423795	-1.917713	1.468939
H	3.565667	-3.185918	-2.873038
H	3.084941	-4.024608	2.307221
H	5.688151	0.206136	0.555158
Ta	-1.792454	-0.011808	0.084111
N	-1.863996	-1.724699	-0.963531
C	-2.053354	-3.184518	-0.789224
C	-2.680115	-3.451549	0.592020
H	-2.828756	-4.539800	0.746401
H	-2.013899	-3.086955	1.401739
H	-3.664873	-2.951439	0.693410
C	-2.972759	-3.732093	-1.907434
H	-2.541586	-3.523998	-2.910285
H	-3.090740	-4.832068	-1.816593
H	-3.982677	-3.275703	-1.867044
C	-0.682537	-3.896790	-0.876378
H	-0.188814	-3.690841	-1.848483
H	-0.007042	-3.547183	-0.071410
H	-0.804220	-4.996686	-0.780999
N	-3.840983	0.162462	0.147028
N	-1.672089	0.212980	2.091695
C	-4.831856	-0.525305	-0.689817
H	-5.689777	-0.845345	-0.044681
H	-4.361309	-1.444234	-1.087856
C	-5.386130	0.293819	-1.869492
H	-6.126162	-0.308879	-2.437344
H	-5.900839	1.219462	-1.538636
H	-4.576380	0.585247	-2.570965
C	-0.693895	1.109390	2.727399
H	-0.105004	0.523237	3.476282
H	0.035253	1.435818	1.959002
C	-1.296223	2.351797	3.402275
H	-0.493444	2.952860	3.878435
H	-1.808086	2.997517	2.658858
H	-2.026575	2.090925	4.196169
C	-4.463137	1.243324	0.912535
H	-4.739551	2.111785	0.266994
H	-5.398981	0.896069	1.414856
H	-3.767645	1.625550	1.683925
C	-2.480246	-0.536100	3.047283
H	-3.224490	-1.163784	2.519481
H	-1.846995	-1.204777	3.679121
H	-3.043140	0.133877	3.739521
N	0.410762	2.818513	-0.677091
C	1.366946	3.837725	-0.538345
C	2.729405	3.461109	-0.400511
C	1.041161	5.216816	-0.474364
C	3.725543	4.432263	-0.234559
H	2.991991	2.391688	-0.415401
C	2.051870	6.179743	-0.321685
H	-0.006720	5.541333	-0.509772
C	3.400093	5.801332	-0.206739
H	4.775223	4.112772	-0.131574
H	1.771977	7.244713	-0.275390
H	4.186463	6.562107	-0.083831
H	-1.543986	-1.532280	-1.931032
C	-1.722267	1.761859	-1.105770
H	-2.651089	1.906980	-1.691577
C	-0.830133	2.813907	-1.285061
H	0.673418	1.883521	-0.316406
C	-1.188967	3.972081	-2.198398
H	-1.930990	3.630423	-2.945177
H	-1.651672	4.815558	-1.643431
H	-0.302111	4.372450	-2.730396

D3-F2-M

E = -2994.90919644 A.U.

O	-3.373083	0.172933	-0.367660
Si	-4.765706	-0.773228	-0.350802
O	-4.537553	-1.920332	0.875457
Si	-3.150916	-2.869085	0.719930
O	-1.843059	-1.792008	0.650523
Si	-1.876993	-0.604107	-0.605729
O	-2.086808	-1.508272	-2.024679
Si	-3.398334	-2.560489	-2.108963
O	-3.240500	-3.612847	-0.790409
O	-0.624563	0.386939	-0.525948
O	-4.781622	-1.637664	-1.802406
H	-3.005398	-3.841741	1.825077

