

Supporting Information for:

# SOMC Grafting of Vanadium Oxytriisopropoxide (VO(O<sup>i</sup>Pr)<sub>3</sub>) on Dehydroxylated Silica; Analysis of Surface Complexes and Thermal Restructuring Mechanism

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## Summary

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## 1. Experimental Methods

**General sample handling and synthesis.** All experiments were carried out using Schlenk equipment or in Argon filled gloveboxes ( $< 0.1$  ppm  $\text{H}_2\text{O}$ ,  $< 0.1$  ppm  $\text{O}_2$ ), and by using high-vacuum lines ( $\sim 10^{-5}$  mbar). Solvents were dried by use of a commercial solvent purification system (CuO catalysts/Alox) and degassed by two freeze-pump-thaw cycles. Molecular sieves were dried in vacuum  $10^{-3}$  mbar for 12 h at  $300^\circ\text{C}$ .

**Elemental analyses** were done at the Mikroanalytisches Labor Pascher, Germany.

**Infrared (IR)** spectra were recorded on Nicolet 6700 FT-IR spectrometer equipped with a DTGS detector. Samples were prepared in a glovebox.

**Custom made high-vacuum transmission IR cell for pellets.** A T-shaped reaction vessel custom made from pyrex glass or quartz, equipped with a interface to the high-vacuum line and with two parallel windows transparent for transmission IR (CaF or KBr windows, 2mm thick), accommodates a self-supporting silica pellet of about 30-100 mg in a glass or quartz sample holder. The sample holder can be transferred from a heating/reaction zone to the measurement zone. A measurement of the evacuated cell without pellet in the beam was performed prior to the measurement of the pellet as background, and automatically subtracted from the sample spectra.

**IR data processing.** Typically 16 scans at a resolution  $4\text{ cm}^{-1}$  were averaged for each spectrum. Corrections for y-offset and a linear baseline correction were performed when necessary using Thermo Fisher Omnic software. Spectra of surface complexes on silica were normalized at the band of silica matrix vibration ( $1868\text{ cm}^{-1}$ ) before plotting them using software Origin 8.0.

**Solid State Nuclear Magnetic Resonance Spectroscopy.** All samples were packed into rotors under inert atmosphere of argon inside gloveboxes. One dimensional  $^1\text{H}$  MAS and  $^{13}\text{C}$  CP/MAS solid state NMR spectra were recorded on Bruker Ultrashield Plus spectrometers operating at 600 MHz resonance frequencies for  $^1\text{H}$ , equipped a conventional double resonance 3.2 mm CP/MAS probe. Dry nitrogen gas was utilized for sample spinning to prevent degradation of the samples. NMR chemical shifts are reported with respect to the external references TMS and adamantane. All experiments were performed nominally at room temperature of  $23^\circ\text{C}$ . For  $^{13}\text{C}$  CP/MAS NMR experiments, the following sequence was used:  $90^\circ$  pulse on the proton (pulse length 2.4 s), then a cross-polarization step with a contact time of typically 2 ms, and finally acquisition of the  $^{13}\text{C}$  signal under high power proton decoupling. The delay between the scans was set to 5 s to allow for a complete relaxation of the  $^1\text{H}$  nuclei and the number of scans ranged between 7 000 - 70 000 for  $^{13}\text{C}$ , and was 32 for  $^1\text{H}$ . An exponential apodization function corresponding to a line broadening of 80 Hz was applied prior to Fourier transformation. The  $^{51}\text{V}$  MAS NMR spectra were recorded on a Bruker AVANCE III operating at 236.7 MHz (21.2 T) using a 3.2 mm MAS probe. The  $^{51}\text{V}$  MAS NMR spectrum was recorded using a single pulse excitation with a small pulse angle ( $\pi/8$ ). Three spinning rates (22, 20, and 18 KHz) were used to determine the isotropic chemical shift. The delay between the scans was set to 0.25 s and the number of scans ranged between 30 000 - 100 000. The  $^{51}\text{V}$  chemical shift was referenced with respect to neat  $\text{VOCl}_3$  ( $\delta = 0\text{ ppm}$ ).

