Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting information for the manuscript

CO_2 Conversion to Isocyanate via Multiple N-Si Bond Cleavage at a Bulky Uranium(III) Complex

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Table of Contents :

1. General considerations.

All manipulations were carried out under an inert argon atmosphere using Schlenk techniques and an MBraun glovebox equipped with a purifier unit. The water and oxygen level were always kept at less than 1 ppm. The solvents were purchased from Aldrich in their anhydrous form conditioned under argon and were vacuum distilled from K/benzophenone (hexane, THF). Depleted uranium turnings were purchased from the "Société Industrielle du Combustible Nucléaire" of Annecy (France). [K(18c6)][U{N(SiMe$_3$)$_2$}$_4$] was synthesized as previously described.[1] Elemental analyses were performed under argon by Analytische Laboratorien GMBH at Lindlar, Germany. ^{1}H NMR experiments were carried out using NMR tubes adapted with J. Young valves. ^{1}H NMR spectra were recorded on Bruker 200 MHz and 400 MHz spectrometers. NMR chemical shifts are reported in ppm with solvent as internal reference. Mass spectra were acquired on a LXQ-linear ion trap (Thermo Scientific, San Jose, CA,USA), equipped with an electrospray source in a THF solution which was prepared and filtered on microporous filters in the glove-box and maintained under argon until injection into the spectrometer. Electrospray full scan spectra, in the range of m/z 50 –3000 amu, were obtained by infusion through fused silica tubing at 2-10 μL.min^{-1}. The LXQ calibration (m/z 50-2000) was achieved according to the standard calibration procedure from the manufacturer (mixture of caffeine/MRFA and Ultramark 1621). The LXQ calibration (m/z 2000-4000) was performed with ES tuning mix (Agilent). The temperature of the heated capillary of the LXQ was set to the range of 180-220 °C, the ion spray voltage was in the range of 1-3 kV with an injection time of 5-100 ms. The experimental isotopic profile was compared in each case to the theoretical one. IR spectra were recorded with a Perkin Elmer 1600 Series FTIR spectrophotometer.

Caution: Depleted uranium (primary isotope ^{238}U) is a weak α-emitter (4.197 MeV) with a half-life of 4.47×10^9 years. Manipulations and reactions should be carried out in monitored fume hoods or in an inert atmosphere glovebox in a radiation laboratory equipped with α- and β-counting equipment.

2. Synthesis

2.1 Synthesis of [K(18c6)] [U{N(SiMe$_3$)$_2$}$_3$(NCO)$_2$], 2

CO_2 (2-3 equiv) was condensed on a liquid nitrogen frozen suspension of **1** (84.0 mg, 0.071 mmol, 1equiv) in THF (1 mL). The dark purple suspension was allowed to warm up at room temperature and the reaction was stirred at room temperature over a period of 48 h resulting in a color change of the solution from dark purple to light pink. The mixture was centrifuged and the pink THF supernatant was recovered. The solvent volume was reduced to 3 mL, layered with 10 mL hexane and let stand at room temperature overnight. This produced [K(18c6)] [U(N(SiMe$_3$)$_2$)$_3$(NCO)$_2$], **2** as a pink microcrystalline solid which was collected by centrifugation and dried *in vacuo* (37.7 mg, 0.034 mmol, 48%). THF solutions of **2** are stable for at least 10days at room temperature.

The same procedure was followed to produce the ^{13}C carbon dioxide analogue of **2.** The reaction with $^{13}CO_2$ was followed by ^{13}C NMR.

Pink single crystals of **2** suitable for X-ray diffraction studies were grown by slow diffusion of hexane into a THF solution of **2**.

ES-MS: m/z = 802.7 [U(N(SiMe$_3$)$_2$)$_3$(NCO)$_2$]$^-$.

^{1}H NMR (200 MHz, THF-d_8, 298 K): δ = 4.7 (s, 24H, 18c6); -10.9 (s, 54H, CH3).

^{13}C NMR (400 MHz, THF-d_8, 298K): δ = 492 (NCO), 71.54 (18c6).

FT-IR (KBr, cm^{-1}): 2954 (m, ν_{CH}), 2902 (m, ν_{CH}), 2201 (s, ν_{NCO}), 1351 (m), 1248, (m) 1117 (m), 965 (m).

Anal. Calcd for **2**: $C_{32}H_{78}N_5O_8Si_6UK$: C 34.73; H 7.10; N 6.33; Found C, 34.34; H, 7.01; N, 6.35.

2.2 Reaction of [K(18c6)] [U{N(SiMe$_3$)$_2$}$_4$] with 1 equivalent of $^{13}CO_2$

One equivalent of $^{13}CO_2$ (1 equiv) was condensed on a dark purple liquid nitrogen frozen suspension of [K(18c6)][U{N(SiMe$_3$)$_2$}$_4$] (24.3 mg, 0.021 mmol, 1 equiv) in THF-d_8 (0.5 mL). The dark purple suspension was allowed to warm up at room temperature and the ^{1}H and ^{13}C NMR spectra were recorded over a period of 4 days following the addition of $^{13}CO_2$. No color change was observed in this period of time. Attempts of crystallization failed in various solvent at room temperature or -40°C.

Computational Details

All the structures reported in this study were fully optimized with the Becke's 3-parameter hybrid functional combined with the non-local correlation functional provided by Perdew/Wang (denoted as B3PW91).[2] The choice of the basis set for the uranium atom, which has a fixed oxidation state (IV) in all the calculations, is the quasi-relativistic energy-consistent 5*f*-in-core RECP (Relativistic Effective Core Potential) in combination with its adapted basis set, augmented by an extra *f* polarization function.[3] In addition, for the silicon atoms the quasi-relativistic energy-adjusted ab-initio pseudopotential is used, along with its corresponding energy-optimized valence basis set,[4] augmented by a d polarization function.[5] Since the full system has been considered, a more sophisticate combination of basis set is used for the sake of the computational cost. In particular, the 6-31G(d) basis set is used for the nitrogen atoms of the amide groups and the inserted CO_2 molecules, being directly connected to uranium atom.[6] For the remaining atoms (carbon and hydrogen atoms of the amide ligands) the minimal 3-21G basis set is applied.[7] It should be noted that this computational protocol was found to give rational results in related studies.[8] In all computations no constrains are imposed on the geometry. All stationary points have been identified for minimum (number of imaginary frequencies $N_{imag}=0$) or transition states ($N_{imag}=1$). Intrinsic Reaction Paths (IRPs) are traced from the various transition structures to verify the reactant to product linkage.[9] Enthalpy energies are obtained at T=298.15K within the harmonic approximation. GAUSSIAN09 program suite is used in all calculations.[10]

3. X-ray Crystallography.

Diffraction data were taken using an Oxford-Diffraction XCallibur S kappa geometry diffractometer (Mo-Kα radiation, graphite monochromator, λ = 0.71073 Å). To prevent evaporation of co-crystallised solvent molecules the crystals were coated with light hydrocarbon oil and the data were collected at 150 K. The cell parameters were obtained with intensities detected on three batches of 5 frames. The crystal-detector distance was 4.5 cm. The number of settings and frames has been established taking in consideration the Laue symmetry of the cell by CrysAlisPro Oxford-diffraction software.[11] 996 for **2** narrow data were collected for 1° increments in ω with a 4 s exposure time. Unique intensities detected on all frames using the Oxford-diffraction Red program were used to refine the values of the cell parameters. The substantial redundancy in data allows empirical absorption corrections to be applied using with the ABSPACK Oxford-diffraction program[11] for **2**. Space groups were determined from systematic absences, and they were confirmed by the successful solution of the structure. The structures were solved by direct methods using the SHELXTL 6.14 package.[12] All non-hydrogen atoms were found by difference Fourier syntheses and refined on F^2. Hydrogen atoms were fixed in ideal position. Experimental details for X-ray data collections of **2** are given in Table S1.

Table *S1*. Crystallographic data of **2**.

	2
Formula	C32 H78 K N5 O8 Si6 U
Crystal size (mm)	0.480 x 0.371 x 0.246
cryst syst	Monoclinic
space group	P 21/m
volume (Å^3)	2735.75(11)
a (Å)	11.5823(2)
b (Å)	17.9907(5)
c (Å)	14.1292(3)
α (deg)	90
β (deg)	111.687(2)
γ (deg)	90
Z	2
formula weight (g/mol)	1106.66

density (g cm^{-3})	1.343
absorption coefficient (mm^{-1})	3.216
F(000)	1128
temp (K)	150(2)
total no. reflections	67035
unique reflections [R(int)]	8579 [R(int) = 0.0509]
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0353, wR2 = 0.0673
Largest diff. peak and hole ($e.Å^{-3}$)	1.274 and -0.994
GOF	1.091

4. NMR spectra

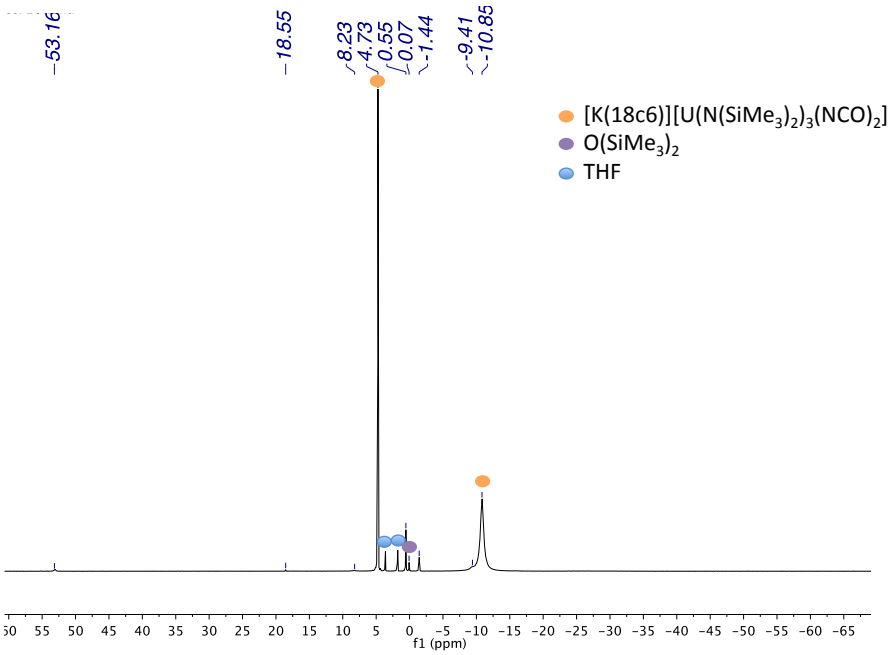

Figure S1. ^{1}H NMR spectrum (200MHz, THF-d_8, 298 K) of the crude reaction mixture between $[U(N(SiMe_3)_2)_4]$ and 2.5 equivalents of CO_2.

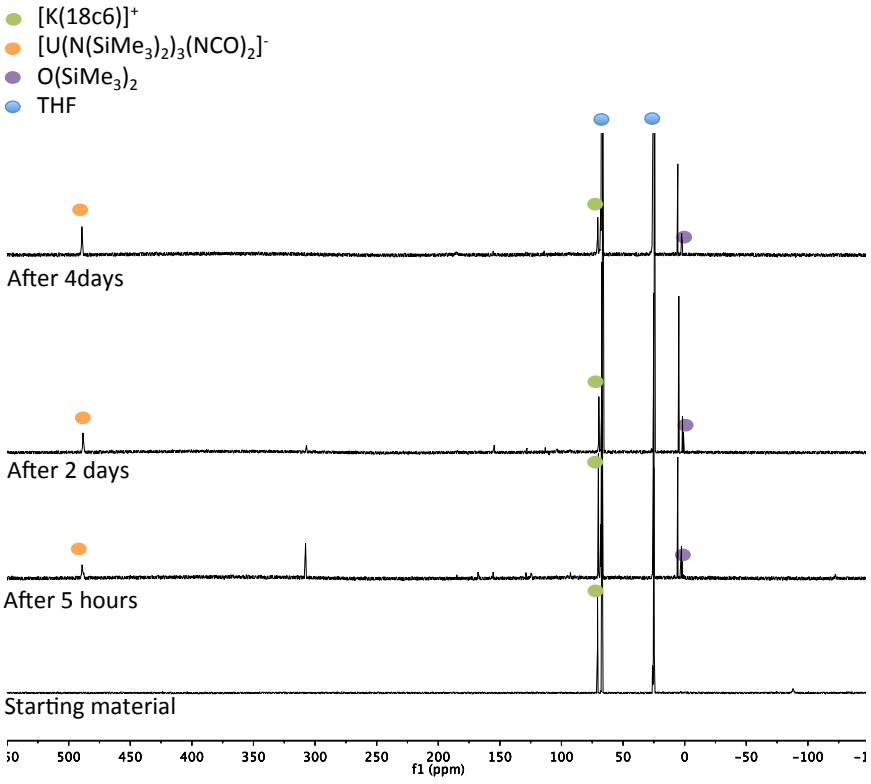

Figure S2. Evolution over time of the ^{13}C NMR spectrum (400MHz, THF-d_8, 298 K) of the crude reaction mixture between $[U(N(SiMe_3)_2)_4]$ and 2.5 equivalents of $^{13}CO_2$

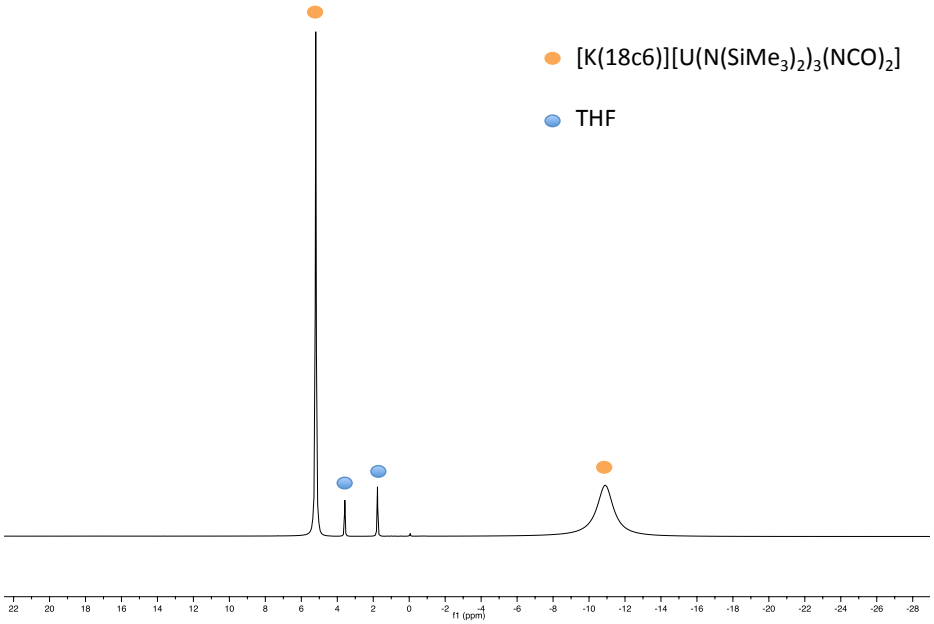

Figure S3. ^{1}H NMR spectrum (400MHz, THF-d_8, 298 K) of crystals of [K(18c6)] [U{N(SiMe$_3$)$_2$}$_3$(NCO)$_2$], 2

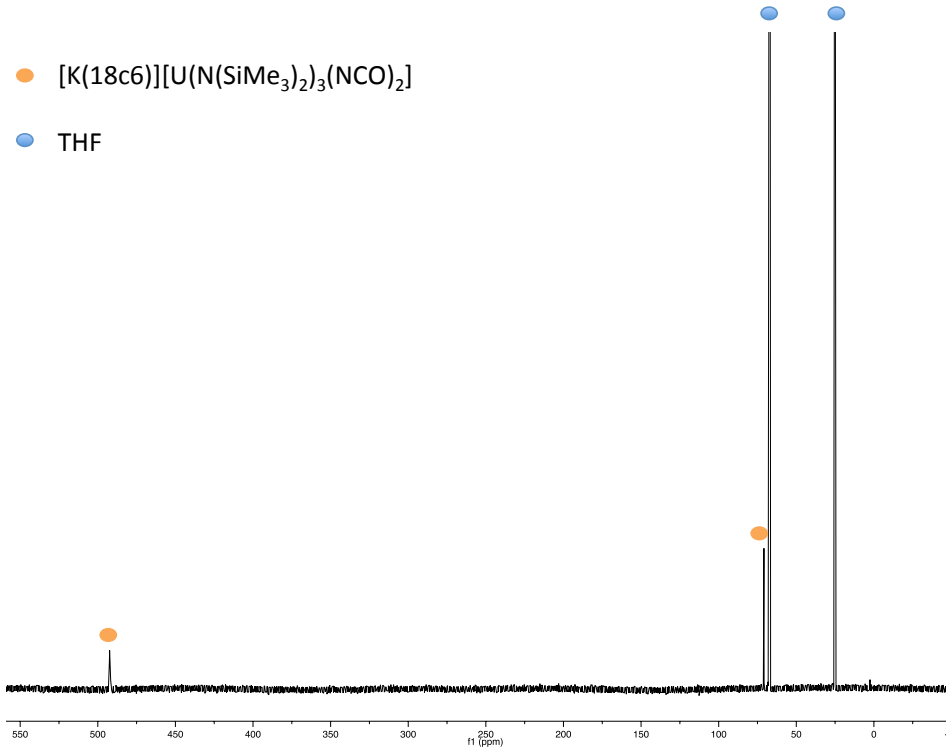

Figure S4. ^{13}C NMR spectrum (400MHz, THF-d_8, 298 K) of crystals of [K(18c6)] [U{N(SiMe$_3$)$_2$}$_3$(N^{13}CO)$_2$], 2.