H	-3.478172	-3.283028	-3.395322
H	-5.996894	0.019677	-0.151378
Ta	1.523688	0.498066	-0.941584
N	1.899270	-1.324136	-0.823694
C	2.167605	-2.633260	-1.414512
C	2.552985	-2.480475	-2.906342
H	2.766975	-3.466722	-3.371265
H	1.724349	-2.002962	-3.468675
H	3.455600	-1.844425	-3.016778
C	3.326130	-3.326741	-0.652074
H	3.070062	-3.467361	0.419570
H	3.544942	-4.327566	-1.081503
H	4.253919	-2.720618	-0.704247
C	0.899315	-3.518475	-1.315011
H	0.597399	-3.669797	-0.257243
H	0.051662	-3.043208	-1.847557
H	1.079193	-4.520834	-1.759194
N	3.438409	1.189429	-1.149554
N	0.940744	1.368269	-2.725338
C	4.698295	0.460265	-0.997631
H	5.374760	0.718638	-1.853536
H	4.479285	-0.622642	-1.076597
C	5.457439	0.721513	0.315628
H	6.398091	0.131275	0.342669
H	5.734188	1.789480	0.436549
H	4.844200	0.429487	1.193926
C	-0.304217	2.088036	-3.013331
H	-0.782207	1.648455	-3.925894
H	-1.012497	1.914314	-2.179349
C	-0.142227	3.605447	-3.218317
H	-1.120242	4.068480	-3.469686
H	0.235731	4.094304	-2.295571
H	0.558276	3.848760	-4.044657
C	3.647262	2.624000	-1.329184
H	3.970051	3.137879	-0.391363
H	4.430473	2.826306	-2.101385
H	2.707292	3.110037	-1.664054
C	1.775104	1.230550	-3.917259
H	2.717396	0.700094	-3.677396
H	1.250883	0.654669	-4.720147
H	2.056435	2.217399	-4.360059
N	-0.532205	2.552059	1.278735
C	-1.482360	3.533400	1.607383
C	-2.845440	3.244319	1.327160
C	-1.163427	4.807619	2.143005
C	-3.847312	4.184827	1.599440
H	-3.107028	2.268569	0.886994
C	-2.180339	5.735056	2.423401
H	-0.118312	5.095453	2.310705
C	-3.527603	5.434851	2.161759
H	-4.896001	3.933480	1.372418
H	-1.905221	6.718197	2.838511
H	-4.317517	6.169999	2.380331
H	1.342426	-1.579673	0.895637
C	1.506512	1.269625	1.182639
H	2.495258	1.209179	1.683775
C	0.725060	2.267860	1.774886
H	-0.826511	1.861472	0.559973
C	1.207853	3.019680	2.999452
H	2.000075	2.431907	3.500644
H	1.650749	4.002662	2.730723
H	0.390432	3.213774	3.724123
C	3.148120	-2.522754	4.480656
C	2.245650	-2.950824	5.470839
C	0.861854	-2.856580	5.238866
C	0.380157	-2.338202	4.025839
C	1.288389	-1.914196	3.035839
C	2.676933	-2.003369	3.264045
H	4.233391	-2.594168	4.654294
H	2.620526	-3.358234	6.422544
H	0.147467	-3.189033	6.008368
H	-0.703503	-2.260571	3.843293
H	3.380870	-1.669971	2.485988
N	0.805868	-1.341318	1.808759
H	-0.200686	-1.536259	1.612769
H	0.968375	-0.190345	1.693074

F2-M

E = -404.019510552 A.U.

C	-3.441993	-0.697348	0.288138
H	-4.403408	-0.198998	0.105152
C	-2.270237	-0.066148	-0.001009
C	-2.256224	1.344390	-0.545155
H	-1.534201	1.456636	-1.380086
H	-3.266189	1.604234	-0.914961
H	-1.987906	2.094596	0.228114
H	-3.465955	-1.721382	0.694984
N	-1.054954	-0.750478	0.143019
H	-1.168063	-1.759816	0.259699
C	0.279870	-0.337626	0.087986
C	1.263668	-1.322950	-0.202667
C	0.722705	0.986483	0.342800
C	2.624366	-0.996826	-0.248503
H	0.940431	-2.358746	-0.401821
C	2.088949	1.303864	0.274249
H	0.006520	1.767636	0.625248
C	3.052239	0.324599	-0.021365
H	3.359233	-1.786019	-0.475411
H	2.403043	2.340790	0.476236
H	4.121116	0.583787	-0.065123

G

E = -2590.92485197 A.U.