**$^1\text{H}$ - $^1\text{H}$  multiple-quantum solid-state NMR spectroscopy.** Two-di-mensional double-quantum (DQ) and triple-quantum (TQ) experiments were recorded on a Bruker Ultrashield Plus spectrometer operating at 600 MHz for  $^1\text{H}$ , equipped with a conventional double resonance 3.2 mm CP/MAS probe, according to the following general scheme: excitation of DQ coherences,  $t_1$  evolution, z-filter, and detection. The spectra were recorded in a rotor synchronized fashion in  $t_1$  by setting the  $t_1$  increment equal to one rotor period ( $45.45\ \mu\text{s}$ ). One cycle of the standard back-to-back (BABA) recoupling sequences was used for the excitation and reconversion period. Quadrature detection in  $w_1$  was achieved using the States-TPPI method. MAS samples were spun at 22 kHz. The  $90^\circ$  proton pulse length was  $2.5\ \mu\text{s}$ , while a recycle delay of 5 s was used. A total of 128  $t_1$  increments with 32 scans per each increment were recorded. The DQ frequency in the  $w_1$  dimension corresponds to the sum of two single quantum (SQ) frequencies of the two coupled protons and correlates in the  $w_2$  dimension with the two corresponding proton resonances.<sup>1</sup> The TQ frequency in the  $w_1$  dimension corresponds to the sum of the three SQ frequencies of the three coupled protons and correlates in the  $w_2$  dimension with the three individual proton resonances. Conversely, groups of less than three equivalent spins will not give rise to diagonal signals in this spectrum.

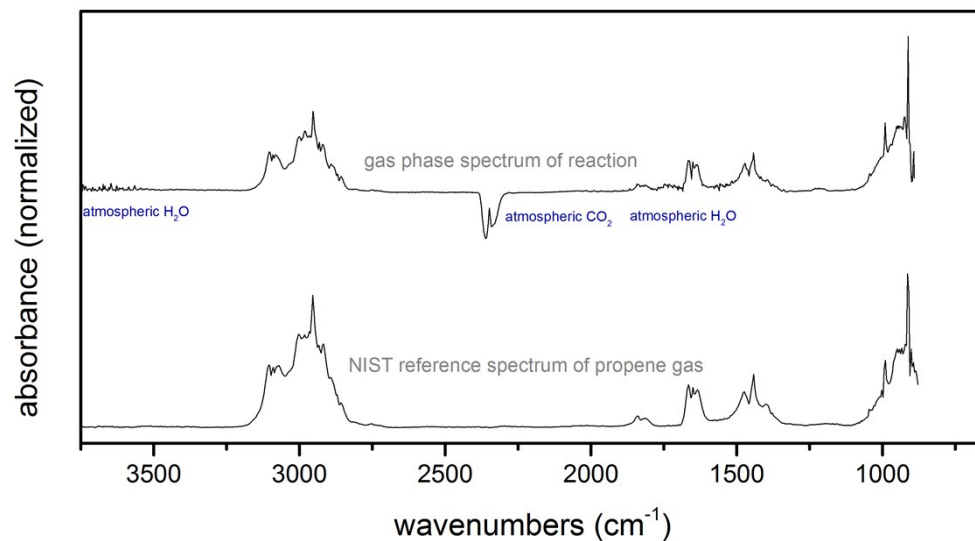
The 2D  $^1\text{H}$ - $^{13}\text{C}$  heteronuclear correlation (HETCOR) solid state NMR spectroscopy experiments were conducted on a Bruker AVANCE III spectrometer using a 3.2 mm MAS probe. The experiments were performed according to the following scheme:  $90^\circ$  proton pulse,  $t_1$  evolution period, CP to  $^{13}\text{C}$ , and detection of the  $^{13}\text{C}$  magnetization under TPPM decoupling. For the cross-polarization step, a ramped radio frequency (RF) field centered at 75 kHz was applied to the protons, while the  $^{13}\text{C}$  channel RF field was matched to obtain optimal signal. A total of 32  $t_1$  increments with 1500 scans each were collected. The sample spinning frequency was 8.5 kHz. Using a short contact time (0.2 ms) for the CP step, the polarization transfer in the dipolar correlation experiment was verified to be selective for the first coordination sphere about the metal center, that is to lead to correlations only between pairs of attached  $^1\text{H}$ - $^{13}\text{C}$  spins (C-H directly bonded).