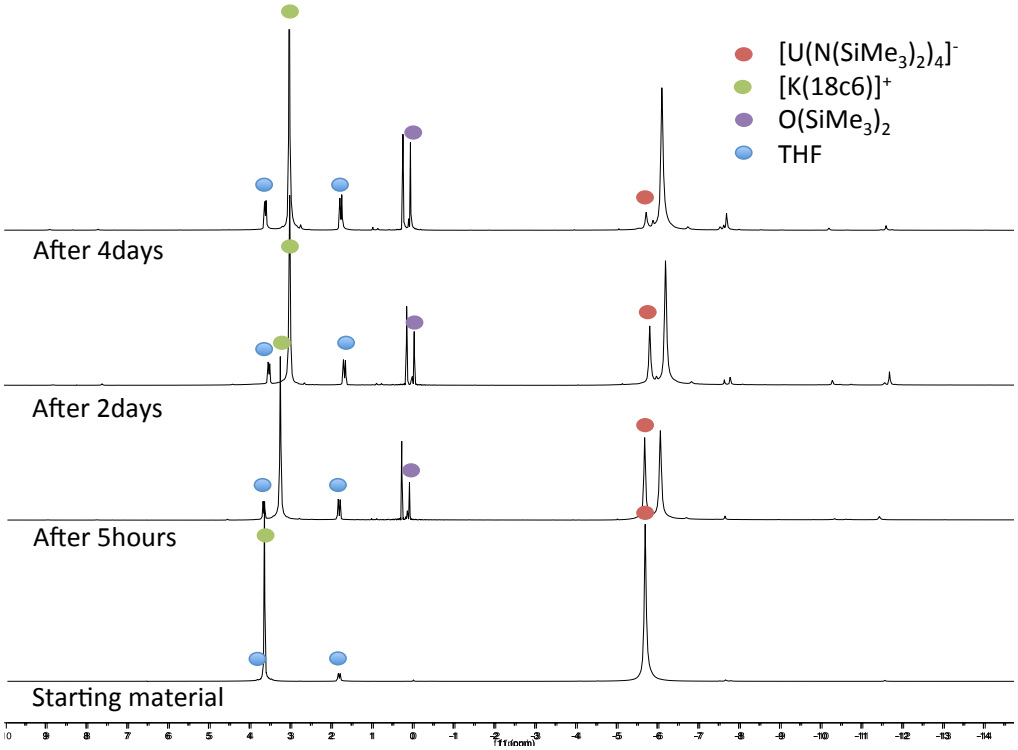

Figure S5. Evolution over time of the ^{1}H NMR spectrum (400MHz, THF-d_8, 298 K) of the crude reaction mixture between $[U(N(SiMe_3)_2)_4]$ and 1 equivalent of $^{13}CO_2$

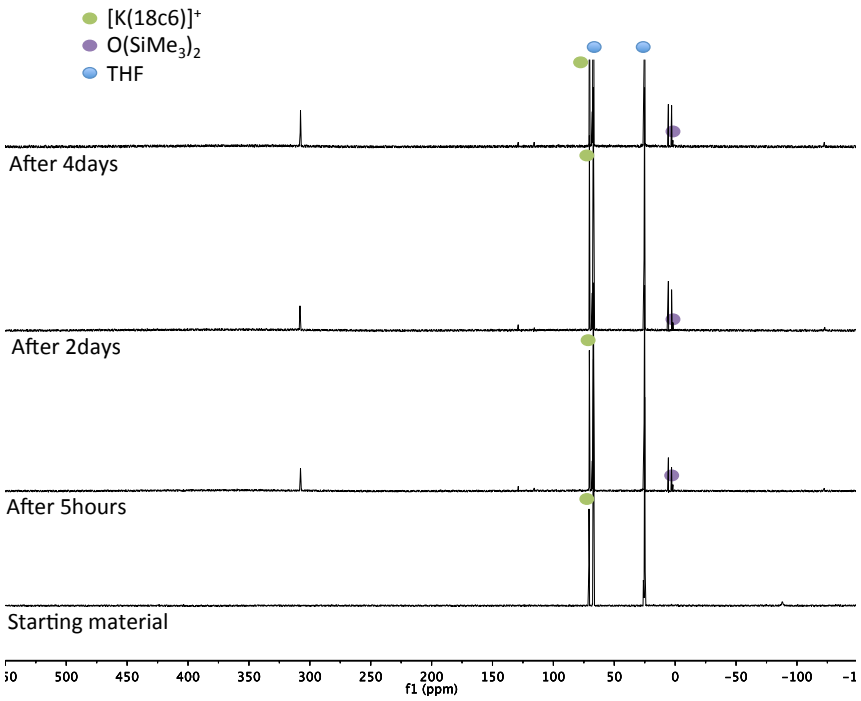

Figure S6. Evolution over time of the ^{13}C NMR spectrum (400MHz, THF-d_8, 298 K) of the crude reaction mixture between $[U(N(SiMe_3)_2)_4]$ and 1 equivalents of $^{13}CO_2$

5. Mass spectroscopy

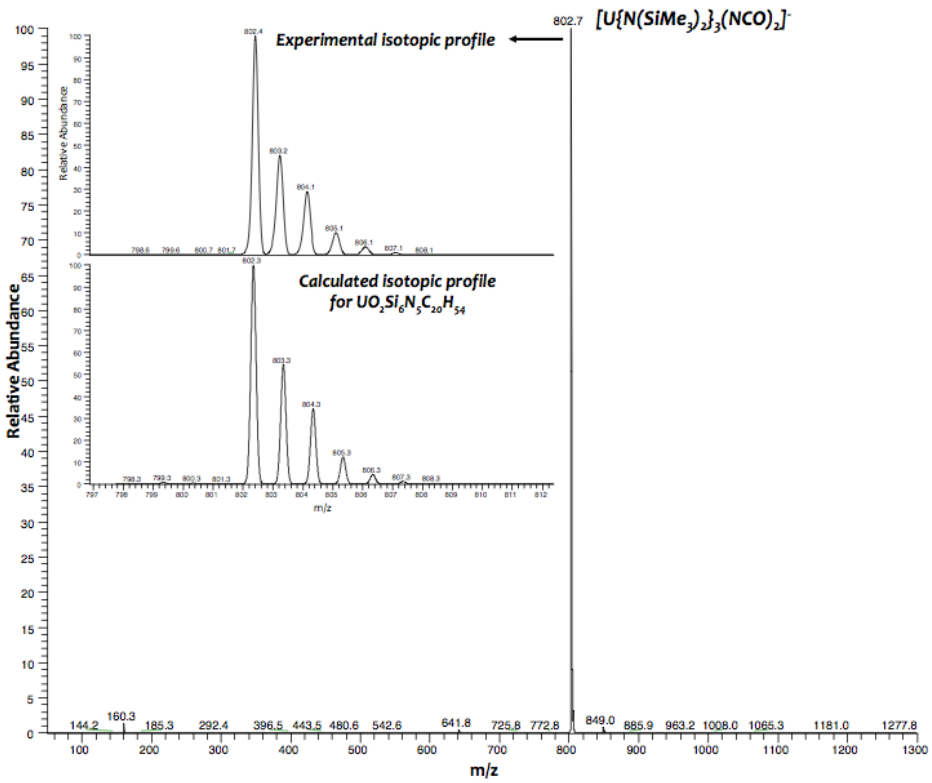

Figure S7. ESI/MS spectrum of 2 in THF.

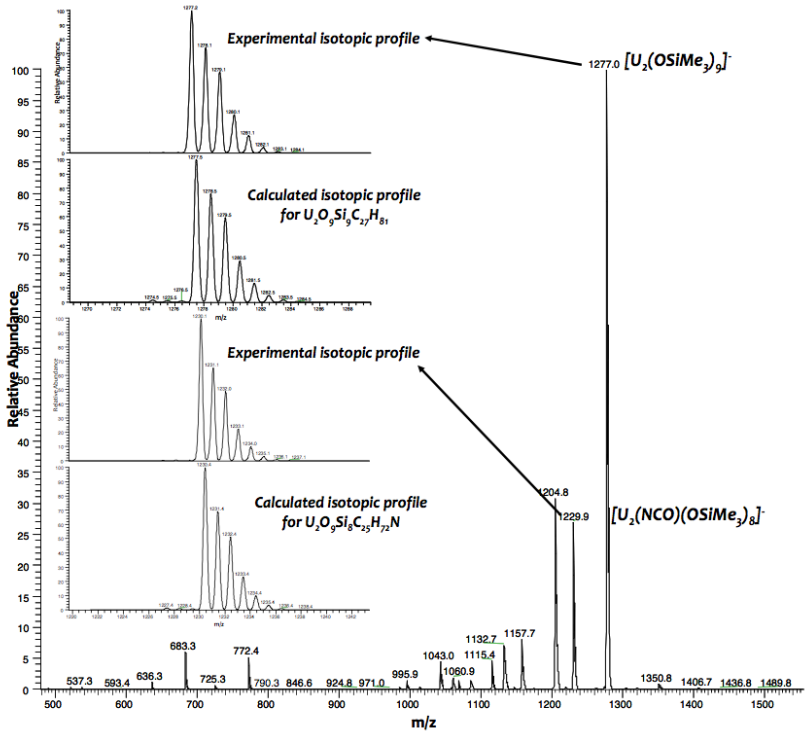

Figure S8. ESI/MS spectrum of supernatant of the crystals of 2 in THF.

6. Infrared spectrum

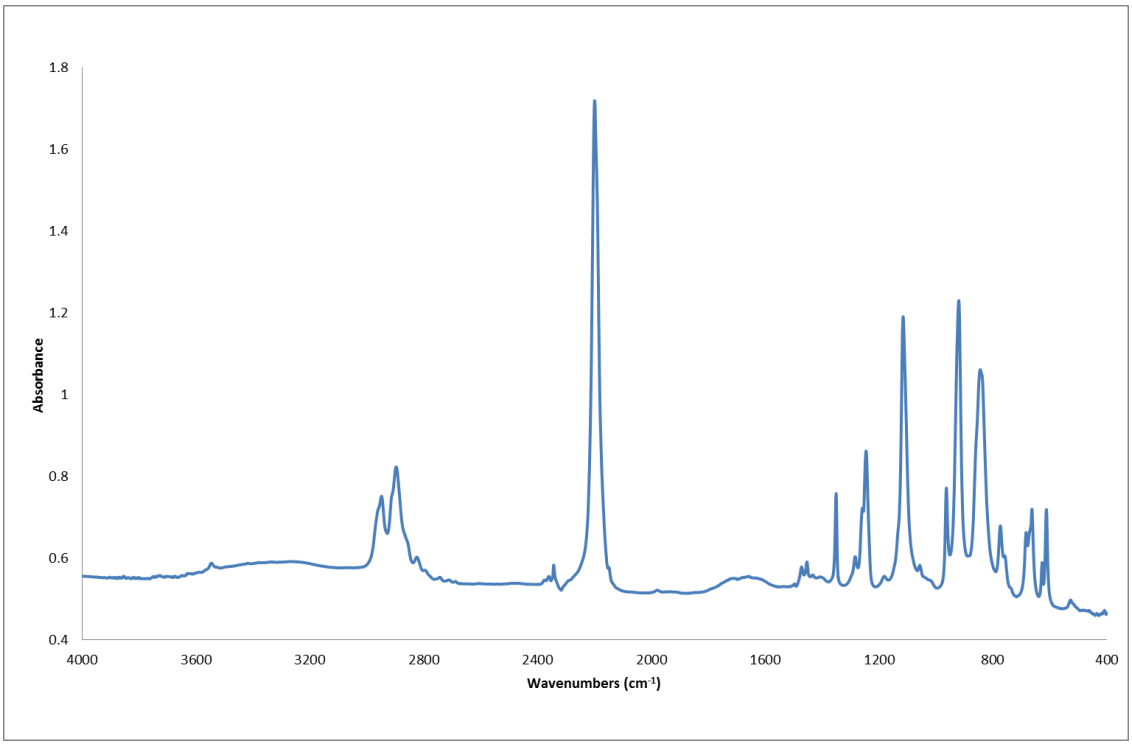

Figure S9. FT-IR spectrum of complex [K(18c6)][U{N(SiMe$_3$)$_2$}$_3$(NCO)$_2$] 2 in KBr pellet.

Table *S2*. FT-IR data for complex **2**.

Wavenumbers (cm^{-1})	Assignment
2954	C-H$_2$ (stretch)
2902	C-H$_3$ (stretch)
2201	NCO
1351	CH (bend)
1248	Si-Me$_3$
1117	Si-NR$_2$
965	C-O

7. Computational Data

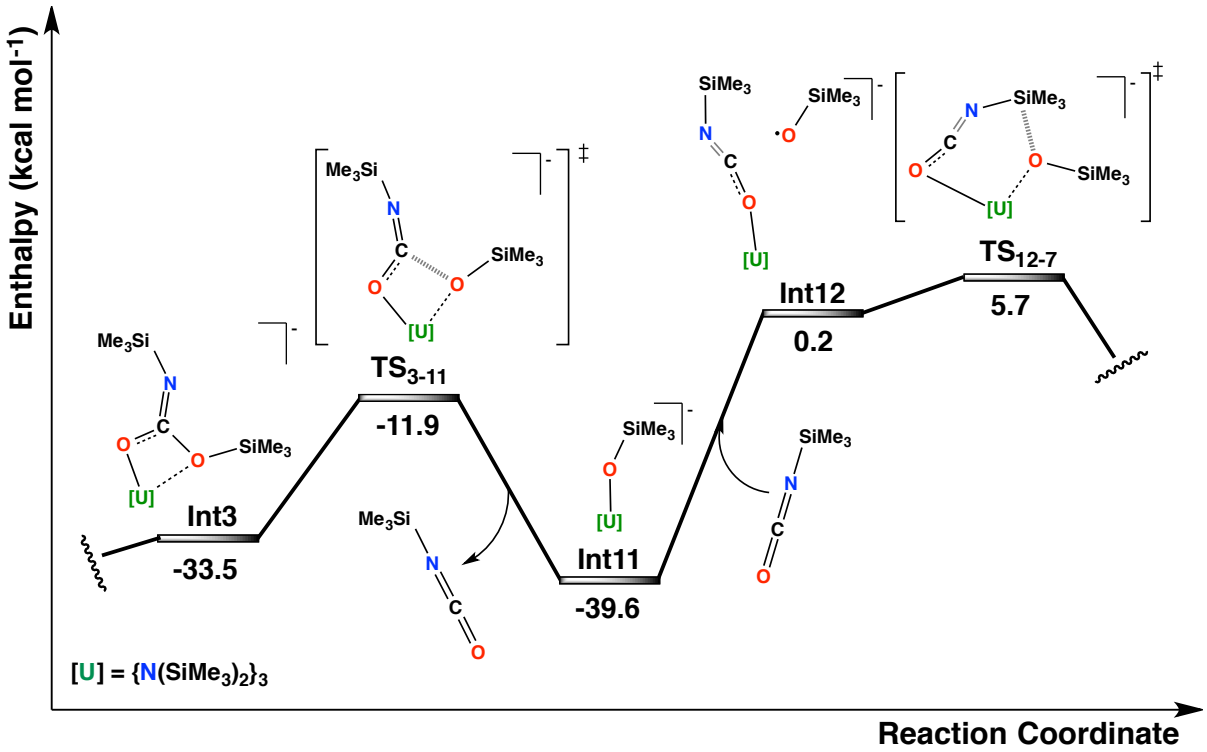

Figure S10. Part of the energy profile that leads to the formation of the siloxide complex 2.

When investigating how a siloxide by-product can be generated in this reaction, as it is experimentally observed by mass-spectroscopy, we located another plausible reaction route starting from **Int3** (depicted schematically in ESI). Hence, instead of undergoing an isomerization step to give **Int4**, the cleavage of the C-O($SiMe_3$) bond can be considered. This process will lead essentially to the formation of a siloxy intermediate, **Int11**, with concomitant release of the trimethylsilyl-isocyanate fragment ($OCNSiMe_3$), passing through the $\mathbf{TS_{3\text{-}11}}$. From **Int3,** an activation energy of 21.6 kcal.mol^{-1} is necessary to reach the transition state, which is stabilized energetically by the formation of the strong siloxide bond with the uranium(IV) center. Then the reaction can proceed through the re-association of the $OCNSiMe_3$ substrate in a concerted type transition state, $\mathbf{TS_{12\text{-}7}}$, that yields directly **Int7**. This occurs through the insertion of the U=O bond into the N-Si bond of the reinserted inorganic fragment. This involves a four-membered ring transition state that requires a relative low energy barrier of 5.5 kcal.mol^{-1}. However, this step is highly endothermic and requires almost 40 kcal.mol^{-1}, hence, prohibiting such a transition state. This extremely high endotermicity is due to the nature of the intermediate in which the siloxy ligand is fully dissociated, being in a radical form, with the $OCNSiMe_3$ ligand now being reduced and linked to the uranium center. It should be noted that the **Int12** is the outcome of the IRC calculation of $\mathbf{TS_{12\text{-}7}}$. The main

factor determining the high energy $\mathbf{TS_{12\text{-}7}}$ is the sterical hinder induced by the arrangement of the trimethylsilyl group of the siloxide pointing towards and in close proximity to the ligand environment.