O	3.041879	0.750629	1.518392
Si	4.687295	0.833841	1.161129
O	4.792651	1.408492	-0.428274
Si	3.961449	0.497632	-1.582288
O	2.349744	0.430780	-1.065824
Si	2.077358	-0.205499	0.506227
O	2.812114	-1.728918	0.489706
Si	4.441157	-1.792569	0.063647
O	4.558571	-1.077235	-1.466693
O	0.515374	-0.165760	0.872171
O	5.255988	-0.757424	1.124526
H	4.092825	1.055992	-2.944988
H	4.986713	-3.165550	0.085122
H	5.437065	1.679139	2.113581
Ta	-1.416788	-0.526471	0.272675
N	-1.766474	-1.432139	-1.253692
C	-1.884507	-2.169140	-2.491797
C	-0.749949	-3.219052	-2.599185
H	-0.823136	-3.791278	-3.548580
H	0.242974	-2.725465	-2.563983
H	-0.801073	-3.939919	-1.757750
C	-3.261089	-2.880137	-2.538085
H	-4.084757	-2.139380	-2.475569
H	-3.382041	-3.457041	-3.479622
H	-3.367198	-3.580881	-1.684995
C	-1.780100	-1.182106	-3.683189
H	-2.571598	-0.406079	-3.617456
H	-0.788606	-0.681648	-3.692395
H	-1.899155	-1.711094	-4.652472
N	-3.033912	0.643432	0.668730
N	-1.667747	-2.006432	1.634671
C	-4.417590	0.436142	0.246174
H	-5.046206	0.210839	1.147504
H	-4.448158	-0.474576	-0.386278
C	-5.059585	1.604472	-0.520109
H	-6.116925	1.369303	-0.765769
H	-5.058410	2.545154	0.068746
H	-4.523563	1.798630	-1.472465
C	-1.565500	-1.619672	3.043963
H	-0.777219	-2.238514	3.544377
H	-1.185435	-0.572632	3.105980
C	-2.876120	-1.716071	3.844662
H	-2.718595	-1.383462	4.892614
H	-3.662303	-1.077946	3.390164
H	-3.262209	-2.755600	3.882032
C	-2.863968	1.644092	1.716321
H	-3.106369	2.678458	1.376763
H	-3.496043	1.424461	2.614404
H	-1.804878	1.685413	2.061661
C	-1.852470	-3.433632	1.434084
H	-1.860115	-3.665534	0.352881
H	-1.025866	-4.022283	1.906024
H	-2.809571	-3.813299	1.867707
N	-0.579950	1.391506	-1.224481
H	0.406509	1.117783	-1.383460
H	-1.112089	1.200409	-2.082492
C	-0.687008	2.763164	-0.831457
C	-1.766467	3.555032	-1.277376
C	0.264694	3.328428	0.045922
C	-1.896719	4.885420	-0.846738
H	-2.509505	3.122749	-1.966266
C	0.129006	4.660805	0.468038
H	1.113951	2.723801	0.397226
C	-0.951684	5.446853	0.029906
H	-2.744740	5.489247	-1.207395
H	0.882883	5.087731	1.148597
H	-1.052897	6.491118	0.363817

G-H

E = -2590.89156401 A.U.

O	-2.558134	1.048844	0.605007
Si	-4.182556	1.369475	0.949619
O	-4.789288	-0.019058	1.698646
Si	-4.619662	-1.453591	0.819333
O	-2.972669	-1.612706	0.484020
Si	-2.244276	-0.326777	-0.343300
O	-3.151115	-0.116780	-1.753213
Si	-4.808820	0.132376	-1.552487
O	-5.383944	-1.188010	-0.664952
O	-0.669905	-0.556467	-0.618034
O	-4.967564	1.481045	-0.543810
H	-5.169442	-2.623505	1.535472
H	-5.517620	0.300893	-2.838011
H	-4.359410	2.582474	1.774376
Ta	1.305208	-0.521591	-0.255097
N	1.856383	-0.569120	1.567305
C	2.294681	-1.226174	2.798721
C	2.164675	-2.759901	2.670451
H	2.524461	-3.264580	3.591988
H	1.105454	-3.049363	2.511057
H	2.757913	-3.137292	1.813240
C	3.773800	-0.849381	3.062421
H	3.890210	0.251574	3.138509
H	4.137984	-1.301558	4.009273
H	4.420851	-1.209839	2.235747
C	1.417010	-0.731686	3.974607
H	1.496692	0.368964	4.093428
H	0.350287	-0.981752	3.797417
H	1.728959	-1.204480	4.929658
N	2.700009	0.357469	-1.373275
N	1.546286	-2.418202	-0.935424