**EPR spectroscopy.** EPR spectra were recorded by using a JEOL JES-FA 200 spectrometer at X-band frequency. The spectra were measured at a microwave frequency of approximately 9.27 GHz with a microwave power of 5 mW, modulation amplitude of 0.4 mT, sweep time of 4 min, time constant of 0.1 s, and modulation frequency of 100 kHz. The microwave frequency was measured with a microwave frequency counter Advantest R5372. The temperature was monitored with a JEOL ES DVT4 temperature controller equipped with a calibrated thermocouple. The experimental values of g and A were determined by using Mn(II) (nuclear spin  $I = 5/2$ ) embedded in MgO as a standard; experimental errors:  $\Delta g = \pm 0.003$ ,  $\Delta A = \pm 5 \cdot 10^{-4}\text{ cm}^{-1}$ . For the quantitative determination of V(IV) concentrations, the calibration curve was made with respectively 0.1 mL of frozen solutions of  $\text{VOSO}_4$  in 0.1 M aqueous hydrochloric acid. The EPR spectra of the standard solutions as well as of silica supported vanadium samples were recorded at 153 K. The peak areas were calculated by numerical double integration of the EPR spectra.

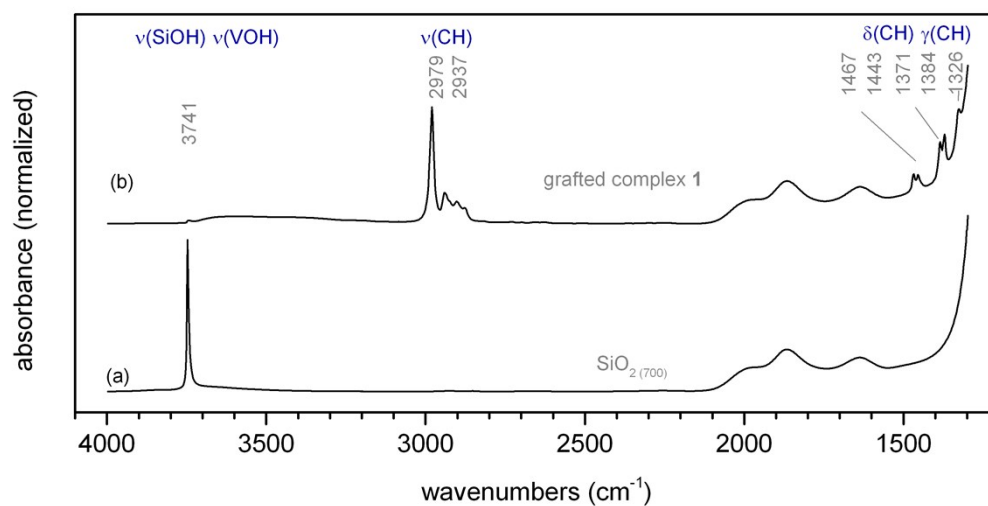
**Gas chromatography.** Gas phases were sampled using an airtight gas syringe and injected into the chromatograph by hand. Gas phase analysis of alkanes was performed on Agilent 6850 gas chromatography with split/splitless injector and equipped with an FID.  $10\ \mu\text{l}$  was injected by the hot needle technique (thermospray) at an injector temperature of  $180^\circ\text{C}$  using split mode (split ratio 10:1; 30 ml/min split flow). A HP-PLOT/U  $30\text{m} \times 0.53\text{mm}$ ;  $20.00\ \mu\text{m}$  capillary column coated with a stationary phasedivinylbenzene/ethylene glycol dimethacrylate was used with nitrogen as carrier gas at 4.65 Psi pressure. Each analysis was carried under the same conditions: a flow rate of 3 ml/min, an isotherm at  $150^\circ\text{C}$ , and a detector sets with a data rate of 5 Hz and a minimum peak width of 0.04 min. Gas phase compounds were further identified by GC/MS.