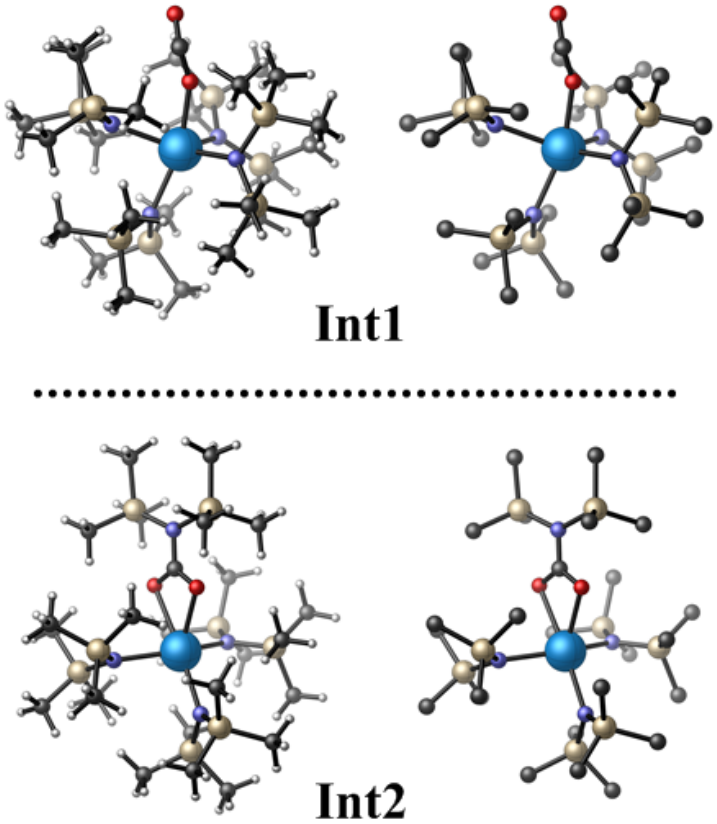

Figure S11. Geometries of the reactant and the product of the insertion step of CO_2, **Int1** and **Int2** respectively. At the right side is depicted the corresponding geometry with the hydrogen atoms being omitted for clarity.

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

Int1

H= -1428.165713 au

U	0.03773700	-0.19448700	-0.06066600
Si	1.82272800	2.63320200	1.85556800
Si	0.70592200	0.44077800	3.44644500
Si	-3.42433600	0.81183100	1.07155300
Si	-3.28617600	-0.95958700	-1.31714500
Si	0.79445100	-3.57210800	1.36427200
Si	3.13928400	-2.09345000	0.33091000
Si	1.48261300	0.86258700	-3.33617400
Si	-0.48346100	2.71716800	-2.12669800
N	0.88566900	1.13081300	1.82176700
N	-2.36383800	-0.05664100	-0.05942900
N	0.46436100	1.22287700	-1.91961400
N	1.42682100	-2.05277600	0.72908400
C	-0.37416300	-3.13731100	-1.97601100
O	0.16282100	-3.67498800	-2.92057500
O	-0.39234200	-1.93044100	-1.56638800
C	-2.10058600	2.54090200	-3.12706400
H	-2.80993100	1.90628100	-2.58485600
H	-2.54359900	3.54215400	-3.23857000
H	-1.94404100	2.11368500	-4.12313400
C	0.48864100	4.14709500	-2.96201600
H	0.77957500	3.93130000	-3.99607900
H	-0.17209400	5.02702700	-2.96710800
H	1.38868600	4.39630400	-2.38700000
C	-1.01274800	3.46100700	-0.46181000
H	-0.14876500	3.80082100	0.11509700
H	-1.65736000	4.32875000	-0.66711600
H	-1.58870400	2.75827900	0.14696800
C	-2.57369300	-0.84118300	-3.09297800
H	-2.39231900	-1.84955700	-3.48555000
H	-3.29714100	-0.32998900	-3.74251100
H	-1.62691600	-0.29618200	-3.12150200
C	-5.09048700	-0.34269200	-1.59985000
H	-5.49489100	-1.02961800	-2.35968400
H	-5.73817600	-0.39502200	-0.71750000
H	-5.12495000	0.67232500	-2.01267100
C	-3.57232300	-2.80022600	-0.90101300
H	-2.65033800	-3.38010700	-1.01238500
H	-3.95783300	-2.93072100	0.11804600
H	-4.31757300	-3.19341400	-1.60879900
C	-4.53995500	-0.40015900	2.05176600
H	-5.14848100	-1.02330900	1.38513600
H	-3.91905500	-1.06477000	2.66757900
H	-5.21211000	0.16384700	2.71498400
C	-4.56883100	2.14611000	0.28943400
H	-5.48346900	1.74073300	-0.15031700
H	-4.85078200	2.84333600	1.09240200
H	-4.03068100	2.71449500	-0.48017700
C	-2.48419300	1.85063400	2.38363800
H	-2.76894900	1.52229700	3.39217100
H	-1.39488300	1.79103800	2.29616500
H	-2.77500100	2.90370000	2.27128500
C	2.58851500	3.10463800	0.17065600
H	2.75733400	4.19120300	0.14562000
H	3.55789900	2.60290200	0.05809600
H	1.96315900	2.82029800	-0.67984200
C	0.81646000	4.14474400	2.50481800
H	1.01927400	4.29482800	3.57330200
H	1.11498800	5.05747500	1.96929700
H	-0.26245100	4.00424700	2.37919400
C	3.36763400	2.58880900	2.99871600
H	4.05220500	1.77945500	2.71385300
H	3.89576900	3.54581200	2.86647200
H	3.11849200	2.48077400	4.06062300
C	-0.70185200	-0.84764500	3.51361600
H	-1.66977600	-0.44831800	3.19582700
H	-0.46894600	-1.73290100	2.91632300
H	-0.79981800	-1.18034600	4.55826500
C	0.24739100	1.72436300	4.80089500
H	1.07250500	2.41448100	5.01324500
H	-0.63679000	2.30979500	4.52401700
H	0.02297200	1.16884000	5.72411400
C	2.24707600	-0.46321700	4.11645800
H	1.99722000	-0.95210000	5.06958800
H	2.54809900	-1.23241700	3.39997100
H	3.08896100	0.21735700	4.28392900
C	0.56132900	1.10733000	-5.00053700
H	-0.32156900	0.45613900	-5.03431200
H	0.24325800	2.13988300	-5.18457500
H	1.24043800	0.80549400	-5.81143400
C	3.07529400	1.92737900	-3.40786900
H	2.87093700	2.99773500	-3.51427400
H	3.67857900	1.78065400	-2.50273400
H	3.67026300	1.59748300	-4.27255900
C	2.10779600	-0.92351000	-3.40483200
H	2.76686200	-1.00074700	-4.28339800
H	2.70293700	-1.19046200	-2.52715600
H	1.30433200	-1.66038400	-3.50488200
C	1.32398900	-3.95235200	3.17298900
H	0.83950000	-4.89408900	3.47382400
H	2.40865700	-4.08208400	3.26401900
H	1.01133000	-3.16530300	3.86819700
C	-1.12398000	-3.62124200	1.38595200
H	-1.47725400	-3.94135600	2.37626600
H	-1.61629800	-2.67188400	1.14425300
H	-1.45945900	-4.35205200	0.64052300
C	1.33497300	-5.13653700	0.40015900
H	1.08175600	-5.05090000	-0.66296300
H	2.41160400	-5.32822100	0.49284000
H	0.79717400	-5.99961300	0.82131400
C	4.30948900	-2.76223100	1.69916300
H	4.14839400	-3.83477300	1.86874800
H	5.34414300	-2.62759400	1.34866600
H	4.19321700	-2.23518400	2.65250400
C	3.75149400	-0.31374900	0.00292800
H	4.82025000	-0.34459300	-0.25499200
H	3.23267300	0.19113200	-0.82231100
H	3.62221400	0.28960000	0.90805400
C	3.59564600	-3.19054000	-1.18022600
H	3.90934400	-4.18322200	-0.83130800
H	2.75358500	-3.32217600	-1.86815800
H	4.43592300	-2.74549600	-1.73313000

TS_{1-2}

H= -1428.142161 au

U	-0.38603100	0.67367900	-0.06028300
Si	1.63387500	3.11561600	1.99160000
Si	0.32317200	0.78672800	3.35355500
Si	-3.78372100	1.71908800	1.01069400
Si	-3.56590100	-0.30234000	-1.20206000
Si	1.09992000	-3.74318000	1.76809300
Si	3.08835000	-1.90871900	0.48951900
Si	1.07036500	1.44382900	-3.33470600
Si	-0.75723700	3.51460300	-2.19133800
N	0.59179600	1.69437300	1.85040300
N	-2.71411400	0.81048300	-0.07486800
N	0.07060600	1.96517700	-1.94874400
N	1.49636000	-2.21881400	1.05538500
C	-0.07878000	-2.59091400	-0.95222300
O	0.27586200	-3.27188800	-1.88220800

O	-0.39197600	-1.30911200	-0.98797000
C	-2.38485700	3.37312900	-3.17779300
H	-3.06539500	2.68266700	-2.66591100
H	-2.86570400	4.36096900	-3.22932100
H	-2.22171500	3.01120100	-4.19935200
C	0.32446200	4.85011400	-3.03811900
H	0.63037300	4.58346000	-4.05556600
H	-0.26233200	5.77947500	-3.08726900
H	1.22543800	5.04420500	-2.44216200
C	-1.21715000	4.31981500	-0.52863100
H	-0.32090300	4.57410900	0.04505300
H	-1.76335000	5.25087900	-0.74144500
H	-1.86875000	3.69494000	0.09044900
C	-2.68974400	-0.47629000	-2.88673300
H	-1.85605200	-1.18190900	-2.83788300
H	-3.42791600	-0.84419300	-3.61470900
H	-2.30836000	0.48928900	-3.23833500
C	-5.31791200	0.30304200	-1.70122600
H	-5.74317900	-0.48252900	-2.34394800
H	-6.00076500	0.45940300	-0.85952500
H	-5.26249800	1.22746000	-2.29044300
C	-3.78380100	-2.02881100	-0.42905500
H	-2.80775900	-2.45310600	-0.16583100
H	-4.40104600	-1.98520200	0.47710000
H	-4.26792100	-2.70237600	-1.15072700
C	-5.01137500	0.58715700	1.94998900
H	-5.68155500	0.03102800	1.28481700
H	-4.45716400	-0.13708000	2.56210200
H	-5.62396100	1.20763200	2.62074600
C	-4.80951600	3.07980600	0.13630100
H	-5.56850800	2.67073800	-0.53705500
H	-5.31664800	3.67647300	0.90928200
H	-4.15827900	3.74794300	-0.44026200
C	-2.82385600	2.63235400	2.39165000
H	-2.93596100	2.07871400	3.33223200
H	-1.75019100	2.74138800	2.20058600
H	-3.25474600	3.63411600	2.52747700
C	2.43377400	3.60100000	0.32922700
H	2.87691800	4.60321000	0.42327700
H	3.23363900	2.88834800	0.09102200
H	1.73130900	3.60329200	-0.50970100
C	0.71264700	4.64288300	2.69859900
H	0.45909800	4.47687900	3.75327500
H	1.37063000	5.52243300	2.63777000
H	-0.21354900	4.86364000	2.15661000
C	3.12699300	2.88882700	3.17141500
H	3.75504900	2.04522800	2.85989300
H	3.73356800	3.80583000	3.12922200
H	2.81905900	2.73001100	4.21215500
C	-1.04149100	-0.49971400	2.99478800
H	-1.99409200	-0.08734100	2.64062400
H	-0.66062000	-1.25458800	2.28809800
H	-1.24566000	-1.04615900	3.92765100
C	-0.22598400	1.88782800	4.82448100
H	0.60630300	2.51565200	5.16956200
H	-1.07371800	2.53526300	4.57667400
H	-0.51720700	1.22907600	5.65610900
C	1.80784600	-0.21930000	3.96949900
H	1.51682100	-0.77495800	4.87312800
H	2.06707400	-0.94455200	3.18767200
H	2.67845500	0.40074200	4.20746500
C	0.21808100	1.78349700	-5.01797300
H	-0.71909000	1.21564500	-5.08382100
H	0.00170500	2.84186400	-5.20071600
H	0.88841900	1.42707800	-5.81360400
C	2.76858400	2.32310700	-3.34777400
H	2.68360300	3.40983100	-3.46092700
H	3.30349900	2.11270100	-2.41315800
H	3.36803700	1.93029100	-4.18200600
C	1.45161600	-0.41328700	-3.37614700
H	2.02362900	-0.59331200	-4.29978700
H	2.06672000	-0.75379200	-2.53793900
H	0.55296000	-1.03634200	-3.39624400
C	1.80411200	-3.99647200	3.54764400
H	1.51671200	-4.98950900	3.92565400
H	2.89962300	-3.92559200	3.55355600
H	1.41002300	-3.23608100	4.23476400
C	-0.78521800	-4.05115300	1.99291900
H	-0.93114500	-5.08118500	2.35145300
H	-1.23786300	-3.36897600	2.72356800
H	-1.30656600	-3.93660600	1.03492800
C	1.71367800	-5.27810700	0.78160200
H	1.38053900	-5.19616900	-0.26071200
H	2.81071400	-5.34655000	0.79202300
H	1.30692300	-6.20264000	1.21834500
C	4.51697800	-2.22955700	1.74797500
H	4.60001300	-3.30285800	1.96909600
H	5.47649200	-1.88962700	1.32950000
H	4.33517600	-1.69783600	2.69115200
C	3.27660200	-0.03677800	0.07540100
H	4.29744600	0.18545900	-0.26946500
H	2.59591400	0.28082700	-0.73150900
H	3.06479800	0.56106100	0.96945700
C	3.64772300	-2.84978900	-1.09044500
H	3.83867700	-3.90417500	-0.85084100
H	2.86705700	-2.82105800	-1.85964000
H	4.57313100	-2.41121000	-1.49335100

Int2

H= -1428.234187 au

U	-0.13558400	0.40144300	-0.19925600
Si	2.59707000	2.31870200	1.06944400
Si	0.76135500	1.37997300	3.25148700
Si	-3.76355400	-0.60441100	0.01768600
Si	-2.16687700	-1.68003300	-2.25224500
Si	0.59798800	-4.35197800	2.19851700
Si	3.30502700	-3.51400300	0.48244600
Si	0.30382400	2.54044000	-3.25133600
Si	-1.51044700	3.59398400	-1.14002100
N	1.12931900	1.48269800	1.54142600
N	-2.23053800	-0.65503100	-0.83113600
N	-0.39004000	2.34346200	-1.65434300
N	1.65044500	-3.30411800	1.16987800
C	1.02911500	-2.11523900	0.80494000
O	-0.04061300	-1.74652800	1.37015700
O	1.54812900	-1.40078300	-0.13169200
C	-3.27950100	3.33011800	-1.82599100
H	-3.59655300	2.29423600	-1.65685400
H	-3.99411200	4.00509200	-1.33257500
H	-3.30766300	3.52181000	-2.90613200
C	-1.02163900	5.38410300	-1.63777600
H	-1.00296700	5.52765300	-2.72507600
H	-1.76273000	6.07695800	-1.21174800
H	-0.03465700	5.64389100	-1.23370900
C	-1.61909400	3.67041300	0.76644200
H	-1.81222300	2.69495600	1.23005300
H	-0.67180100	4.04214400	1.17370200
H	-2.43023500	4.35330400	1.06007900
C	-0.39199600	-2.30986700	-2.60761700
H	0.36714900	-1.52065400	-2.68175900
H	-0.07079900	-3.01101800	-1.82776000
H	-0.41123200	-2.84763100	-3.56808000

C	-2.75947200	-0.78350900	-3.83605300
H	-2.63216900	-1.42333400	-4.72139700
H	-3.81662800	-0.50093300	-3.75461400
H	-2.17247100	0.13285800	-3.97573000
C	-3.16079800	-3.31920200	-2.12551000
H	-4.23247900	-3.16295800	-1.95836400
H	-3.03568900	-3.87849300	-3.06498300
H	-2.76603200	-3.93257200	-1.30522600
C	-4.05239500	-2.11976900	1.15312900
H	-4.11233400	-3.05623200	0.58579900
H	-3.21817800	-2.19881600	1.86239000
H	-4.98559200	-1.99316700	1.72143200
C	-5.27375200	-0.48072300	-1.17091600
H	-6.19887000	-0.45665700	-0.57588300
H	-5.21544300	0.45095800	-1.75031200
H	-5.34019600	-1.31904600	-1.87436800
C	-4.00806500	0.89730700	1.17006700
H	-3.32953200	0.86871200	2.02854200
H	-3.87468800	1.84788100	0.64372500
H	-5.04141300	0.85548400	1.54781600
C	3.28275900	1.64073500	-0.58169400
H	4.18924300	2.20237800	-0.85524600
H	3.54266300	0.58023300	-0.48990500
H	2.56212800	1.74778400	-1.40050700
C	2.34051700	4.19940400	0.83004900
H	2.03179200	4.67760200	1.76878000
H	3.26802500	4.67637200	0.48139800
H	1.55795600	4.36484300	0.07992000
C	4.06590400	2.12674700	2.29186000
H	4.35117000	1.07089100	2.38353100
H	4.92618700	2.68442700	1.89264600
H	3.83749200	2.51584500	3.29146500
C	-1.01808900	0.78826700	3.59881600
H	-1.75099500	1.53584800	3.27301000
H	-1.22029700	-0.15697700	3.08075400
H	-1.13774600	0.63382400	4.68231700
C	0.90863700	3.07319300	4.14921700
H	1.91962000	3.49408000	4.07694700
H	0.20362300	3.79075200	3.70810300
H	0.66018700	2.95247100	5.21392800
C	1.88276600	0.14434100	4.19466600
H	1.55376000	0.06740800	5.24167500
H	1.79592400	-0.84628000	3.73081400
H	2.93638700	0.44578200	4.18121000
C	-0.97799100	3.02829000	-4.59879700
H	-1.76661100	2.26798800	-4.66863400
H	-1.44965600	3.99730000	-4.39290500
H	-0.47102300	3.09261500	-5.57299500
C	1.67376500	3.88319900	-3.34100800
H	1.26081900	4.88662300	-3.18289100
H	2.44466100	3.70543300	-2.58156200
H	2.14917600	3.85523600	-4.33279900
C	1.10835200	0.95275900	-3.94972200
H	1.53300500	1.19180300	-4.93739300
H	1.91111700	0.56663600	-3.31015300
H	0.36034000	0.16229300	-4.08074700
C	1.39187800	-6.06277400	2.48619500
H	0.65231800	-6.65036500	3.05085700
H	1.59319300	-6.59093600	1.54660100
H	2.31341600	-6.02094500	3.07609100
C	0.31325100	-3.59570100	3.91526100
H	1.26688600	-3.47623500	4.44630600
H	-0.16009300	-2.61489100	3.81520300
H	-0.33580900	-4.25473600	4.50924600
C	-1.02497800	-4.70832300	1.28355600
H	-1.52420600	-3.77333300	1.01461600
H	-0.82170800	-5.28209000	0.36897500
H	-1.69444900	-5.30125400	1.92268100
C	4.40526300	-2.05403600	0.99202800
H	4.47429500	-2.00134100	2.08688500
H	5.41733600	-2.19007300	0.58496000
H	3.99457300	-1.11175200	0.62264500
C	3.25157000	-3.75555800	-1.39938300
H	4.27302700	-3.83884300	-1.79685300
H	2.70349800	-4.67253700	-1.65411500
H	2.74983800	-2.90270900	-1.86584700
C	4.17062000	-5.04825600	1.21477900
H	4.22542300	-5.00623800	2.30921500
H	3.70616900	-5.99430200	0.91811300
H	5.19955700	-5.03613800	0.82492900