C	2.144075	0.946639	-2.607303
H	2.211804	2.058487	-2.529777
H	1.049671	0.719459	-2.641063
C	2.786341	0.469565	-3.917517
H	2.295802	0.967217	-4.779323
H	3.865754	0.721003	-3.962987
H	2.678506	-0.626496	-4.049092
C	2.627097	-2.937205	-1.785479
H	2.171771	-3.473833	-2.655577
H	3.185171	-2.072683	-2.196946
C	3.617901	-3.880061	-1.082812
H	4.380761	-4.238359	-1.805819
H	4.146980	-3.359743	-0.257532
H	3.120559	-4.776726	-0.659010
C	4.091815	0.698822	-1.104420
H	4.780001	0.209993	-1.832206
H	4.254947	1.799468	-1.165670
H	4.377456	0.358568	-0.090696
C	0.556696	-3.446288	-0.602406
H	-0.294707	-3.012845	-0.042283
H	0.145567	-3.912861	-1.530098
H	0.988597	-4.262142	0.021357
N	0.685898	1.554590	0.793554
H	1.342393	0.596118	1.572453
C	1.184536	2.846900	0.583906
C	0.331633	3.922695	0.208786
C	2.565901	3.140767	0.754249
C	0.836776	5.215303	0.002956
H	-0.745290	3.722499	0.080425
C	3.064603	4.434918	0.539970
H	3.242798	2.338278	1.084945
C	2.209234	5.485680	0.158423
H	0.145354	6.024404	-0.285689
H	4.140092	4.628905	0.689117
H	2.603984	6.500678	-0.003966
H	-0.339864	1.582805	0.891303

H

E = -2590.93043138 A.U.

O	2.768313	-1.339313	0.182221
Si	4.401057	-1.701327	-0.041578
O	5.268460	-0.653574	0.962770
Si	4.963924	0.993273	0.717586
O	3.301362	1.199788	0.899664
Si	2.294330	0.270369	-0.101338
O	2.816524	0.606434	-1.681881
Si	4.448964	0.358834	-2.018737
O	5.315332	1.296302	-0.908809
O	0.725279	0.548272	0.120359
O	4.777747	-1.255307	-1.628399
H	5.749106	1.850680	1.630582
H	4.799070	0.678685	-3.418905
H	4.708365	-3.121926	0.230575
Ta	-1.210062	-0.064803	0.412625
N	-1.705404	1.886446	0.564998
C	-1.104591	3.239594	0.392299
C	-0.026102	3.482706	1.472970
H	0.424192	4.492240	1.364096
H	-0.470948	3.414039	2.488020
H	0.783485	2.731735	1.392009
C	-0.483738	3.391759	-1.014198
H	-1.249905	3.225451	-1.800219
H	-0.064427	4.410769	-1.151968
H	0.336682	2.662595	-1.159411
C	-2.237102	4.277503	0.557507
H	-3.028146	4.130166	-0.208478
H	-2.705051	4.198905	1.562469
H	-1.845556	5.309876	0.448063
N	-1.207746	-0.964627	-1.399946
N	-0.827060	-1.070879	2.106228
C	-1.815780	-2.268687	-1.695172
H	-2.507750	-2.159283	-2.566239
H	-2.455017	-2.558947	-0.834402
C	-0.804953	-3.389332	-1.989694
H	-1.336811	-4.340954	-2.200321
H	-0.175508	-3.159918	-2.874026
H	-0.124498	-3.554887	-1.128264
C	-0.816206	-2.535285	2.159856
H	-1.584113	-2.885470	2.897635
H	-1.147126	-2.920952	1.169605
C	0.549582	-3.152706	2.499950
H	0.491270	-4.259790	2.445538
H	1.323007	-2.799844	1.787232
H	0.878854	-2.890502	3.526518
C	-0.642784	-0.312737	-2.580926
H	0.213618	-0.885745	-3.005790
H	-1.411049	-0.206512	-3.384803
H	-0.260249	0.695719	-2.335371
C	-0.599361	-0.403883	3.383772
H	-0.708533	0.693437	3.271234
H	-1.329972	-0.746421	4.157604
H	0.424939	-0.595174	3.779364
N	-3.227142	-0.557414	0.688613
H	-2.707222	1.971882	0.783552
C	-4.397537	-0.386563	-0.055870
C	-5.643283	-0.888925	0.414997
C	-4.391892	0.293477	-1.305675
C	-6.819736	-0.729583	-0.330055
H	-5.673234	-1.416488	1.384116
C	-5.573219	0.442915	-2.047015
H	-3.444995	0.704896	-1.685874
C	-6.795994	-0.064940	-1.570476