**Computational details.** All calculations have been performed using a cluster silica (2T) model (fig-SF1) with B3LYP density functional<sup>2</sup> as implemented in the Gaussian09 package<sup>3</sup>. The triple- $\zeta$  basis set TZVP<sup>4,5</sup> was used. The whole study was performed assuming a singlet spin state. All stationary points were characterized through frequency calculations. The transition states were located using the synchronous transit-guided quasi-newton (QST2) approach and the character of the stationary points has been checked by analytical frequency calculations. The Gibbs Free energies were computed assuming an ideal gas, unscaled harmonic vibrational frequencies and the rigid rotor approximation at 298.15 K and 1 atm. Since we reaction pathways, we assume the complex 1 (V bis-isopropoxy) as reference states at 0 kcal mol<sup>-1</sup>. All the other species are thus referred to this reference state, by adding/subtracting the energy of the propene and water molecules needed to connect chemically the species under discussion with the assumed reference state.

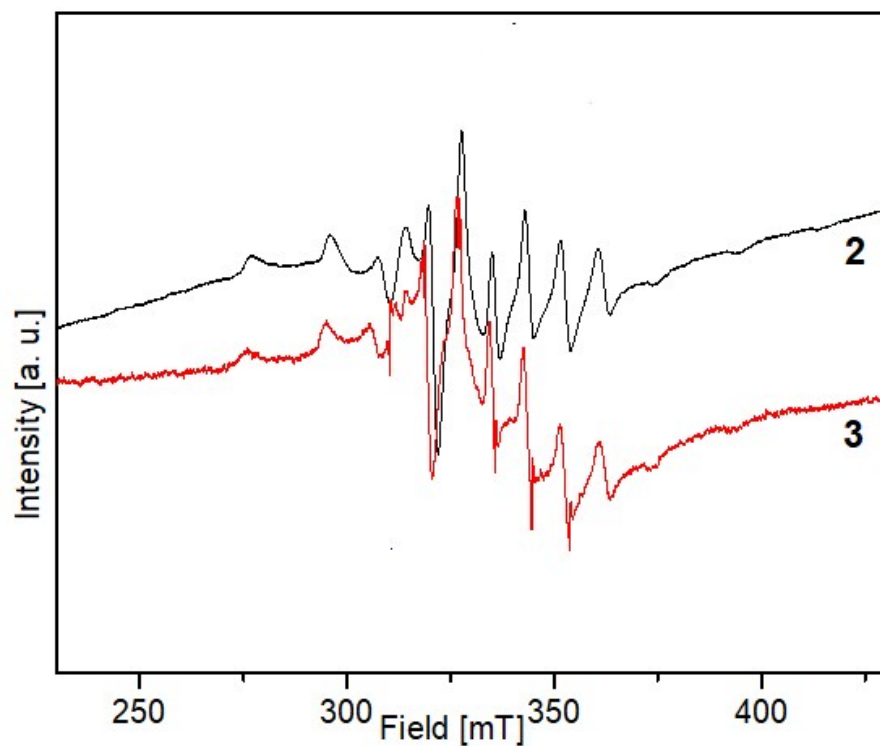
## 2. Supplementary Spectra and Figures



**Figure S1:** Transmission IR spectrum of the gas phase of the thermolysis reaction (top) in comparison with NIST reference spectrum of propene gas (bottom). (The reaction spectrum shows signals of atmospheric H<sub>2</sub>O (noise at 1400-1800 $\text{cm}^{-1}$  and > 3500  $\text{cm}^{-1}$ ) and atmospheric CO<sub>2</sub> (2400 $\text{cm}^{-1}$ ) from insufficient purging of the instrument during measurement).