$TS_{2\text{-}3}$

H= -1428.211253 au

U	-0.18422700	0.90694400	0.06237700
Si	2.60145700	2.65668600	1.40283300
Si	0.70493300	1.82549400	3.56765700
Si	-3.77914900	-0.15844500	0.27463500
Si	-2.17087400	-1.24509700	-1.97922700
Si	0.55781300	-3.31804100	2.49809900
Si	3.50936600	-3.20684700	0.41271500
Si	0.28597500	3.03603000	-2.91823500
Si	-1.49600500	4.13522200	-0.78227200
N	1.08329600	1.89564700	1.85653400
N	-2.23601900	-0.20758900	-0.56196900
N	-0.41677700	2.85408600	-1.31956800
N	1.97070900	-2.76578800	1.17553000
C	1.27839900	-1.67905700	0.84836300
O	0.18125900	-1.59312000	1.56821600
O	1.53762600	-0.79005700	-0.02834000
C	-3.27203000	3.93655000	-1.46957700
H	-3.62678900	2.91236200	-1.30054400
H	-3.96153500	4.63548100	-0.97403800
H	-3.29526900	4.13025400	-2.54924700
C	-0.93259000	5.90841100	-1.25270500
H	-0.90346300	6.06707200	-2.33769000
H	-1.64538900	6.62579000	-0.81942800
H	0.06299300	6.12066200	-0.84198200
C	-1.60256600	4.16875700	1.12318400
H	-1.95205400	3.22017600	1.54841700
H	-0.61477200	4.37639200	1.54971200
H	-2.30366100	4.95770300	1.43410300
C	-0.40520200	-1.88853300	-2.34656200
H	0.36785800	-1.11391900	-2.40833400
H	-0.09560300	-2.61092100	-1.58106300
H	-0.43746700	-2.40964600	-3.31573200
C	-2.77253100	-0.35679100	-3.56526200
H	-2.66633400	-1.01059400	-4.44314200
H	-3.82439300	-0.05879600	-3.47360900
H	-2.17568800	0.54951200	-3.72868500
C	-3.16764000	-2.87924800	-1.83011800
H	-4.24155600	-2.72156100	-1.67954500
H	-3.02948500	-3.45936700	-2.75481400
H	-2.78175300	-3.47334700	-0.99125100
C	-4.09555800	-1.69371800	1.37353300
H	-4.23007200	-2.60507400	0.77913700
H	-3.23919600	-1.84649400	2.04136100
H	-4.99470200	-1.53928700	1.98767000
C	-5.27590400	-0.00034800	-0.92464100
H	-6.20435600	0.03526000	-0.33557100
H	-5.19974600	0.93223000	-1.50049100
H	-5.35019200	-0.83582000	-1.63088600
C	-4.00385500	1.33280200	1.44284800

H	-3.30434400	1.30326600	2.28420200
H	-3.88585900	2.28609500	0.91659500
H	-5.02793000	1.28759700	1.84431400
C	3.27693400	1.94998400	-0.24050200
H	4.23968400	2.43417900	-0.46534800
H	3.43204800	0.86798100	-0.15861200
H	2.60574600	2.13505900	-1.08790500
C	2.43721500	4.54883800	1.16990400
H	2.15980900	5.04013400	2.11142000
H	3.38587200	4.97831200	0.81658500
H	1.65978000	4.75852100	0.42505600
C	4.05012500	2.38310200	2.63319900
H	4.28905100	1.31448900	2.71042800
H	4.93635500	2.90754700	2.24568700
H	3.83600300	2.76658300	3.63780700
C	-1.10894600	1.36598800	3.93768800
H	-1.79304600	2.15460300	3.60250700
H	-1.39211500	0.42231600	3.45671100
H	-1.22264000	1.24934300	5.02647700
C	0.96428300	3.51023200	4.45654800
H	2.00477700	3.85431800	4.40610800
H	0.32474500	4.27607400	3.99702700
H	0.68296000	3.41491400	5.51562200
C	1.74010400	0.52067800	4.51531400
H	1.42234800	0.48402200	5.56789900
H	1.57005000	-0.46739800	4.06936100
H	2.81401200	0.73626800	4.48180200
C	-0.99355800	3.56222200	-4.25061200
H	-1.80534800	2.82543100	-4.30823100
H	-1.43329100	4.54519300	-4.04015300
H	-0.49795300	3.60991600	-5.23139400
C	1.69440300	4.33580700	-2.99218100
H	1.31345800	5.35119700	-2.83133600
H	2.45291500	4.12802600	-2.22767300
H	2.17651500	4.29745800	-3.98018500
C	1.04394000	1.42807300	-3.61987400
H	1.45266700	1.65502700	-4.61736300
H	1.85347500	1.02881500	-2.99715800
H	0.27940300	0.65093900	-3.73342000
C	1.85471000	-4.02651300	3.73515100
H	1.34833200	-4.62034700	4.50872200
H	2.60381500	-4.64679200	3.23179700
H	2.37413200	-3.19530500	4.23419700
C	-0.77947000	-2.78388500	3.78253100
H	-0.42145600	-1.95055000	4.40137100
H	-1.69451900	-2.45946900	3.27437800
H	-1.01450300	-3.63164900	4.44306800
C	-0.25633800	-4.68805800	1.45091900
H	-0.88024800	-4.23636400	0.66857200
H	0.49929200	-5.32292000	0.97307000
H	-0.90092300	-5.31092700	2.08620300
C	4.89500300	-2.06737300	1.04748900
H	5.00657500	-2.16961100	2.13477300
H	5.85468200	-2.30963400	0.57009400
H	4.64567200	-1.02283500	0.82273000
C	3.39099100	-3.07098200	-1.47934900
H	4.36502700	-3.29116900	-1.93871400
H	2.64959800	-3.77858400	-1.87219600
H	3.08086000	-2.05842800	-1.75849700
C	3.91825800	-5.01597200	0.84973400
H	4.23711000	-5.12569800	1.89297300
H	3.04365300	-5.65783000	0.68383700
H	4.73268000	-5.36638100	0.20024500

Int3

H= -1428.219136 au

U	-0.21756100	0.38180400	-0.10460500
Si	2.54802500	2.12668500	1.27298300
Si	0.57063400	1.39113600	3.40126900
Si	-3.83124800	-0.62432700	0.01211100
Si	-2.19067000	-1.85020700	-2.13445800
Si	0.22810600	-3.74235300	2.54664200
Si	3.63083100	-3.53962700	-0.40845000
Si	0.35585700	2.39177100	-3.13279900
Si	-1.44118500	3.61976700	-1.07711100
N	1.00300500	1.40775900	1.70440500
N	-2.24974100	-0.77882700	-0.73626800
N	-0.39367100	2.28715900	-1.54754500
N	2.20029100	-3.38347800	0.57873600
C	1.39959300	-2.37717000	0.58298500
O	0.38360900	-2.35953200	1.51155400
O	1.38152800	-1.33595800	-0.18690200
C	-3.20802600	3.46271800	-1.79863900
H	-3.61374000	2.46355000	-1.59854500
H	-3.87681400	4.21069700	-1.34840500
H	-3.19771900	3.61362400	-2.88538300
C	-0.80981800	5.35577200	-1.59761900
H	-0.74927800	5.47235400	-2.68668500
H	-1.50930200	6.11116200	-1.20948100
H	0.18166300	5.55210600	-1.16955400
C	-1.58661100	3.73025000	0.82372500
H	-1.96279800	2.80818900	1.28333300
H	-0.60267100	3.93557000	1.26013500
H	-2.27565100	4.54676800	1.08685800
C	-0.45594500	-2.58125300	-2.45789300
H	0.33827500	-1.83781400	-2.58019100
H	-0.15907400	-3.25230000	-1.64264200
H	-0.51718300	-3.17135500	-3.38535400
C	-2.71843200	-0.97285600	-3.75328200
H	-2.58701400	-1.64268300	-4.61551500
H	-3.76738800	-0.65553600	-3.71103800
H	-2.09926900	-0.07994300	-3.90698500
C	-3.26963300	-3.43399600	-1.97904800
H	-4.34042600	-3.22784100	-1.86874000
H	-3.12655700	-4.03802200	-2.88755300
H	-2.93736700	-4.02895300	-1.11787600
C	-4.29695100	-2.11190700	1.12637400
H	-4.41072300	-3.03676400	0.54941800
H	-3.51152000	-2.26980100	1.87501000
H	-5.24089200	-1.90655400	1.65198500
C	-5.25428500	-0.42626500	-1.26789900
H	-6.20848900	-0.32662600	-0.72962100
H	-5.09907600	0.48470400	-1.86201300
H	-5.33528600	-1.27528000	-1.95667600
C	-4.05451100	0.90442300	1.13173100
H	-3.46082200	0.83880100	2.04899900
H	-3.79875900	1.83253100	0.61000700
H	-5.11836800	0.95369100	1.41165400
C	3.24490800	1.37484000	-0.34033400
H	4.22998200	1.82410600	-0.53991100
H	3.36261200	0.28943800	-0.24365600
H	2.60826700	1.57314900	-1.21095300
C	2.43133900	4.01732200	0.99839400
H	2.13945800	4.53386200	1.92194500
H	3.39948200	4.41754400	0.66415700
H	1.68055400	4.23032600	0.22753700
C	3.95761300	1.85102300	2.54683700
H	4.17007800	0.77959100	2.65549100
H	4.86534200	2.34632200	2.17103300
H	3.72555000	2.26446100	3.53566900
C	-1.26091200	0.96116800	3.72511900
H	-1.92543700	1.74867100	3.35067600

H	-1.54132000	0.01414300	3.24810600
H	-1.41272800	0.86714000	4.81169700
C	0.82873600	3.09174900	4.25766300
H	1.87867300	3.40976800	4.24052600
H	0.22676300	3.85924100	3.75271700
H	0.50354900	3.03097100	5.30666900
C	1.55156500	0.09230600	4.41186300
H	1.18184600	0.05960000	5.44735400
H	1.40463600	-0.89474800	3.95580700
H	2.62613900	0.30646700	4.42988600
C	-0.87906700	2.89404600	-4.51509200
H	-1.70464300	2.17230400	-4.56689300
H	-1.30228600	3.89279100	-4.34930100
H	-0.35951900	2.89715200	-5.48457100
C	1.79449600	3.65678700	-3.22526500
H	1.43400600	4.68594800	-3.11321600
H	2.53339800	3.46336600	-2.43829700
H	2.29516700	3.56837700	-4.20078100
C	1.09251900	0.73722400	-3.73862200
H	1.53961200	0.90762200	-4.73081600
H	1.87055200	0.34637000	-3.07205900
H	0.31349400	-0.02649900	-3.84439300
C	1.74828700	-4.06472300	3.63402800
H	1.47546500	-4.75280300	4.44744200
H	2.55610400	-4.49250700	3.03541300
H	2.09723400	-3.12455700	4.07970000
C	-1.18826400	-3.20700400	3.69302800
H	-0.90731800	-2.30416100	4.24937200
H	-2.09379000	-2.98650300	3.11746500
H	-1.41706200	-4.00588200	4.41243000
C	-0.30309900	-5.26538700	1.55102600
H	-1.17189500	-5.01980500	0.92655600
H	0.51957200	-5.59002500	0.90670700
H	-0.58283800	-6.08231900	2.23121600
C	5.06156000	-2.51339100	0.33061600
H	5.23944300	-2.80174500	1.37493400
H	5.98830800	-2.66772300	-0.24000400
H	4.81118400	-1.44550100	0.30627700
C	3.41403800	-3.04719100	-2.23641400
H	4.35544000	-3.18185300	-2.78800600
H	2.63533200	-3.65594700	-2.71337900
H	3.10757200	-1.99694300	-2.29685400
C	4.12596800	-5.38211100	-0.33446500
H	4.27665700	-5.69373900	0.70764000
H	3.33347900	-6.00666200	-0.76813800
H	5.05556500	-5.56128900	-0.89238000

Int4

H= -1428.21218 au

U	-0.27700500	0.32920400	0.30524300
Si	1.43877600	3.06228400	2.22450700
Si	0.22999900	0.76739100	3.74255800
Si	-3.81627800	1.47916000	1.03598700
Si	-3.49853200	-0.78025600	-0.85227300
Si	-0.04619300	-4.95779800	0.31164900
Si	3.17170200	-1.68017400	0.82042900
Si	1.27285200	0.42890100	-3.04121800
Si	-0.45747100	2.76299800	-2.30725700
N	0.49018500	1.58593600	2.20343000
N	-2.70870500	0.44387200	0.15217600
N	0.26302900	1.23081500	-1.82964100
N	1.46651900	-1.31372400	0.64352000
C	0.53778900	-2.34767000	0.71906200
O	0.92584600	-3.58012100	0.16481500
O	-0.70443000	-1.92208400	0.38766200
C	-1.98544400	2.57882600	-3.43948300
H	-2.72781100	1.94269700	-2.94145600
H	-2.43783100	3.56428200	-3.62307400
H	-1.72827600	2.12706100	-4.40464500
C	0.77365800	3.97132500	-3.14824800
H	1.20137800	3.57322400	-4.07489000
H	0.24741500	4.90806400	-3.38470400
H	1.59597300	4.20392500	-2.45840400
C	-1.05359300	3.73491900	-0.77760500
H	-0.21015800	4.06673700	-0.16412100
H	-1.59346700	4.62833800	-1.12526100
H	-1.74861700	3.16086900	-0.15440700
C	-2.39260400	-1.33541100	-2.30207600
H	-1.55333600	-1.93633000	-1.93635300
H	-2.99270300	-1.94818400	-2.99155400
H	-1.99613600	-0.47408500	-2.85314400
C	-5.09727000	-0.16093900	-1.72720600
H	-5.46802300	-0.98118700	-2.36021000
H	-5.89503700	0.11908400	-1.02887900
H	-4.88071900	0.69955900	-2.37391800
C	-3.98836300	-2.34605500	0.12459300
H	-4.71833000	-2.12297800	0.91233500
H	-4.41990000	-3.10008700	-0.55017000
H	-3.07910800	-2.75257700	0.58158500
C	-5.22140700	0.53194300	1.94072500
H	-5.89314400	0.01283000	1.24677700
H	-4.79450400	-0.20963500	2.62920700
H	-5.81522000	1.24851900	2.52750500
C	-4.69856200	2.80792300	-0.03544400
H	-5.26042200	3.48082800	0.62980100
H	-3.97447000	3.40775400	-0.60005000
H	-5.40139500	2.35955500	-0.74656500
C	-2.96678400	2.45538700	2.44019100
H	-2.83928000	1.80837400	3.31593600
H	-1.98036500	2.84867400	2.17363000
H	-3.61729000	3.29556800	2.72448900
C	2.36714000	3.32552900	0.57101700
H	2.57730800	4.39447600	0.42062000
H	3.32278200	2.78745900	0.61186000
H	1.81606400	2.95540600	-0.30144200
C	0.39583500	4.62615600	2.60793500
H	-0.02963500	4.55411900	3.61768800
H	1.04093500	5.51660700	2.56811000
H	-0.42991300	4.76368600	1.90037800
C	2.83126300	3.11095700	3.54448100
H	3.53193100	2.27914400	3.40393300
H	3.38461100	4.05383800	3.41916600
H	2.44458500	3.07532500	4.57039900
C	-1.00950100	-0.66771700	3.50074500
H	-1.94853800	-0.37218000	3.01445100
H	-0.56459800	-1.49248200	2.92432800
H	-1.26253400	-1.06133500	4.49707700
C	-0.44470600	1.91998100	5.12026500
H	0.30740600	2.66792300	5.40494200
H	-1.35229400	2.44523300	4.80266200
H	-0.67859000	1.31869500	6.01138600
C	1.78680700	-0.04798400	4.49236700
H	1.48595200	-0.72299400	5.30728900
H	2.29254700	-0.63939600	3.72237700
H	2.49186600	0.68915900	4.89414700
C	0.71388300	0.74888400	-4.85343100
H	-0.29031900	0.33321000	-5.01185500
H	0.70639600	1.80417100	-5.14825200
H	1.40952200	0.21160500	-5.51542200
C	3.08595900	1.01722500	-2.89612000
H	3.15312800	2.10733700	-3.00291100
H	3.48626300	0.74309500	-1.91203300