H	-7.767791	-1.131200	0.063266
H	-5.537731	0.972699	-3.013059
H	-7.720144	0.060453	-2.155659
H	-3.454652	-0.983059	1.596386

H-I-anti

E = -2707.44845724 A.U.

O	-3.193735	-1.592410	0.903696
Si	-4.861101	-1.390490	1.039748
O	-5.469155	-1.358688	-0.538527
Si	-4.784106	-0.190162	-1.551162
O	-3.119621	-0.459107	-1.537979
Si	-2.356333	-0.450384	-0.022746
O	-2.759428	1.063746	0.654419
Si	-4.406440	1.420364	0.779772
O	-5.034059	1.298299	-0.785209
O	-0.767679	-0.677144	-0.065465
O	-5.103257	0.162690	1.667215
H	-5.355800	-0.222274	-2.913958
H	-4.655552	2.745658	1.385400
H	-5.498452	-2.436414	1.866776
Ta	1.243256	-0.407468	-0.279701
N	2.118489	-1.122802	1.276212
C	2.720227	-2.374437	1.799399
C	3.106492	-3.311156	0.638889
H	3.587157	-4.229292	1.035667
H	2.218688	-3.606756	0.048064
H	3.821257	-2.813944	-0.048700
C	3.997973	-2.021211	2.597214
H	3.772081	-1.357864	3.454339
H	4.472743	-2.942130	2.995705
H	4.735571	-1.506363	1.947506
C	1.697492	-3.085151	2.717599
H	1.387318	-2.428235	3.555461
H	0.785624	-3.357331	2.147590
H	2.129996	-4.012878	3.148454
N	1.114814	-1.920462	-1.677401
N	2.687714	0.581839	-1.273178
C	2.009934	-2.130412	-2.824575
H	2.440159	-3.162902	-2.761156
H	2.863631	-1.433035	-2.733956
C	1.357132	-1.959016	-4.207818
H	2.118372	-2.083565	-5.006917
H	0.558720	-2.705724	-4.395794
H	0.906716	-0.949949	-4.316230
C	4.101573	0.779069	-0.921547
H	4.327001	1.872685	-0.950106
H	4.241350	0.449774	0.127785
C	5.102674	0.038935	-1.823538
H	6.141164	0.285018	-1.517365
H	4.977202	-1.060680	-1.747797
H	4.998462	0.324641	-2.890838
C	0.049973	-2.931555	-1.665310
H	-0.727239	-2.751577	-2.444018
H	0.479633	-3.944477	-1.858299
H	-0.467059	-2.960824	-0.688995
C	2.269436	1.335605	-2.456045
H	1.181352	1.200522	-2.646825
H	2.450462	2.427708	-2.323825
H	2.800050	1.003807	-3.378641
N	0.637144	1.484399	0.729839
H	1.939704	-0.390274	2.148404
C	0.937172	2.802845	0.286438
C	2.235131	3.344486	0.447701
C	-0.065493	3.616537	-0.296888
C	2.528429	4.641214	-0.002533
H	3.002157	2.738636	0.951772
C	0.234270	4.913705	-0.745511
H	-1.085417	3.211431	-0.401817
C	1.534359	5.432088	-0.609653
H	3.544762	5.044896	0.135307
H	-0.559840	5.525486	-1.203385
H	1.767890	6.450073	-0.958760
H	-0.387764	1.417665	0.838117
C	1.591122	0.676592	3.355309
C	0.953347	1.591598	2.749561
C	2.073532	0.321276	4.721155
H	3.180482	0.411376	4.778157
H	1.645940	0.973309	5.514169
H	1.837350	-0.731977	4.985256
H	0.437834	2.554396	2.770439