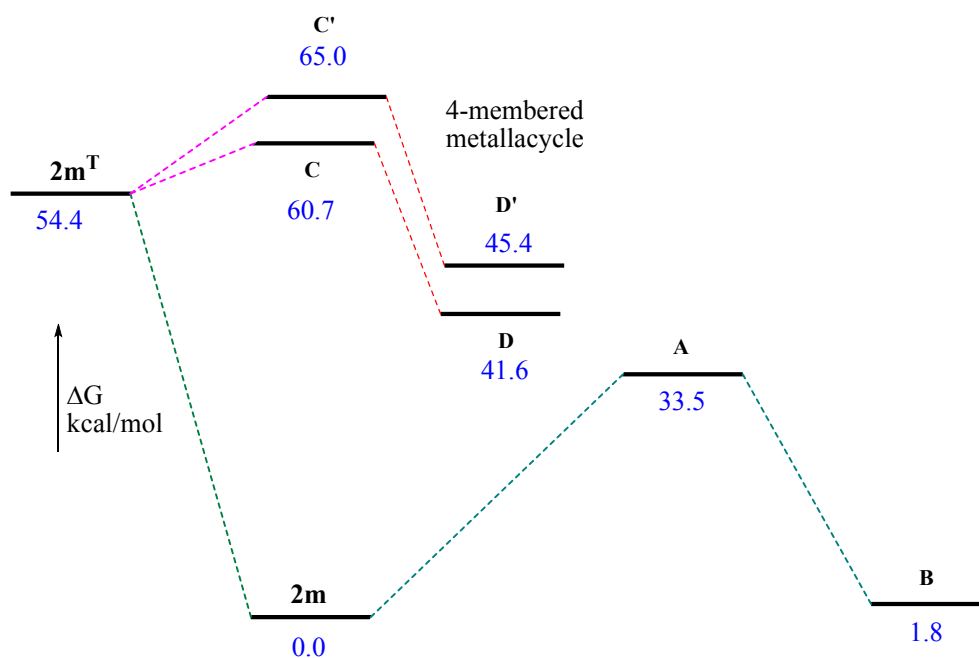


**Figure S2:** Transmission IR spectra of self-supporting pellets of silica 700 (bottom) and grafted complex 2 (top) showing the consumption of free SiOH of partially dehydroxylated silica upon grafting and the appearance of CH-stretch and CH-deformation modes.

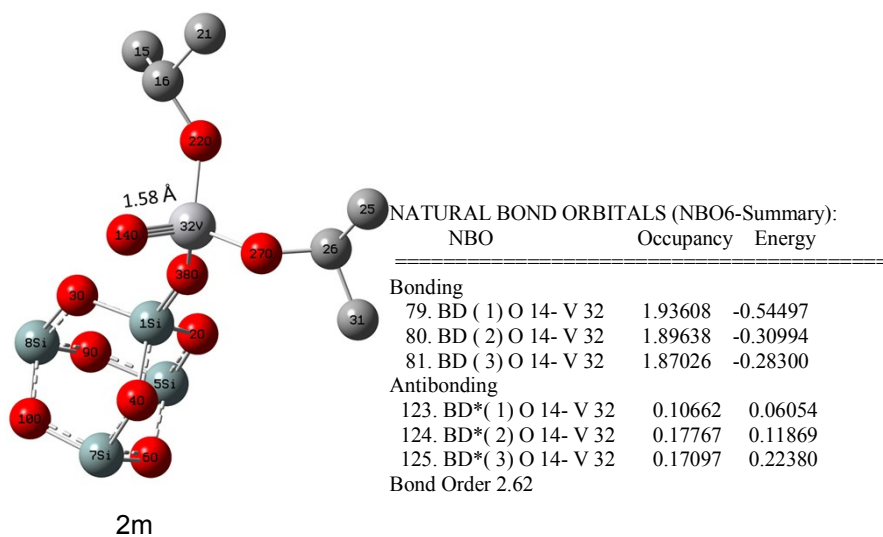


**Figure S3:** X-band EPR spectra of **2** (black trace) and **3** (red trace).  $\nu \approx 9.27$  GHz, mod. = 0.4 mT, recording temperature: 286 K, \*reference signals deriving from Mn<sup>2+</sup>/MgO. Spectral parameters for **2**:  $g_{\parallel} = 1.928$ ,  $g_{\perp} = 1.982$ ;  $A_{\parallel} = 527$  MHz,  $A_{\perp} = 202$  MHz. Spectral parameters for **3**:  $g_{\parallel} = 1.932$  ( $\Delta g_{\parallel} = + 0.002$ ),  $A_{\parallel} = 536$  MHz (nearly unchanged),  $g_{\perp} = 1.991$  ( $\Delta g_{\perp} = + 0.003$ ),  $A_{\perp} = 229$  MHz ( $\Delta A_{\perp} = + 20$  MHz).

### 3. Supplementary Computational Data



**Figure S4:** Energies (kcal/mol) of the reaction intermediates, reagents and products discussed in the DFT study.



**Figure S5:** Geometry of  $2m$  as obtained by the DFT study. The natural bonding orbital analysis summary indicates a  $V=O$  with calculated bond order of 2.62.

#### 4. Computational Coordinates

2m

38

E= 3094.33331284 A.U.