H	3.71170400	0.54711500	-3.66830500
C	1.24819500	-1.46918200	-2.92901700
H	2.05761900	-1.87124200	-3.55680400
H	1.39209800	-1.83024600	-1.90579300
H	0.29374700	-1.85549300	-3.30669800
C	1.18335600	-6.41143900	0.24448500
H	0.64875300	-7.37099000	0.28123500
H	1.76719000	-6.37360700	-0.68445800
H	1.87976000	-6.36475000	1.09160900
C	-0.97844500	-4.96987800	1.96386000
H	-0.27954800	-4.81810900	2.79597600
H	-1.71431700	-4.15834800	1.97886300
H	-1.49711600	-5.92890600	2.10354000
C	-1.26217800	-5.11818100	-1.13589500
H	-1.91963100	-4.24269000	-1.16243400
H	-0.71922000	-5.17623700	-2.08804900
H	-1.87634400	-6.02329300	-1.02458700
C	3.51203700	-2.88895300	2.26446300
H	2.97583500	-3.82581100	2.07185900
H	4.58830900	-3.10419700	2.33306300
H	3.17258700	-2.48344700	3.22444000
C	4.11895200	-0.05432300	1.12837200
H	5.17144200	-0.26681600	1.36368400
H	4.08652400	0.58001200	0.23358500
H	3.67273100	0.50350500	1.95926100
C	3.96651500	-2.49464900	-0.71674800
H	3.44168200	-3.42824500	-0.95120400
H	3.91065100	-1.83475000	-1.59067200
H	5.02431900	-2.71902900	-0.51247500

TS_{4-5}

H= -1428.169345 au

U	-0.37993600	0.46459700	0.34475100
Si	1.42872700	3.06319600	2.22841400
Si	0.01848100	0.89493300	3.77957000
Si	-3.88122600	1.70766500	1.00732800
Si	-3.57212300	-0.72432800	-0.67491200
Si	1.38396700	-5.23120800	0.05119500
Si	3.05133600	-1.98210500	0.74477400
Si	1.18965300	0.38062200	-2.95368600
Si	-0.48162700	2.80482600	-2.32064100
N	0.34515400	1.66673500	2.21324800
N	-2.77089100	0.58204900	0.22863200
N	0.18000600	1.26280700	-1.77857900
N	1.36502500	-1.24789900	0.66097700
C	0.42501600	-2.13626100	0.86436000
O	1.78508700	-3.64555900	0.02033000
O	-0.82154700	-1.85659400	0.68434700
C	-1.99743700	2.61093200	-3.46342200
H	-2.76382300	2.01827800	-2.94768400
H	-2.42156400	3.59699100	-3.70186400
H	-1.73826400	2.10614500	-4.40096300
C	0.80053300	3.95074900	-3.16534500
H	1.23035600	3.52237800	-4.07689900
H	0.30755800	4.89850600	-3.42780400
H	1.61879600	4.17215600	-2.46713900
C	-1.07082000	3.83605500	-0.82643900
H	-0.23370400	4.13135600	-0.18534200
H	-1.54050400	4.75373400	-1.21120600
H	-1.82432100	3.32132200	-0.22023200
C	-2.42928500	-1.42223800	-2.03098800
H	-1.66542200	-2.08130000	-1.60405300
H	-3.04140600	-2.01516000	-2.72662100
H	-1.94061700	-0.62276600	-2.60164900
C	-5.13153300	-0.15232500	-1.63989000
H	-5.49648000	-1.01655600	-2.21482800
H	-5.94519000	0.19056100	-0.98974800
H	-4.88514200	0.64920400	-2.34832600
C	-4.10527900	-2.18798300	0.42499600
H	-4.83175400	-1.88709400	1.18960300
H	-4.55733600	-2.97465600	-0.19669300
H	-3.21535800	-2.59639500	0.91738100
C	-5.30196800	0.84400900	1.96365400
H	-5.97251600	0.28282600	1.30215300
H	-4.89175300	0.14945900	2.70860500
H	-5.89377900	1.60797000	2.48917100
C	-4.72621800	2.93498400	-0.20186400
H	-5.29823600	3.66955900	0.38436300
H	-3.98538000	3.47653900	-0.80208800
H	-5.41545000	2.42803600	-0.88600800
C	-3.05074800	2.80614400	2.33449300
H	-2.92508200	2.24136600	3.26521700
H	-2.06836200	3.19458100	2.04783700
H	-3.71868500	3.65634900	2.53725500
C	2.37292400	3.22717300	0.57622700
H	2.78897200	4.24175100	0.49152000
H	3.20373200	2.51053600	0.57244200
H	1.75962200	3.03138000	-0.31026000
C	0.49910700	4.69953000	2.58627400
H	0.04557200	4.66626600	3.58535800
H	1.20989300	5.53849100	2.55685400
H	-0.29702600	4.89396700	1.85805600
C	2.81804100	2.98259400	3.54264100
H	3.44127500	2.09400400	3.38609200
H	3.45075900	3.87380200	3.41617800
H	2.44038000	2.97533300	4.57191300
C	-1.40899200	-0.36435900	3.61322600
H	-2.33032600	0.06855800	3.20843200
H	-1.14375800	-1.23495500	2.99978300
H	-1.62474200	-0.73452800	4.62712300
C	-0.49738600	2.15282700	5.12881100
H	0.32224700	2.84124100	5.37050100
H	-1.36481800	2.74200600	4.80925600
H	-0.76291800	1.60541600	6.04503800
C	1.48566600	-0.10953200	4.46482500
H	1.14041500	-0.73031300	5.30442100
H	1.87504900	-0.77018200	3.68164300
H	2.30206100	0.53032300	4.81796300
C	0.66942200	0.69718100	-4.77566300
H	-0.33934400	0.30103600	-4.95387800
H	0.69336800	1.74809400	-5.08348300
H	1.36764500	0.13659500	-5.41493300
C	3.01025800	0.91375100	-2.76393200
H	3.11607300	1.99943300	-2.88476600
H	3.37443900	0.63740500	-1.76682700
H	3.64172400	0.41209400	-3.51075500
C	1.06779800	-1.51253300	-2.83156100
H	1.81690000	-1.92701500	-3.52414900
H	1.26439800	-1.94656500	-1.84454200
H	0.07999100	-1.84628600	-3.17162900
C	2.87792400	-6.37181000	-0.35655700
H	2.57661700	-7.42938600	-0.32506500
H	3.26917400	-6.15070700	-1.35914400
H	3.68846100	-6.21983600	0.36963300
C	0.70967300	-5.82348500	1.74602500
H	1.47917900	-5.72502500	2.52330800
H	-0.15366700	-5.21028400	2.03674300
H	0.39453600	-6.87615200	1.69537800
C	0.02556500	-5.62678500	-1.24249700
H	-0.87314100	-5.03107900	-1.03330700
H	0.37604200	-5.37400600	-2.25231400
H	-0.24635100	-6.69234500	-1.22085900

C	3.38989300	-3.08030200	2.27651900
H	3.79261100	-4.04708900	1.95107000
H	4.09400200	-2.60287000	2.97137400
H	2.44332900	-3.27606800	2.79584200
C	3.95205000	-0.32835300	1.24891900
H	5.01029500	-0.52783900	1.47900200
H	3.91885400	0.40031900	0.42455000
H	3.48145900	0.13409800	2.12726400
C	4.07978500	-2.37582200	-0.82340100
H	4.08185300	-3.45308200	-1.01098900
H	3.64434000	-1.87902400	-1.69855100
H	5.10699700	-2.00524100	-0.69407100

Int5

H= -1428.17395 au

U	-0.29926200	0.35671000	0.04641500
Si	1.57862400	2.89548500	1.94033800
Si	0.07146900	0.79098600	3.49333200
Si	-3.74750600	1.73738200	0.68899100
Si	-3.51111900	-0.70213700	-1.00381000
Si	2.19202000	-5.43147200	-0.14554800
Si	3.14316600	-2.24955800	0.32808500
Si	1.23091100	0.32010900	-3.30386500
Si	-0.38332400	2.74054400	-2.56664800
N	0.45700500	1.52097600	1.91492300
N	-2.67413300	0.57223400	-0.08859500
N	0.26772400	1.17575100	-2.06894900
N	1.32795500	-1.53409700	0.22080500
C	0.32433200	-2.28790500	0.49516300
O	2.32689800	-3.81102100	-0.29657100
O	-0.91066400	-1.91541500	0.50325400
C	-1.94307200	2.59642500	-3.65714000
H	-2.68602600	1.97614500	-3.14068600
H	-2.37769300	3.59276000	-3.82401500
H	-1.72376800	2.14310900	-4.63032000
C	0.88990900	3.86703700	-3.44967200
H	1.28203500	3.43375600	-4.37605700
H	0.40301600	4.82282200	-3.69381000
H	1.73415200	4.07360400	-2.77848300
C	-0.89331800	3.77449400	-1.04404700
H	-0.01918400	4.08462000	-0.46243800
H	-1.39668100	4.68175600	-1.41052400
H	-1.60223600	3.26394900	-0.38245200
C	-2.35940400	-1.45369600	-2.32450400
H	-1.61931900	-2.12421900	-1.87360500
H	-2.97272100	-2.04775600	-3.01795900
H	-1.84366900	-0.67794500	-2.90338500
C	-5.01612500	-0.05921500	-2.00893600
H	-5.39137600	-0.89497600	-2.61821100
H	-5.83726400	0.29248900	-1.37262700
H	-4.72273200	0.75392800	-2.68486700
C	-4.14775300	-2.13970800	0.07561200
H	-4.87675000	-1.80045200	0.82106200
H	-4.62726200	-2.89669000	-0.56231500
H	-3.29652000	-2.59912700	0.59029800
C	-5.20537400	0.91816500	1.62786700
H	-5.88882800	0.38468400	0.95627700
H	-4.82910800	0.20715100	2.37517000
H	-5.77536600	1.70207300	2.14846800
C	-4.55034700	2.98960000	-0.52302700
H	-5.06213000	3.76498400	0.06678000
H	-3.79254900	3.47625600	-1.14840900
H	-5.28670200	2.51578600	-1.18158800
C	-2.86163300	2.81205800	2.00787000
H	-1.76877000	2.75460100	1.95726300
H	-3.16186400	3.86228700	1.88862700
H	-3.16506100	2.48012800	3.00997100
C	2.49683300	3.08461400	0.27713100
H	2.87166300	4.11420100	0.18209500
H	3.35053500	2.39666700	0.27103400
H	1.88371500	2.85804700	-0.60248900
C	0.68811400	4.54218100	2.34476600
H	0.28359500	4.52102300	3.36443900
H	1.40988300	5.36952300	2.27666100
H	-0.13879700	4.74442000	1.65421500
C	2.97749900	2.73456900	3.23482200
H	3.56326300	1.82699700	3.04481200
H	3.64203900	3.60445100	3.12462100
H	2.61030200	2.71323400	4.26761100
C	-1.45103300	-0.35293700	3.35621200
H	-2.35329100	0.18183100	3.03914700
H	-1.30549100	-1.20837800	2.68447500
H	-1.63121300	-0.75567200	4.36481000
C	-0.37055000	2.09304200	4.82513200
H	0.47655600	2.74998500	5.05663200
H	-1.21547300	2.71091200	4.49845500
H	-0.65763400	1.56756600	5.74759000
C	1.47608500	-0.29901000	4.17473900
H	1.10860200	-0.87294400	5.03776500
H	1.80690600	-1.00391200	3.40260400
H	2.34239900	0.29213100	4.49221500
C	0.58806800	0.63237200	-5.08756200
H	-0.42814400	0.23009700	-5.19488200
H	0.58302400	1.68394400	-5.39461300
H	1.24436600	0.07710400	-5.77406200
C	3.05394700	0.87107000	-3.23176000
H	3.14819100	1.95880700	-3.33780600
H	3.49530400	0.57443100	-2.27246600
H	3.62680200	0.38719100	-4.03558400
C	1.16774600	-1.57554600	-3.18065800
H	1.86343000	-1.96786500	-3.93841600
H	1.47001000	-1.98396600	-2.21138200
H	0.16454600	-1.94682700	-3.42284500
C	3.87486300	-6.34607400	-0.26886700
H	3.72628100	-7.43405100	-0.20547500
H	4.36645400	-6.11497400	-1.22350400
H	4.54472100	-6.03863500	0.54532100
C	1.38856700	-5.97406100	1.50477300
H	2.02172800	-5.69161400	2.35567000
H	0.41534100	-5.47903600	1.62103800
H	1.23670100	-7.06323400	1.52541200
C	1.08830100	-6.10971600	-1.55360600
H	0.09039700	-5.65490900	-1.49704600
H	1.52277300	-5.86263700	-2.53143300
H	0.98180200	-7.20182800	-1.48174000
C	3.62844600	-3.04851700	2.01694100
H	4.08802100	-4.03315800	1.86063400
H	4.32101200	-2.41092400	2.58188000
H	2.72204200	-3.20046800	2.62104000
C	3.72142500	-0.41319900	0.77612500
H	4.79281500	-0.42525200	1.03537900
H	3.59514000	0.25187000	-0.09333400
H	3.15802400	0.01301600	1.61821500
C	4.40405100	-2.40769100	-1.13607200
H	4.75210700	-3.44386000	-1.22364700
H	3.90052000	-2.15078800	-2.07863300
H	5.26227500	-1.73326700	-1.00932900

$TS_{5\text{-}6}$

H= -1428.173051 au

U	-0.20040600	0.26530000	0.12782100
Si	1.70406400	2.84170400	1.94681600

Si	0.18419200	0.79849100	3.56466300
Si	-3.65171000	1.66346000	0.73738700
Si	-3.40497800	-0.81556000	-0.90151500
Si	2.29723700	-5.36773400	-0.39433700
Si	3.31688000	-2.36430300	0.40175900
Si	1.33523600	0.17420300	-3.23281100
Si	-0.29003600	2.59430000	-2.53633300
N	0.56937200	1.47954300	1.96542400
N	-2.57858100	0.48312700	-0.01386500
N	0.36947600	1.04270200	-2.00975100
N	1.40560400	-1.60983300	0.34401600
C	0.40566100	-2.34874900	0.64575200
O	2.51489000	-3.74198300	-0.46430800
O	-0.83632000	-1.98135500	0.67455400
C	-1.85290700	2.42355500	-3.61816700
H	-2.59449100	1.81724000	-3.08367200
H	-2.28785700	3.41507000	-3.81073300
H	-1.63553000	1.94416900	-4.57917500
C	0.97393300	3.70885400	-3.44903500
H	1.35710700	3.26306700	-4.37337900
H	0.48293000	4.66037100	-3.70164300
H	1.82469400	3.92618700	-2.78964200
C	-0.79612600	3.65852600	-1.03374300
H	0.07942600	3.97476600	-0.45756100
H	-1.29490200	4.56174200	-1.41623500
H	-1.50715800	3.16218500	-0.36385900
C	-2.23819000	-1.59244100	-2.19486000
H	-1.49742500	-2.24748900	-1.72251300
H	-2.84161300	-2.20674900	-2.87927800
H	-1.72199700	-0.82754500	-2.78770000
C	-4.90565400	-0.20275700	-1.93194400
H	-5.27790600	-1.05472500	-2.52031700
H	-5.72978300	0.16470300	-1.30831100
H	-4.61043300	0.59228200	-2.62832400
C	-4.04847700	-2.22998500	0.20453000
H	-4.78223700	-1.87365000	0.93723100
H	-4.52445600	-3.00047700	-0.41983900
H	-3.19999300	-2.67691800	0.73436100
C	-5.10456000	0.86192200	1.69918700
H	-5.78672700	0.30951100	1.04148600
H	-4.72364600	0.16986700	2.46182300
H	-5.67732500	1.65502100	2.20252600
C	-4.46276000	2.88563000	-0.49949700
H	-5.01230400	3.64671800	0.07482600
H	-3.70418700	3.39353800	-1.10699400
H	-5.16725300	2.38818400	-1.17497100
C	-2.76309800	2.77554500	2.02505000
H	-1.67136700	2.68565500	1.99948100
H	-3.02949600	3.82734700	1.85176300
H	-3.09567400	2.49922800	3.03497200
C	2.61193000	2.98098900	0.27270600
H	2.99384800	4.00509200	0.14993800
H	3.46113400	2.28724500	0.27611300
H	1.99032600	2.73806100	-0.59649400
C	0.83537100	4.50760700	2.31856300
H	0.43962200	4.51515100	3.34180900
H	1.56408600	5.32613300	2.22369700
H	0.00419600	4.70012300	1.63025600
C	3.11589700	2.69905500	3.23091200
H	3.68868000	1.77877600	3.06282000
H	3.79025700	3.55642300	3.08733200
H	2.76057800	2.71336300	4.26801900
C	-1.35409300	-0.32762400	3.47020900
H	-2.25372500	0.21762000	3.16321100
H	-1.23125800	-1.19008700	2.80273000
H	-1.52214200	-0.71833800	4.48558700
C	-0.23042300	2.14384400	4.86188000
H	0.62552800	2.79865900	5.06455400
H	-1.07155000	2.76016800	4.52225300
H	-0.51552400	1.65062200	5.80253000
C	1.58368600	-0.29058800	4.25833200
H	1.22205600	-0.84093600	5.13897400
H	1.89370000	-1.01614100	3.49659500
H	2.46150300	0.29695200	4.54981000
C	0.67834900	0.44395500	-5.01907200
H	-0.33167200	0.02346600	-5.11494000
H	0.65457900	1.48993900	-5.34366300
H	1.34064400	-0.11219100	-5.69906000
C	3.15465500	0.74749700	-3.19643400
H	3.23972100	1.83304300	-3.32822300
H	3.61344400	0.47685000	-2.23776700
H	3.71890600	0.24961800	-3.99799100
C	1.30865600	-1.71721600	-3.07163300
H	1.99562700	-2.11056200	-3.83702700
H	1.63557000	-2.10903500	-2.10298300
H	0.30765200	-2.11139700	-3.28712500
C	3.94771000	-6.33997400	-0.45498100
H	3.75642600	-7.42247300	-0.42060300
H	4.49502400	-6.10988100	-1.37867800
H	4.58609300	-6.07161600	0.39746000
C	1.36621600	-5.93865400	1.17278000
H	1.97590900	-5.77780200	2.07085200
H	0.44032500	-5.35916800	1.27964000
H	1.11462200	-7.00703900	1.10397900
C	1.26220200	-5.90617500	-1.90688300
H	0.28536800	-5.40542700	-1.88923700
H	1.77328500	-5.62808100	-2.83797100
H	1.10031900	-6.99363000	-1.90504200
C	3.58064800	-3.15883100	2.13044500
H	3.91355000	-4.20006500	2.03072900
H	4.33540100	-2.59684100	2.69690200
H	2.64257300	-3.15555900	2.70210500
C	3.79817500	-0.49650600	0.77600100
H	4.83385900	-0.45340100	1.14745400
H	3.74964900	0.09542000	-0.15083800
H	3.12537900	-0.03673700	1.51126500
C	4.87783700	-2.61054700	-0.74559900
H	5.14699700	-3.67031400	-0.83285500
H	4.63582900	-2.24742700	-1.75682200
H	5.74191700	-2.03787000	-0.37916200