H-I-M

E = -2707.45296962 A.U.

O	3.273515	-1.130769	-1.252121
Si	4.938280	-0.874221	-1.236750
O	5.489002	-1.359166	0.287543
Si	4.734667	-0.605212	1.599709
O	3.081090	-0.872732	1.422063
Si	2.367496	-0.377524	-0.036160
O	2.756201	1.284102	-0.159664
Si	4.397675	1.681213	-0.079225
O	4.970900	1.057839	1.382099
O	0.788662	-0.636276	-0.127991
O	5.161781	0.803009	-1.303589
H	5.256967	-1.079939	2.898375
H	4.629961	3.136608	-0.200621
H	5.635345	-1.576111	-2.334713
Ta	-1.239296	-0.541402	0.119524
N	-2.093655	-0.885927	-1.550984
C	-2.728182	-1.934702	-2.379328
C	-3.244965	-3.078290	-1.483101

H	-3.732124	-3.861155	-2.101357
H	-2.415980	-3.541571	-0.913757
H	-3.988288	-2.701351	-0.750454
C	-3.923250	-1.311932	-3.142279
H	-3.597039	-0.480404	-3.798372
H	-4.419858	-2.075361	-3.777160
H	-4.675551	-0.911154	-2.431792
C	-1.691540	-2.492511	-3.384888
H	-1.292199	-1.688359	-4.035296
H	-0.835656	-2.947652	-2.845921
H	-2.148741	-3.268430	-4.034723
N	-1.052255	-2.353382	1.088799
N	-2.708358	0.114476	1.330902
C	-1.873042	-2.858054	2.196880
H	-2.288506	-3.859466	1.913467
H	-2.741296	-2.183422	2.319111
C	-1.142904	-2.997827	3.544705
H	-1.849766	-3.342573	4.329047
H	-0.313904	-3.733864	3.503015
H	-0.713987	-2.026754	3.870563
C	-4.147813	0.263705	1.073974
H	-4.431588	1.330598	1.244634
H	-4.322771	0.052064	-0.000247
C	-5.061122	-0.636629	1.922598
H	-6.124579	-0.415749	1.692435
H	-4.884395	-1.711293	1.711583
H	-4.921050	-0.472656	3.011241
C	0.015431	-3.303391	0.754306
H	0.825563	-3.332267	1.519930
H	-0.398661	-4.338019	0.673064
H	0.492142	-3.050682	-0.210986
C	-2.282139	0.666661	2.616289
H	-1.175646	0.605204	2.725011
H	-2.564922	1.741585	2.708890
H	-2.717739	0.116874	3.482818
N	-0.692223	1.569007	-0.360246
H	-1.796675	0.058042	-2.292248
C	-1.338743	2.735391	0.110188
C	-2.686973	3.003779	-0.236440
C	-0.655491	3.680475	0.919321
C	-3.329888	4.158924	0.233061
H	-3.212298	2.301196	-0.899758
C	-1.305771	4.834357	1.387638
H	0.398000	3.492307	1.187005
C	-2.649417	5.079790	1.053221
H	-4.377010	4.348702	-0.054417
H	-0.753557	5.548622	2.019772
H	-3.158931	5.985259	1.418021
H	0.323259	1.666434	-0.207081
C	-1.289746	1.115264	-3.153324
H	-1.529019	1.001862	-4.217889
C	-0.526944	1.917407	-2.525171
C	0.464942	2.999102	-2.436303
H	0.115819	3.841499	-1.802720
H	1.430497	2.635212	-2.024483
H	0.650689	3.392549	-3.45