Si	-1.110353	0.066354	0.055650
O	-1.794320	0.449780	1.533530
O	-1.678658	-1.465215	-0.307467
O	-1.848322	1.086288	-1.045522
Si	-3.461233	0.372316	1.648085
O	-4.045327	1.375832	0.439519
Si	-3.519140	1.055445	-1.119816
Si	-3.338372	-1.679578	-0.327904
O	-3.875465	-1.183231	1.180877
O	-3.929747	-0.543983	-1.408636
H	-3.963191	0.723599	2.976024
H	-4.070443	1.977833	-2.111312
H	-3.737685	-3.047466	-0.656299
O	2.115505	-0.503670	-2.122374
C	3.070513	-3.457798	0.968879
C	3.717474	-2.407615	0.075669
H	3.543589	-2.661319	-0.975528
H	2.000943	-3.529545	0.768754
H	3.522030	-4.434846	0.783699
H	3.210735	-3.204017	2.021360
C	5.211471	-2.247329	0.322338
O	3.074371	-1.145781	0.325740
H	5.399933	-1.964488	1.359903
H	5.726976	-3.188825	0.121080
C	4.816022	2.604441	0.522115
C	3.314377	2.354026	0.551505
O	2.964743	1.584720	-0.617008
H	5.365476	1.662366	0.522260
H	5.088227	3.164917	-0.374015
H	5.119588	3.179519	1.399745
C	2.489212	3.634122	0.540881
V	2.160499	0.009573	-0.628948
H	1.422820	3.406942	0.550609
H	2.720798	4.237880	1.421201
H	2.711484	4.219812	-0.352920
H	3.064736	1.773773	1.449164
H	5.631269	-1.481307	-0.330919
O	0.497747	0.178059	0.073900

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2m<sup>F</sup>

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E= -3094.24127013 A.U.

Si	1.098619	-0.293254	0.020165
O	1.665738	1.136137	-0.672923
O	1.771942	-1.510153	-0.918738
O	1.904007	-0.390557	1.487872
Si	3.320241	1.306810	-0.846104
O	3.963747	1.103887	0.686661
Si	3.571124	-0.326119	1.473619
Si	3.430184	-1.526440	-1.106790
O	3.829819	-0.020533	-1.731075
O	4.069575	-1.550523	0.442442
H	3.700730	2.580494	-1.459016
H	4.168865	-0.423146	2.804984
H	3.908969	-2.630117	-1.939017
O	-2.482032	-1.086530	2.186251
C	-5.523035	-0.577995	-1.764158
C	-4.633664	-1.561541	-1.008112
H	-4.310833	-2.343938	-1.705783
H	-4.973197	-0.121126	-2.588081
H	-6.397042	-1.088757	-2.174207
H	-5.873097	0.213248	-1.096304
C	-5.347454	-2.213315	0.170459
O	-3.451794	-0.891005	-0.592922
H	-5.678077	-1.456743	0.886249
H	-6.223309	-2.768224	-0.173200
C	-3.587912	3.131610	0.175072
C	-2.235007	2.436571	-0.168587
O	-2.039664	1.532149	0.871476

H	-4.397557	2.405890	0.223032
H	-3.510541	3.660417	1.123892
H	-3.791172	3.844019	-0.625915
C	-1.082139	3.432007	-0.238251
V	-2.281688	-0.514661	0.716200
H	-0.150253	2.907037	-0.446944
H	-1.271187	4.148680	-1.040130
H	-0.983616	3.972724	0.704179
H	-2.365121	1.899856	-1.114863
H	-4.685101	-2.905813	0.691786
O	-0.495929	-0.347279	0.101676

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B

29

E= -2976.35330987 A.U.