Int6

H= -1107.19077 au

U	-0.43034100	0.49665300	0.01924600
Si	1.66943500	2.72482200	1.95466800
Si	0.02225300	0.75759400	3.53712000
Si	-3.88925500	1.78838000	0.71053200
Si	-3.63867300	-0.69591700	-0.93797300
Si	1.20049500	0.34543600	-3.29119500
Si	-0.37072300	2.83352700	-2.67692100
N	0.39790600	1.51124700	1.98024500
N	-2.84298400	0.63995200	-0.10035400
N	0.16350100	1.24666000	-2.16756600
N	1.25673100	-1.15814400	-0.09589000
C	0.41547600	-1.96483900	0.39564600
O	-0.88278200	-1.72384600	0.61559500
C	-1.81186100	2.80356800	-3.93259900
H	-2.64714200	2.23062700	-3.50813400
H	-2.15936000	3.82593600	-4.14137100
H	-1.51425000	2.33580200	-4.87832300
C	1.01724300	3.96729900	-3.36578500
H	1.48858600	3.57290500	-4.27241300

H	0.59103700	4.95464400	-3.59816600
H	1.79730600	4.10071700	-2.60479200
C	-1.03519700	3.81061700	-1.17420300
H	-0.30008900	3.89407200	-0.36318200
H	-1.27950100	4.83131700	-1.50444900
H	-1.95498000	3.36227400	-0.78482000
C	-2.48320300	-1.41083300	-2.27618400
H	-1.66380200	-1.97932900	-1.81968900
H	-3.05681900	-2.09911700	-2.91454700
H	-2.06221400	-0.61897000	-2.90831600
C	-5.22721300	-0.18003700	-1.88912800
H	-5.59117400	-1.05648300	-2.44601600
H	-6.02975900	0.15408500	-1.21930800
H	-5.01472700	0.62150800	-2.60858900
C	-4.13060800	-2.14292300	0.20534600
H	-4.83164300	-1.82829700	0.98844900
H	-4.59833700	-2.94688600	-0.38219100
H	-3.21794100	-2.52737800	0.67571600
C	-5.23788400	0.96019900	1.79559900
H	-5.91905900	0.34491200	1.19376500
H	-4.77536800	0.31664000	2.55506500
H	-5.83008800	1.73511300	2.30407600
C	-4.83376300	2.96095500	-0.48370500
H	-5.31082600	3.76357600	0.09832300
H	-4.14843500	3.42083500	-1.20691700
H	-5.61236900	2.42699800	-1.04063300
C	-2.96149200	2.97129000	1.89782200
H	-2.37768300	2.43417900	2.65101400
H	-2.28134300	3.65145500	1.37260200
H	-3.71966800	3.57987700	2.41382300
C	2.54296200	2.74531100	0.25952700
H	3.27668700	3.56481600	0.24195500
H	3.07713700	1.79757700	0.11143300
H	1.86611700	2.87753200	-0.59193900
C	1.00616700	4.48319900	2.32127600
H	0.58816200	4.52901800	3.33515000
H	1.81931500	5.21970400	2.24435500
H	0.21482300	4.76428700	1.61531300
C	3.09441700	2.42649400	3.19996700
H	3.59747400	1.47740900	2.97632600
H	3.82634100	3.24067900	3.09298100
H	2.75350400	2.40536600	4.24171900
C	-1.58057600	-0.27403500	3.46718900
H	-2.46380200	0.32186500	3.21280500
H	-1.49743900	-1.09534200	2.74377200
H	-1.73520400	-0.70898200	4.46644700
C	-0.23625200	2.05556800	4.92566700
H	0.66554500	2.65373500	5.10638300
H	-1.05672300	2.73675400	4.66345500
H	-0.49938700	1.53838800	5.85993800
C	1.37176000	-0.47424800	4.09768100
H	1.01926400	-1.04195300	4.97116000
H	1.56528500	-1.17895700	3.27776300
H	2.31335600	0.02213300	4.35881900
C	0.88289900	0.80827500	-5.13494800
H	-0.13136400	0.50475700	-5.42793300
H	1.01169100	1.87005900	-5.37150900
H	1.59544000	0.23305300	-5.74517900
C	3.04546600	0.66658600	-2.92332500
H	3.27871600	1.73878700	-2.92987800
H	3.27573000	0.25946900	-1.93039800
H	3.67882600	0.16069600	-3.66619600
C	0.96383100	-1.54311200	-3.30713000
H	1.69421100	-1.96265700	-4.01597700
H	1.15162500	-1.96064700	-2.31279600
H	-0.04216400	-1.82455700	-3.63996900

Int7

H= -1107.224781 au

U	-0.52042900	0.68127300	-0.08777300
Si	1.52354600	2.73452800	2.03930900
Si	0.03338700	0.41855800	3.39150000
Si	-3.87319300	2.00457300	0.88412800
Si	-3.77091700	-0.49509200	-0.79329700
Si	1.14268500	0.20628500	-3.32404800
Si	-0.31166300	2.82276100	-2.94164000
N	1.12622400	-1.03288600	-0.00204100
C	1.93086000	-1.81970900	0.42057600
O	2.72826600	-2.61179000	0.83176300
N	0.36479900	1.42236200	1.99651100
N	-2.92619900	0.84352800	-0.02565000
N	0.10140700	1.23386100	-2.33527000
C	-1.55514600	2.77092800	-4.39966200
H	-2.44106900	2.19316000	-4.10219400
H	-1.87693300	3.79065400	-4.65688100
H	-1.12298100	2.30602600	-5.29310000
C	1.20043000	3.87477100	-3.48183500
H	1.77494500	3.40335800	-4.28806200
H	0.86146500	4.86212300	-3.82826000
H	1.87064100	4.02084100	-2.62407100
C	-1.17813100	3.89769800	-1.61855200
H	-0.51245000	4.12772800	-0.77767300
H	-1.47637100	4.84645800	-2.09254600
H	-2.08452300	3.41660700	-1.23077500
C	-2.83322700	-1.13126100	-2.33182500
H	-1.98286600	-1.76563400	-2.05304400
H	-3.52113600	-1.73181300	-2.94671900
H	-2.45088500	-0.30082800	-2.93892300
C	-5.52109300	-0.04557100	-1.44885200
H	-5.94647800	-0.93528500	-1.93630700
H	-6.20283400	0.26309300	-0.64638300
H	-5.46713500	0.76176000	-2.19065600
C	-4.02276500	-1.99607400	0.36613700
H	-4.63587600	-1.72698400	1.23584600
H	-4.52054700	-2.81408300	-0.17473400
H	-3.04983500	-2.35417100	0.72616400
C	-5.02656700	1.17286400	2.17499300
H	-5.76114700	0.51075700	1.69864100
H	-4.43534200	0.57652900	2.88290600
H	-5.57064100	1.94342400	2.74057400
C	-4.98625100	3.13598300	-0.19494100
H	-5.43623000	3.91072000	0.44380800
H	-4.38507900	3.63491800	-0.96651200
H	-5.79207500	2.58161900	-0.68851500
C	-2.77788200	3.21746500	1.86867600
H	-1.96115600	2.71087000	2.39514900
H	-2.33486700	3.97509400	1.21037800
H	-3.40845700	3.73493500	2.60721200
C	2.61899500	2.76209600	0.47301500
H	3.30918900	3.61821500	0.51553400
H	3.21089700	1.83931600	0.41002800
H	2.02426100	2.84250500	-0.44607500
C	0.69389800	4.45278500	2.19380500
H	0.08750600	4.50598600	3.10771400
H	1.46204400	5.23882200	2.23481100
H	0.03610100	4.65250700	1.33943000
C	2.76209100	2.63899100	3.50225700
H	3.40568200	1.75564900	3.40627700
H	3.39941700	3.53523100	3.48481400
H	2.25586500	2.59781500	4.47513000
C	-1.30296900	-0.86951900	2.92422100
H	-2.19366000	-0.41907200	2.46611900

H	-0.89898300	-1.62249200	2.23250500
H	-1.62247800	-1.39343900	3.83774900
C	-0.65299300	1.41765300	4.87838600
H	0.07138200	2.17300100	5.21102000
H	-1.58251600	1.93158800	4.60167100
H	-0.86278000	0.74492500	5.72265700
C	1.51063300	-0.60946300	4.03918900
H	1.15051200	-1.31985000	4.79848000
H	1.96449000	-1.18191700	3.22020300
H	2.28299600	0.02040900	4.49602700
C	1.08502800	0.60402400	-5.20579300
H	0.09072400	0.38952500	-5.61864000
H	1.34789100	1.64044800	-5.44617800
H	1.80988500	-0.05715000	-5.70415200
C	2.97320300	0.36424900	-2.80184400
H	3.32016400	1.40130800	-2.90194300
H	3.07701600	0.06084400	-1.75326200
H	3.61170800	-0.28281400	-3.42039700
C	0.66982300	-1.64212800	-3.26767300
H	1.44261000	-2.22158700	-3.79471100
H	0.60801200	-2.00431300	-2.23581900
H	-0.29173200	-1.80830100	-3.76920100

Int8

H= -1275.353576 au

U	-0.17870900	0.06213400	0.16416300
Si	-3.18985400	1.64776900	1.31270200
Si	-3.43317900	0.17210900	-1.32027700
Si	-0.17027700	-2.17385400	2.98013200
Si	2.17152100	-0.26551900	2.85953000
Si	2.31002800	-1.00510100	-2.19963000
Si	1.27742200	1.80641000	-2.62409600
C	0.59099700	3.44601300	1.14617000
O	0.81750400	4.58111200	1.43773700
N	-0.80298500	-2.10496300	-0.65564900
N	0.36540200	2.30090700	0.85466400
N	-2.43515000	0.68335200	0.04288800
N	1.23352800	0.30155000	-1.70192900
N	0.66797300	-0.85910100	2.15122900
C	-1.13643100	-3.06735900	-1.29456200
O	-1.46837400	-4.02472500	-1.92664000
C	1.48107500	1.52251200	-4.50978400
H	0.63587100	0.93813900	-4.89664400
H	1.48821600	2.49820700	-5.01746700
H	2.41015900	0.99697600	-4.76011300
C	2.69036100	2.96383300	-2.06597100
H	3.67059500	2.49233100	-2.20763300
H	2.66385400	3.89881500	-2.64410400
H	2.57313400	3.20983500	-1.00362200
C	-0.35196800	2.79390400	-2.47655700
H	-0.66036100	2.95052700	-1.43693800
H	-0.19007300	3.78181500	-2.93324200
H	-1.16836700	2.29710700	-3.01439700
C	-2.39912300	-0.30568900	-2.86837900
H	-2.48682100	-1.38286100	-3.05711600
H	-2.79525300	0.23451500	-3.74066900
H	-1.33068300	-0.07243500	-2.78840700
C	-4.61266000	1.55725500	-1.93103200
H	-5.18059500	1.18034700	-2.79455500
H	-5.32768700	1.88058900	-1.16461900
H	-4.03034400	2.43038000	-2.25434200
C	-4.51406300	-1.34715600	-0.90640300
H	-5.21510900	-1.13799500	-0.08990600
H	-5.08773600	-1.64929800	-1.79478800
H	-3.87107500	-2.18475600	-0.60917500
C	-4.93743000	1.01555700	1.78881500
H	-5.64252800	1.05191300	0.94959100
H	-4.87864000	-0.02073700	2.14756600
H	-5.33581200	1.64120700	2.60101500
C	-3.34970400	3.49227900	0.84036900
H	-3.75048700	4.06388600	1.69013400
H	-2.36130100	3.89668000	0.58811000
H	-4.01451000	3.63365600	-0.02034000
C	-2.20303800	1.60709000	2.94882300
H	-2.06752300	0.59016900	3.33391600
H	-1.21565900	2.06661000	2.83525900
H	-2.77002900	2.18337700	3.69531900
C	1.66145300	-1.97083000	-3.71591700
H	0.68101400	-2.40827400	-3.48994200
H	1.56136400	-1.32610000	-4.59715800
H	2.35608000	-2.78835900	-3.95842800
C	4.07830000	-0.38548600	-2.61438500
H	4.09606200	0.30871800	-3.46350300
H	4.51442900	0.12208800	-1.74365800
H	4.71206200	-1.24912500	-2.86417200
C	2.56711200	-2.31044100	-0.82788500
H	3.26628600	-3.06656200	-1.21586700
H	2.99835000	-1.88570000	0.08533200
H	1.62897800	-2.81126000	-0.56640500
C	-0.17155300	-1.97367900	4.88800600
H	-0.73295100	-2.80856200	5.33255100
H	0.83877500	-1.97346000	5.31517400
H	-0.66806700	-1.03574500	5.17015400
C	-2.01577800	-2.28654200	2.50096700
H	-2.57307200	-1.37506200	2.74450200
H	-2.13895500	-2.49322900	1.43240500
H	-2.45764200	-3.11977200	3.06806200
C	0.57760300	-3.88315900	2.57135400
H	0.54399500	-4.04123700	1.48594900
H	1.61999900	-3.95990100	2.90238500
H	-0.00622400	-4.67782400	3.05796200
C	1.87015000	0.94665500	4.30439000
H	1.33322000	0.46587600	5.13070200
H	2.82900700	1.32922900	4.68293700
H	1.27276900	1.79569300	3.94846300
C	3.25131900	0.67660700	1.59708500
H	4.16026400	1.01220900	2.11859800
H	3.55437900	0.04518600	0.75466100
H	2.73652900	1.55851000	1.20102900
C	3.29913000	-1.68002700	3.49859300
H	2.83521300	-2.26521300	4.30193200
H	3.54914600	-2.36179000	2.67487200
H	4.23374900	-1.24674100	3.88399200

Int8'

H= -1275.353576 au

U	-0.18406700	0.06222700	0.16923700
Si	-3.19428800	1.62758500	1.32207900
Si	-3.44536800	0.14982800	-1.31292800
Si	-0.14220000	-2.18302600	2.96438700
Si	2.20595900	-0.27245100	2.82153800
Si	2.25115800	-0.98636100	-2.23836200
Si	1.22350600	1.84215200	-2.60830200
N	0.36973500	2.25035500	0.90705300
N	-1.12589300	-4.18739200	-1.71493600
O	0.93059300	4.45333300	1.66151800
O	-0.72778900	-2.08002200	-0.57434100
C	0.65069100	3.35727600	1.28603200
N	-2.45115900	0.63594200	0.06494500
N	1.17836100	0.31888900	-1.71712500
N	0.70087500	-0.87710000	2.12599000
C	-0.93302300	-3.16590000	-1.16202000

C	1.42087400	1.59921500	-4.49870900
H	0.57616300	1.02515500	-4.90146700
H	1.43322500	2.58553800	-4.98519000
H	2.34944900	1.07612100	-4.75673800
C	2.64001200	2.98647800	-2.03239500
H	3.61965900	2.52075300	-2.19539800
H	2.60687800	3.93626100	-2.58557900
H	2.53314400	3.20531000	-0.96294900
C	-0.40150800	2.82826500	-2.41309600
H	-0.65171400	3.01941000	-1.36325700
H	-0.26971300	3.79997400	-2.91205900
H	-1.24609100	2.31246400	-2.88580400
C	-2.39829100	-0.47421700	-2.78926400
H	-2.23540100	-1.55634900	-2.72372700
H	-2.96133600	-0.26971300	-3.71225400
H	-1.41935900	0.01173100	-2.88234400
C	-4.48965100	1.60419100	-2.00072800
H	-5.05700500	1.25702100	-2.87668500
H	-5.20207400	1.99449400	-1.26341800
H	-3.83245100	2.42545300	-2.31605100
C	-4.63933000	-1.27951500	-0.89119200
H	-5.38860300	-0.98782800	-0.14606500
H	-5.15928500	-1.60712100	-1.80315200
H	-4.06668900	-2.13037700	-0.50004100
C	-4.99387600	1.10667000	1.72706000
H	-5.66479700	1.21173800	0.86593600
H	-5.02418000	0.06246700	2.06479100
H	-5.37301500	1.74445400	2.53893500
C	-3.22722800	3.48330600	0.87166700
H	-3.64925900	4.06577800	1.70344400
H	-2.20670000	3.83855800	0.68376800
H	-3.82983100	3.66815200	-0.02605300
C	-2.26810100	1.48300500	2.98772100
H	-2.33484900	0.47140600	3.40580100
H	-1.21025800	1.75661000	2.90382500
H	-2.74273600	2.17790700	3.69677000
C	1.62623100	-1.89331800	-3.79717800
H	0.64935100	-2.35037700	-3.59267400
H	1.53172600	-1.22393600	-4.66011400
H	2.32983400	-2.69898800	-4.05391100
C	4.02879800	-0.35955000	-2.59427000
H	4.06180500	0.37231300	-3.41107900
H	4.45491800	0.10547000	-1.69536800
H	4.66054900	-1.21503400	-2.87529000
C	2.44383800	-2.34775500	-0.90389300
H	3.44208700	-2.79604100	-1.01923000
H	2.35872400	-1.98497700	0.12781000
H	1.69729300	-3.13683200	-1.05176100
C	-0.24568100	-1.88221600	4.85523600
H	-0.79358200	-2.71219600	5.32480100
H	0.74434400	-1.81555100	5.32314600
H	-0.78773500	-0.94918700	5.05881900
C	-1.95336300	-2.37391300	2.37757800
H	-2.46046700	-1.41938700	2.19334100
H	-2.00541800	-2.96810500	1.45902500
H	-2.50868800	-2.90430700	3.16554900
C	0.66933400	-3.88813900	2.68033200
H	0.75848200	-4.07629500	1.60259200
H	1.66657800	-3.95138700	3.13142700
H	0.03703100	-4.67557700	3.11560000
C	1.91289400	1.01323500	4.20279000
H	1.33771300	0.58351400	5.03206000
H	2.87588100	1.37344700	4.59278300
H	1.35842000	1.87109600	3.80286500
C	3.31085000	0.56454200	1.50759700
H	4.20042900	0.96257300	2.01836800
H	3.64467900	-0.14967400	0.74530800
H	2.80595100	1.39881900	1.00809900
C	3.30534700	-1.66126500	3.55421700
H	2.82869100	-2.18207100	4.39353600
H	3.55057700	-2.40097500	2.78087400
H	4.24382500	-1.21547500	3.91518700

Int9

H= -1295.691114 au

U	-0.44460700	0.53085300	0.00161200
Si	1.67420300	2.72805500	1.93380400
Si	-0.00484600	0.74955000	3.49081300
Si	-3.89023600	1.81659900	0.72805600
Si	-3.63311000	-0.69892500	-0.87792200
Si	1.18311400	0.32704200	-3.30038700
Si	-0.36761000	2.83744000	-2.66891100
N	0.38099900	1.52836200	1.93675300
N	-2.83033100	0.65440400	-0.06005300
N	0.15950500	1.24360100	-2.16717900
N	1.41408600	-1.05342000	-0.10231500
C	0.59054100	-1.88957100	0.33625300
O	-0.71204000	-1.73344000	0.54389700
C	1.09481900	-3.45302200	0.76715800
O	1.02370000	-4.18974600	-0.20761300
O	1.38625000	-3.48598000	1.95669600
C	-1.82412700	2.82170000	-3.90475100
H	-2.65599300	2.24448100	-3.47949500
H	-2.17250200	3.84705200	-4.09638200
H	-1.53769000	2.36669600	-4.86001700
C	1.01875300	3.96355200	-3.36543200
H	1.46668900	3.57245200	-4.28515500
H	0.59946600	4.95766500	-3.58017900
H	1.81517500	4.08012000	-2.61919300
C	-1.00813300	3.79356400	-1.14100400
H	-0.26125400	3.86809000	-0.33981100
H	-1.25233500	4.81924700	-1.45494300
H	-1.92774600	3.35106300	-0.74317000
C	-2.48799100	-1.41863500	-2.22033000
H	-1.69227900	-2.03143900	-1.77966200
H	-3.08367300	-2.06954300	-2.87722800
H	-2.03958700	-0.62861300	-2.83604500
C	-5.23341000	-0.20033500	-1.81297700
H	-5.60642200	-1.09111200	-2.33996300
H	-6.02644800	0.15495700	-1.14361500
H	-5.02706700	0.57869000	-2.55837500
C	-4.08207700	-2.12537500	0.30403600
H	-4.76939000	-1.80494800	1.09657400
H	-4.55184600	-2.94566000	-0.25799900
H	-3.15937100	-2.49990400	0.76355100
C	-5.25732100	1.00006700	1.79539600
H	-5.92683600	0.37388000	1.19246000
H	-4.81286400	0.37240400	2.57837600
H	-5.85950400	1.78474600	2.27631900
C	-4.80202500	2.97481600	-0.50183100
H	-5.28707800	3.78653200	0.06034600
H	-4.10184000	3.42257400	-1.21810700
H	-5.57196700	2.43634700	-1.06605000
C	-2.97608300	2.99627300	1.92528800
H	-2.46515500	2.45356900	2.72622800
H	-2.23477200	3.63090100	1.42705900
H	-3.73469200	3.65190300	2.37897600
C	2.55338600	2.74964400	0.24248100
H	3.33751200	3.52099000	0.25829500
H	3.02820700	1.77624800	0.06295500
H	1.89144700	2.95732400	-0.60515900
C	1.02538300	4.48754000	2.31566000

H	0.59779100	4.52374500	3.32578100
H	1.84996100	5.21300700	2.25917900
H	0.24642700	4.79252000	1.60588200
C	3.08025200	2.39320800	3.18552100
H	3.57804100	1.44465400	2.94928000
H	3.81908700	3.20367000	3.10068000
H	2.72860600	2.35538900	4.22296600
C	-1.59724400	-0.29425400	3.36819100
H	-2.46503500	0.26316800	3.00169700
H	-1.44999400	-1.17126700	2.72555000
H	-1.82408200	-0.65549000	4.38276700
C	-0.29494200	2.04905000	4.87030000
H	0.61026600	2.63418200	5.07605900
H	-1.09960400	2.74226700	4.59296800
H	-0.58511300	1.53065700	5.79571400
C	1.32616700	-0.47842200	4.08170500
H	0.98806200	-0.94113700	5.02132200
H	1.45459100	-1.27969300	3.34098900
H	2.29754000	-0.00469500	4.26085700
C	0.83870200	0.79791800	-5.13506400
H	-0.18607400	0.51441900	-5.41044400
H	0.98483400	1.85730700	-5.37247700
H	1.52894600	0.21047100	-5.75875500
C	3.02994000	0.64240000	-2.95032700
H	3.26665900	1.71374100	-2.96307700
H	3.27092800	0.23653300	-1.95981100
H	3.65244700	0.13237100	-3.69921000
C	0.91704200	-1.55702800	-3.32057300
H	1.63030900	-1.97175800	-4.04958100
H	1.11377300	-2.02356700	-2.35096300
H	-0.09481600	-1.82026200	-3.65051100

Int10

H= -1127.690134 au

U	-0.02032700	0.92626900	0.34035300
Si	-3.12149300	1.81798000	1.60988900
Si	-3.35450100	0.25694900	-1.00912000
Si	-0.16086300	-2.03485900	2.52560700
Si	2.22279800	-0.24161800	2.93063200
Si	1.84950000	-0.74034100	-2.27544000
Si	1.18429700	2.17407800	-2.79384200
C	0.81354500	3.55421700	0.92741400
O	1.34704800	2.44070700	1.43092500
O	-0.33047400	3.22337000	0.32822000
N	-2.38650900	0.85968100	0.32245500
N	1.01445700	0.72390900	-1.77568900
N	0.74959100	-0.62326900	2.01576700
C	1.63848000	1.79066300	-4.62041400
H	0.83955100	1.22830000	-5.11959700
H	1.74764700	2.75833300	-5.13251100
H	2.58111300	1.24106300	-4.73130600
C	2.53723700	3.34316000	-2.13899700
H	3.49259200	2.81023400	-2.04042100
H	2.67539200	4.18875600	-2.82886400
H	2.25435900	3.73809000	-1.15294800
C	-0.46195700	3.12695600	-2.90169000
H	-0.74940600	3.50845000	-1.91453200
H	-0.34136900	3.98059300	-3.58488200
H	-1.26100500	2.48215900	-3.29149200
C	-2.24597400	-0.67661000	-2.25514300
H	-1.84914300	-1.59986300	-1.80973800
H	-2.85192100	-0.95637400	-3.12927400
H	-1.39920300	-0.06900500	-2.59648100
C	-4.25469200	1.63943500	-1.97775300
H	-4.75463500	1.21813100	-2.86187900
H	-5.01388000	2.12545700	-1.35107700
H	-3.53972600	2.40438400	-2.30490900
C	-4.70561700	-1.00997900	-0.51459900
H	-5.49997900	-0.55348800	0.08757500
H	-5.15825700	-1.41859100	-1.43029800
H	-4.26976000	-1.83935900	0.05610200
C	-4.71127100	1.01398000	2.31900400
H	-5.54967300	1.08298500	1.61387000
H	-4.54537400	-0.04395200	2.55977300
H	-4.99713800	1.54148600	3.24085600
C	-3.55112800	3.60119600	1.09827400
H	-3.90422000	4.17343900	1.96838700
H	-2.63657800	4.06549700	0.70979800
H	-4.32644100	3.62996600	0.32258300
C	-1.90228400	1.92803100	3.07814400
H	-1.57607000	0.93992300	3.42621500
H	-1.01378700	2.52835500	2.84316900
H	-2.41847700	2.42775900	3.91169700
C	1.22432000	-1.50318100	-3.91939300
H	0.12917000	-1.57766200	-3.90681600
H	1.52573200	-0.92294600	-4.79783800
H	1.63771900	-2.51830100	-4.01413300
C	3.74146100	-0.49543900	-2.42442700
H	3.98881400	0.26955900	-3.17139000
H	4.14947000	-0.17375000	-1.45749200
H	4.22915200	-1.43672700	-2.71619600
C	1.57770900	-2.13746800	-1.00340200
H	2.16905400	-3.00902200	-1.32166100
H	1.88133000	-1.85762200	0.01153400
H	0.52268800	-2.44494700	-0.96926900
C	-0.75096500	-1.92746200	4.34776600
H	-1.31733800	-2.83083800	4.61701900
H	0.09451800	-1.82828200	5.04028000
H	-1.40427500	-1.05530000	4.48097600
C	-1.74680700	-2.27870000	1.48987600
H	-2.41044400	-1.40986300	1.53531600
H	-1.51501600	-2.47341400	0.43326800
H	-2.27482500	-3.15925300	1.88525500
C	0.74112800	-3.71886700	2.33164000
H	1.16655000	-3.81050700	1.32400300
H	1.54253200	-3.85992400	3.06395000
H	0.00215100	-4.52283100	2.46738800
C	1.92937100	1.06798300	4.28339000
H	1.14560300	0.74268500	4.98055100
H	2.85406300	1.24433100	4.85196100
H	1.62224600	2.00242400	3.80182200
C	3.62654700	0.34484800	1.77824400
H	4.55390600	0.44859700	2.36069800
H	3.80570000	-0.38324600	0.97524100
H	3.37477000	1.31818800	1.34390600
C	3.00209300	-1.74595400	3.84477300
H	2.32942700	-2.21895700	4.57056400
H	3.35292600	-2.50885900	3.13846800
H	3.87556500	-1.36136300	4.39306200

$TS_{3\text{-}11}$

H= -1428.184649 au

U	-0.14436300	0.22620700	0.07781200
Si	2.48776100	2.56946500	1.06958200
Si	0.73555700	1.78370300	3.32609300
Si	-3.83003100	-0.84851200	0.35759100
Si	-2.16022900	-1.95758900	-1.82235100
Si	0.20167700	-3.00146800	2.31364300
Si	3.90325900	-4.13002400	-0.52835800
Si	0.20078100	2.15755100	-3.15294700
Si	-1.67069500	3.29275800	-1.15818000
N	1.07807500	1.66464800	1.60743000

N	-2.26013500	-0.89789000	-0.42209700
N	-0.50924300	2.03626900	-1.55552100
N	2.62815800	-3.17099400	0.19760900
C	2.23303100	-2.02141900	0.09240100
O	0.53830700	-1.80936900	1.19247800
O	2.21607900	-0.88398200	-0.31898800
C	-3.42840900	2.90083300	-1.80419100
H	-3.72019800	1.89986700	-1.46699900
H	-4.15694700	3.63129800	-1.42324000
H	-3.45765000	2.91294500	-2.90102500
C	-1.25124200	5.05111700	-1.81074400
H	-1.25632400	5.10709800	-2.90618900
H	-2.00981400	5.74945800	-1.42637600
H	-0.26810700	5.37602400	-1.44809400
C	-1.80855900	3.53344700	0.73016800
H	-2.06493500	2.60750900	1.25941800
H	-0.85368800	3.88854800	1.13323600
H	-2.59250100	4.27551600	0.94441500
C	-0.38192300	-2.62038400	-2.09751300
H	0.36283600	-1.84491100	-2.31830800
H	-0.05215300	-3.18072200	-1.21462700
H	-0.41023200	-3.30740500	-2.95764300
C	-2.70515100	-1.11609200	-3.44994400
H	-2.54275200	-1.78507100	-4.30762000
H	-3.76756200	-0.84396400	-3.41148500
H	-2.12477400	-0.19920800	-3.60111500
C	-3.18651300	-3.57774300	-1.70506700
H	-4.26385000	-3.39192500	-1.62502600
H	-3.00542300	-4.16364700	-2.61892800
H	-2.86981100	-4.17799900	-0.84324600
C	-4.28743900	-2.43659700	1.33904000
H	-4.57988400	-3.25160800	0.66612800
H	-3.44756100	-2.78231400	1.95145800
H	-5.13551900	-2.21782700	2.00494900
C	-5.29223300	-0.60852200	-0.86980000
H	-6.23296900	-0.56587500	-0.30080900
H	-5.18253800	0.33046300	-1.42617200
H	-5.36637900	-1.43045000	-1.59287200
C	-4.01737000	0.58254600	1.60224200
H	-3.25307700	0.54607800	2.38628800
H	-3.95603600	1.55529500	1.10080700
H	-5.00714700	0.50131700	2.07633700
C	3.26187800	1.91483000	-0.54936600
H	3.98688000	2.66081700	-0.90856600
H	3.78359100	0.96898700	-0.37156300
H	2.52258100	1.75682800	-1.34085800
C	2.11508500	4.42117300	0.75084000
H	1.74282800	4.92228900	1.65250800
H	3.02636700	4.93660300	0.41323500
H	1.35458800	4.50919300	-0.03478000
C	3.98354900	2.50282600	2.27848100
H	4.30211000	1.46027400	2.41333800
H	4.81736000	3.06097600	1.82650800
H	3.77578500	2.93328300	3.26460200
C	-1.06278900	1.40876200	3.84954500
H	-1.76489800	2.09634200	3.36491000
H	-1.36905000	0.38136500	3.63109700
H	-1.12507000	1.56414500	4.93839800
C	0.98282700	3.55206800	4.05191300
H	1.99092100	3.95453900	3.90098700
H	0.26232500	4.24369000	3.59353300
H	0.78232200	3.51862900	5.13343300
C	1.81806300	0.59356200	4.36727600
H	1.51831900	0.62432100	5.42508200
H	1.68431400	-0.42947500	3.99454600
H	2.88210100	0.84827700	4.29508100
C	-1.07389300	2.47271500	-4.55973400
H	-1.81461700	1.66550300	-4.61203000
H	-1.60750700	3.42122200	-4.41824200
H	-0.54117300	2.51884900	-5.52139000
C	1.46821100	3.59117500	-3.35289700
H	0.95463600	4.55301800	-3.47124200
H	2.13661100	3.66242400	-2.48784600
H	2.07874300	3.41412500	-4.25105700
C	1.12730000	0.57712900	-3.70765100
H	1.57016200	0.77490000	-4.69639400
H	1.93198000	0.28967900	-3.01966700
H	0.43499300	-0.26725500	-3.80676200
C	1.74438800	-3.49912800	3.32682300
H	1.44756600	-4.19229600	4.12778500
H	2.49322900	-3.98321100	2.69204700
H	2.19670300	-2.61218200	3.78931400
C	-1.06793200	-2.39958500	3.60066000
H	-0.60008100	-1.67106000	4.27389500
H	-1.92643100	-1.92081500	3.11772200
H	-1.42892800	-3.24821400	4.20026100
C	-0.47839400	-4.56443800	1.45829900
H	-1.36474700	-4.31032500	0.86434500
H	0.28131500	-4.98689200	0.78847600
H	-0.75779100	-5.32572500	2.20059400
C	3.34670100	-5.94048000	-0.44082700
H	2.41926000	-6.08105300	-1.01040200
H	4.11684500	-6.60566600	-0.85437400
H	3.15645000	-6.22719200	0.60125700
C	5.48333900	-3.88080900	0.49574800
H	6.29583800	-4.51381800	0.11328700
H	5.80545000	-2.83263500	0.45076700
H	5.30022600	-4.13983800	1.54625300
C	4.18505600	-3.60323100	-2.33110800
H	3.26064900	-3.72079800	-2.91053600
H	4.48707100	-2.54933900	-2.38012600
H	4.97094300	-4.21556900	-2.79474800

Int11

H= -1137.316928 au

U	-0.61678100	0.69576700	0.38693800
Si	1.94684600	2.55681500	1.99736200
Si	-0.62327000	2.78805700	3.49160900
Si	-3.88627200	-0.64391500	1.21089300
Si	-2.82522800	-1.54695400	-1.46075100
Si	1.08625100	-2.54314000	1.56074000
Si	0.93657400	1.90777000	-2.84339300
Si	-1.55328900	3.27147700	-1.92428600
N	0.22502100	2.23516700	2.06143800
N	-2.64317700	-0.56664900	-0.02328800
N	-0.34465700	2.03526300	-1.65526500
O	0.42647700	-1.06629200	1.23220800
C	-2.92042200	2.76453600	-3.16590100
H	-3.37978500	1.82111000	-2.84599600
H	-3.70186400	3.53752000	-3.20308300
H	-2.51727400	2.62582700	-4.17663000
C	-0.88219100	4.96546700	-2.53281300
H	-0.41607400	4.89708000	-3.52408700
H	-1.71863100	5.67745200	-2.59482100
H	-0.14130900	5.36136300	-1.82597800
C	-2.43723200	3.66262300	-0.28036200
H	-2.96659100	2.79292400	0.13471700
H	-1.71308300	4.01313500	0.46527000
H	-3.18311400	4.45390400	-0.44721400
C	-1.38091100	-1.26221000	-2.67272000
H	-1.23207700	-0.19712700	-2.88387600
H	-0.44459700	-1.67102100	-2.26947500

H	-1.60230200	-1.78403000	-3.61592900
C	-4.42448400	-1.14912100	-2.44517700
H	-4.49028700	-1.78152800	-3.34275600
H	-5.32551800	-1.31055900	-1.84019200
H	-4.40929800	-0.09861900	-2.76268400
C	-2.79286600	-3.44299200	-1.15941900
H	-3.70030400	-3.81256200	-0.66924600
H	-2.68240900	-3.96069700	-2.12403500
H	-1.92906400	-3.69888900	-0.53133900
C	-3.18451000	-0.78985100	2.98422800
H	-2.46576900	-1.61910700	3.01937300
H	-2.67340700	0.11845100	3.31774100
H	-4.00501400	-1.00589400	3.68581700
C	-5.03417800	-2.18654100	1.10402600
H	-5.83559800	-2.06240300	1.84787600
H	-5.49928100	-2.31315000	0.11924600
H	-4.48060800	-3.10170200	1.34993200
C	-5.09118200	0.84145600	1.12405200
H	-4.56682900	1.79298800	1.26865000
H	-5.57433800	0.86259500	0.13734100
H	-5.87110000	0.75298200	1.89445100
C	2.81914200	1.41176300	0.73927400
H	3.90509000	1.57240500	0.82248000
H	2.60678200	0.35603800	0.94890100
H	2.53093300	1.63299700	-0.29412200
C	2.36177300	4.34551100	1.45103200
H	1.98462700	5.08351700	2.16918100
H	3.44978200	4.47546700	1.35383500
H	1.89969500	4.54413500	0.47476900
C	2.88696100	2.21500600	3.63726200
H	2.77365700	1.15642800	3.90670200
H	3.95733900	2.42239800	3.48967500
H	2.52870100	2.82662900	4.47369900
C	-2.49138200	3.12143900	3.26039800
H	-2.65872200	3.93250400	2.54178200
H	-3.03454700	2.23765700	2.91252600
H	-2.90682300	3.42705400	4.23308500
C	0.01363300	4.48151000	4.15057300
H	1.07894000	4.47063800	4.40951100
H	-0.15170200	5.26388900	3.39734000
H	-0.55735200	4.74828500	5.05235100
C	-0.46970100	1.55019500	4.94654600
H	-1.06847700	1.88382100	5.80671600
H	-0.82582500	0.56028200	4.63404200
H	0.57599400	1.45182000	5.26413600
C	0.30524700	2.01498000	-4.65697900
H	-0.42460300	1.21875500	-4.85572700
H	-0.16801200	2.98127300	-4.87426000
H	1.15424300	1.88591100	-5.34462900
C	2.25692400	3.29363900	-2.68873300
H	1.81984400	4.27785700	-2.89583500
H	2.68664800	3.31693100	-1.67985300
H	3.06987700	3.11550400	-3.40839300
C	1.90180000	0.25518700	-2.78452600
H	2.80605600	0.35843500	-3.40365300
H	2.20422300	-0.02135000	-1.76806800
H	1.29178100	-0.55810900	-3.19376400
C	2.57612200	-2.35681500	2.74187800
H	2.99976000	-3.33833200	2.99845300
H	3.36248300	-1.74684200	2.27809900
H	2.25905300	-1.85889700	3.66789400
C	-0.18717900	-3.69446700	2.39416000
H	-0.51674700	-3.26925500	3.35130800
H	-1.06806900	-3.80911400	1.74950100
H	0.24405800	-4.68835100	2.58139700
C	1.68944200	-3.39018500	-0.04070100
H	0.84612500	-3.54648400	-0.72650100
H	2.43049400	-2.76006800	-0.54999000
H	2.14742100	-4.36558800	0.17725900

Int12

H= -1428.165469 au

U	-0.06002100	0.51189100	-0.46903500
Si	2.17677700	2.33798200	1.50086900
Si	0.07245300	0.94732400	3.15911700
Si	-3.66961600	0.44690600	-0.40863100
Si	-2.24584200	-2.23518300	-0.39353600
Si	0.38296700	-4.67584900	3.03359800
Si	3.95777700	-2.94291900	0.15628800
Si	-0.29705500	1.48582400	-3.80393500
Si	-0.69356900	3.86447000	-2.02504400
N	0.64363800	1.44339800	1.52834600
N	-2.15005900	-0.45114300	-0.34378300
N	-0.41949500	2.12169500	-2.13932700
N	3.15774900	-1.73603900	-0.85827600
C	2.16623800	-1.00011800	-0.94359700
O	0.57527400	-3.32564000	2.17001900
O	1.60350300	-0.32644100	-1.89647500
C	-2.45240300	4.42184400	-2.53802400
H	-3.22244900	3.82198200	-2.03977000
H	-2.58582700	5.47171200	-2.23803200
H	-2.60691100	4.35118200	-3.62003600
C	0.53080500	4.87550700	-3.09684400
H	0.39785900	4.68837200	-4.16922000
H	0.36849700	5.94739200	-2.91148900
H	1.56745400	4.63157000	-2.82961100
C	-0.42825000	4.51607400	-0.25371400
H	-0.83714300	5.53564200	-0.19766500
H	-0.90996100	3.90901800	0.52124400
H	0.64149900	4.56463200	-0.02654200
C	-0.52001500	-2.93368700	-0.76203500
H	0.02246300	-2.45920000	-1.59090900
H	0.07612800	-2.96297900	0.17291400
H	-0.66654300	-3.98738700	-1.04932500
C	-3.43296600	-2.82835300	-1.77767700
H	-3.40854900	-3.92751000	-1.80356400
H	-4.47087600	-2.51364800	-1.61111400
H	-3.10554800	-2.45444500	-2.75653900
C	-2.76176800	-2.97893600	1.27298500
H	-3.56018300	-2.41997200	1.77231800
H	-3.08839700	-4.01990600	1.13702200
H	-1.85570000	-2.99199700	1.89777100
C	-5.08393700	-0.37563000	0.58040400
H	-5.30353900	-1.39329000	0.23779500
H	-4.82896200	-0.41733700	1.64705100
H	-5.99266800	0.23328700	0.46491800
C	-4.28246500	0.70364300	-2.19938200
H	-5.18871700	1.32627200	-2.20200000
H	-3.50714900	1.21399600	-2.78380500
H	-4.51314400	-0.25180700	-2.68594600
C	-3.48241800	2.18528000	0.35375100
H	-3.26774300	2.12382800	1.42529700
H	-2.69254000	2.76801300	-0.13092100
H	-4.42567800	2.73516300	0.21962700
C	2.81668000	2.47692000	-0.29928900
H	3.70696200	3.12328700	-0.27066900
H	3.13230300	1.50493000	-0.69836300
H	2.10507000	2.92708100	-1.00291000
C	2.06173300	4.11773800	2.21416400
H	1.03938200	4.50790700	2.18628800
H	2.40582100	4.12409400	3.25582800
H	2.70918100	4.79232200	1.63548400

C	3.58522200	1.49483700	2.47063600
H	3.72137500	0.46138100	2.13481800
H	4.52036100	2.04818300	2.29966200
H	3.38261400	1.48497200	3.54888600
C	-1.79759800	0.57703000	3.17025700
H	-2.38600700	1.50257900	3.20183800
H	-2.11663700	-0.02141300	2.30926600
H	-2.01071900	-0.00166400	4.08000000
C	0.29735000	2.36026100	4.43561500
H	1.35300300	2.55840400	4.65788200
H	-0.17204800	3.29319600	4.09885500
H	-0.19085900	2.04266000	5.36876700
C	0.95351100	-0.58856400	3.81894800
H	0.58206400	-0.78224500	4.83790400
H	0.75171100	-1.49192600	3.21067900
H	2.03974100	-0.44864800	3.87351800
C	-1.48287000	2.34143400	-5.04366500
H	-2.52958900	2.23610700	-4.73257100
H	-1.26212900	3.40547000	-5.18868100
H	-1.35997900	1.83361300	-6.01198100
C	1.46087600	1.64075900	-4.52288900
H	1.78466600	2.68690200	-4.58144700
H	2.15875100	1.08508200	-3.88613200
H	1.48789000	1.20899300	-5.53398900
C	-0.79533600	-0.35659600	-3.87163800
H	-1.02934700	-0.60185200	-4.91811800
H	0.02229400	-1.00893800	-3.54590100
H	-1.68825400	-0.56678800	-3.26961900
C	2.00585100	-5.38822100	3.80914200
H	1.78862900	-6.29828900	4.38894600
H	2.73270600	-5.64061400	3.02420300
H	2.46946400	-4.65037700	4.47902000
C	-0.80205300	-4.49606700	4.55066000
H	-0.41656100	-3.73187100	5.24070300
H	-1.80538800	-4.18790100	4.22467500
H	-0.88849700	-5.44734200	5.09768000
C	-0.33267200	-6.16216000	2.02529600
H	-1.31599700	-5.90509100	1.60768500
H	0.33860300	-6.41110900	1.19072200
H	-0.44453400	-7.05437200	2.65989900
C	3.21648500	-4.62631900	-0.29960500
H	2.21349300	-4.66716700	0.14416600
H	3.14638600	-4.76251600	-1.38567400
H	3.81921000	-5.44064700	0.12583000
C	3.70651800	-2.62091000	1.99236900
H	4.30622900	-3.32492900	2.58660100
H	3.97953900	-1.59784900	2.27391900
H	2.63409200	-2.79954300	2.20291900
C	5.79041400	-2.84187200	-0.35707200
H	5.90409200	-3.03845400	-1.43078800
H	6.19421700	-1.84418100	-0.14057100
H	6.37809800	-3.58353600	0.20143700

$TS_{12\text{-}7}$

H= -1428.156604 au

U	-0.49908500	0.73649500	-0.34089100
Si	1.79912900	2.48084000	1.62215700
Si	-0.30786800	1.07289500	3.26298200
Si	-4.03643400	0.63065900	-0.31790900
Si	-2.69550600	-2.10156000	-0.29616300
Si	0.56982600	-4.55019100	2.77595300
Si	3.34058000	-2.93342300	0.63861400
Si	-0.58743500	1.57534400	-3.74169100
Si	-1.00778300	4.02019400	-2.05159100
N	0.22963700	1.65491300	1.66208500
N	-2.55452900	-0.32379500	-0.24334900
N	-0.76594600	2.27471900	-2.11453600
N	2.40686700	-1.70078500	-0.22640500
C	1.53690500	-0.89712900	-0.53289700
O	1.02003000	-3.30392500	1.84586300
O	1.17520500	-0.25454300	-1.61561100
C	-2.75282600	4.59028100	-2.59960000
H	-3.53713500	4.06390000	-2.04288100
H	-2.85016600	5.66742400	-2.39797400
H	-2.92019400	4.42412000	-3.66944100
C	0.24372700	4.98783100	-3.13206300
H	0.12873300	4.76875700	-4.20045900
H	0.09123500	6.06681200	-2.98290700
H	1.27209100	4.73996400	-2.83748400
C	-0.74923100	4.71544300	-0.29059000
H	-1.24446800	5.69511500	-0.22571900
H	-1.14333800	4.07920100	0.51079000
H	0.32097700	4.86085500	-0.10630000
C	-1.01924100	-2.90028500	-0.67148800
H	-0.51315000	-2.45986400	-1.54100400
H	-0.33323000	-2.91785100	0.19814700
H	-1.22551700	-3.95366800	-0.92087800
C	-3.91496600	-2.65814100	-1.66642700
H	-3.94029000	-3.75730200	-1.68499200
H	-4.93677200	-2.29534900	-1.49712800
H	-3.57609000	-2.30627700	-2.64960500
C	-3.30797500	-2.82344000	1.35595200
H	-4.32851900	-2.51279400	1.60729100
H	-3.27582800	-3.92061600	1.29906400
H	-2.63091700	-2.51860900	2.16294400
C	-5.47346300	-0.09394700	0.71224000
H	-5.79527700	-1.07539200	0.34455300
H	-5.17818400	-0.19571100	1.76416400
H	-6.33021100	0.59331900	0.65570400
C	-4.66055000	0.88832100	-2.10384400
H	-5.53049000	1.56074400	-2.10739000
H	-3.86484600	1.34507100	-2.70548300
H	-4.95038700	-0.06038600	-2.57145400
C	-3.73798200	2.37718400	0.39712500
H	-3.43390200	2.33819100	1.44832000
H	-2.98813600	2.94034200	-0.16950200
H	-4.67892400	2.94397700	0.33360800
C	2.41662600	2.61744200	-0.18532100
H	3.33378900	3.22526200	-0.16430400
H	2.68360900	1.63715400	-0.59985500
H	1.71514300	3.10533300	-0.87333500
C	1.75193700	4.25139700	2.35120100
H	0.85411700	4.79701000	2.04120500
H	1.77419100	4.21543500	3.44676300
H	2.63659700	4.80779100	2.00803200
C	3.18136600	1.55707300	2.55486000
H	3.25274900	0.52051200	2.20502600
H	4.14118000	2.05990400	2.36593100
H	3.00754400	1.54697300	3.63810500
C	-2.18284500	0.71422400	3.28395000
H	-2.76235000	1.64564400	3.32020800
H	-2.51596500	0.12349800	2.42218700
H	-2.40052300	0.13856100	4.19476900
C	-0.04847600	2.38961100	4.63113600
H	1.01479600	2.55488100	4.84563900
H	-0.50577600	3.34912100	4.35739800
H	-0.52732200	2.02473600	5.55152100
C	0.58369200	-0.50836700	3.80697300
H	0.09753800	-0.89268800	4.71597200
H	0.56854100	-1.31057500	3.04989900
H	1.63448500	-0.30178300	4.04562700
C	-1.70886700	2.40822800	-5.05534100

H	-2.76823900	2.31026900	-4.78569400
H	-1.48102600	3.46975000	-5.20804300
H	-1.54803600	1.88414600	-6.00917000
C	1.20679400	1.66296900	-4.37736400
H	1.55932500	2.69831700	-4.46036000
H	1.85503100	1.12051900	-3.67858600
H	1.28093800	1.18678800	-5.36577900
C	-1.11728800	-0.25907600	-3.76313800
H	-1.29410900	-0.54784100	-4.80970500
H	-0.33248500	-0.90883500	-3.35990200
H	-2.04697600	-0.42725100	-3.20482700
C	2.00099000	-5.44507700	3.72309900
H	1.59599000	-6.28098300	4.31368800
H	2.75508300	-5.84407600	3.03091400
H	2.50194800	-4.74758000	4.40886500
C	-0.65299900	-4.09920000	4.20208400
H	-0.18526900	-3.38686600	4.89557000
H	-1.57002500	-3.64224900	3.80766400
H	-0.92996800	-5.00361500	4.76506300
C	-0.32305000	-5.97496100	1.82193300
H	-1.23072700	-5.59244500	1.33419100
H	0.33161100	-6.39250600	1.04418000
H	-0.61299200	-6.78620000	2.50683100
C	2.86583400	-4.67273300	0.03662400
H	1.81166500	-4.66749900	-0.24968300
H	3.49789100	-4.96827800	-0.81169100
H	2.98544700	-5.39777200	0.84974300
C	3.76906000	-2.53971600	2.44612600
H	4.25229800	-3.42247300	2.88895300
H	4.47234400	-1.69758700	2.49352000
H	2.85077400	-2.32886300	2.99352300
C	5.04430400	-2.63511000	-0.23031100
H	4.96567800	-2.79192000	-1.31472200
H	5.40723000	-1.61333900	-0.05157200
H	5.79025800	-3.34008300	0.16942800

CO_2

H= -188.488908 au

C	1.19942200	0.05780300	0.00000000
O	2.36728600	0.05780300	0.00000000
O	0.03155800	0.05780300	0.00000000

$OCNSiMe_3$

H=-290.911871 au

Si	4.07202900	-5.08710100	-1.90439300
N	3.63952200	-3.51799500	-1.24717800
C	3.34980000	-2.44300800	-0.80909300
O	3.06247900	-1.38253500	-0.37572300
C	2.85941200	-6.35208700	-1.19004000
H	1.82878800	-6.10277300	-1.47155000
H	3.09061100	-7.35563300	-1.57198600
H	2.92549300	-6.37426500	-0.09510500
C	5.84932300	-5.45535300	-1.36856800
H	6.16946400	-6.42873200	-1.76409900
H	6.53476800	-4.68580700	-1.74489500
H	5.92499300	-5.48377600	-0.27442500
C	3.92480800	-4.97124500	-3.78741500
H	2.89936000	-4.71272900	-4.07948400
H	4.60287600	-4.20421400	-4.18180300
H	4.18448400	-5.93403600	-4.24791100

$Me_3SiOSiMe_3$

H= -321.017671 au

Si	2.04054100	-5.48114800	-0.07641200
O	2.05246500	-3.80122900	-0.15429600
C	3.80151000	-6.17286300	-0.25388200
H	3.77791300	-7.27097800	-0.22383400
H	4.24724800	-5.86442600	-1.20842000
H	4.44729300	-5.82271800	0.56186700
C	1.30125900	-6.02924500	1.58433700
H	1.91850100	-5.68147400	2.42270900
H	0.28918700	-5.62228400	1.70648800
H	1.24114200	-7.12533100	1.63188000
C	0.95366000	-6.08555500	-1.50682800
H	-0.05919900	-5.67250600	-1.41728700
H	1.37213500	-5.76664700	-2.46994900
H	0.88354300	-7.18170000	-1.50352000
Si	2.95913700	-2.47107000	0.33237700
C	3.78568300	-2.79606200	2.01316300
H	4.36630000	-1.91534200	2.32091900
H	3.03201600	-2.99753300	2.78537900
H	4.46923600	-3.65342900	1.96025300
C	1.75868600	-1.01073500	0.47481900
H	2.29567500	-0.09555600	0.75875300
H	1.25322900	-0.83415000	-0.48316000
H	0.99458000	-1.21542600	1.23557000
C	4.28871700	-2.10583600	-0.97232500
H	3.82856700	-1.94208200	-1.95523600
H	4.85121500	-1.20252900	-0.69877700
H	4.99661600	-2.94067400	-1.05506700

NCO

H= -167.914783 au

O	0.00000000	0.00000000	1.14314400
C	0.00000000	0.00000000	-0.04093300
N	0.00000000	0.00000000	-1.27136500

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