Si	0.743916	-0.192415	-0.226445
O	1.069754	1.431816	0.006102
O	1.678052	-0.649219	-1.534630
O	1.412042	-0.972180	1.091241
Si	2.673437	1.861748	0.223327
O	3.215821	0.946030	1.517325
Si	3.038470	-0.716279	1.390032
Si	3.325692	-0.371118	-1.428034
O	3.484623	1.268347	-1.117668
O	3.826478	-1.142293	-0.027238
H	2.860629	3.298881	0.417914
H	3.532568	-1.437981	2.561382
H	4.059225	-0.803878	-2.616523
O	-2.973799	-2.521815	-0.624834
O	-0.826538	-0.501038	-0.447660
H	-3.067778	-2.575255	-1.585778
C	-4.229770	2.594976	-0.059102
C	-4.578824	1.142811	0.234435
O	-3.604567	0.305572	-0.417966
H	-3.223482	2.829430	0.289258
H	-4.281431	2.792270	-1.131457
H	-4.933761	3.256589	0.450137
C	-5.963216	0.743016	-0.257021
V	-2.492831	-0.948065	0.078117
H	-6.163475	-0.306966	-0.040272
H	-6.723827	1.347083	0.242073
H	-6.048078	0.900288	-1.333980
H	-4.500415	0.952950	1.310155
O	-2.592545	-1.100202	1.643604

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D

38

E= -3094.25906184 A.U.

Si	1.169599	0.155297	0.123514
O	1.769014	0.986782	-1.201433
O	1.634378	-1.436767	-0.115349
O	2.089347	0.686327	1.419084
Si	3.406271	0.859693	-1.513805
O	4.176210	1.348920	-0.107213
Si	3.749770	0.538353	1.297388
Si	3.261918	-1.738151	-0.348622
O	3.718133	-0.782018	-1.648364
O	4.040924	-1.082277	0.982875
H	3.828636	1.619627	-2.690028
H	4.460837	1.028623	2.477778
H	3.565381	-3.154960	-0.547876
O	-2.218787	-0.789407	2.332210
C	-4.710510	-1.793196	-1.768865
C	-3.716160	-2.331202	-0.738392
H	-3.208822	-3.204023	-1.182949
H	-4.190330	-1.522436	-2.687905
H	-5.456878	-2.555264	-2.002641
H	-5.224678	-0.913459	-1.379411
C	-4.356220	-2.742809	0.538147
O	-2.668324	-1.374859	-0.544683
H	-2.409911	-0.174908	3.053315
H	-5.337792	-3.197149	0.524809
H	-3.792557	-2.731689	1.460695
C	-4.843600	2.519995	-0.625776



C	-3.361456	2.213673	-0.452204
O	-3.230623	1.204404	0.562696
H	-5.394734	1.621679	-0.906349
H	-5.262154	2.902752	0.307143
H	-4.988627	3.270394	-1.406168
C	-2.545393	3.436548	-0.049586
V	-2.122562	-0.184767	0.646944
H	-1.494205	3.174882	0.075558
H	-2.617785	4.210283	-0.817250
H	-2.917709	3.846873	0.891512
H	-2.965338	1.814973	-1.394810
O	-0.410298	0.361732	0.333463

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D'

38

E= -3094.26148416 A.U.

Si	-1.083970	-0.291327	0.160795
O	-1.667395	-1.127933	-1.166060
O	-1.539459	1.302429	-0.088706
O	-2.020295	-0.815394	1.447423
Si	-3.299939	-0.998525	-1.501395
O	-4.089634	-1.478805	-0.102600
Si	-3.679222	-0.664234	1.304067
Si	-3.164606	1.604570	-0.345345
O	-3.604862	0.643911	-1.646237
O	-3.960668	0.956312	0.979317
H	-3.708891	-1.761992	-2.679818
H	-4.406491	-1.147083	2.477477
H	-3.461112	3.021512	-0.554361
O	2.053763	0.492988	2.433177
C	4.033522	2.638720	-1.437396
C	2.733342	2.365364	-0.706066
H	1.968869	3.080211	-1.027008
H	3.898167	2.535167	-2.515577
H	4.370187	3.656914	-1.227253
H	4.812901	1.944667	-1.115022
C	2.810260	2.224756	0.790229
O	2.244183	1.037564	-0.992736
H	1.802801	-0.350874	2.844803
H	3.795009	2.214237	1.250925
H	2.076178	2.754163	1.389159
C	5.519073	-1.894749	-0.298363
C	4.039038	-1.683813	-0.584460
O	3.492680	-0.904117	0.497185
H	6.032673	-0.938888	-0.190293
H	5.653383	-2.466061	0.622039
H	5.983059	-2.445099	-1.119732
C	3.261392	-2.986739	-0.715653
V	2.158001	0.217331	0.632279
H	2.204205	-2.793559	-0.901936
H	3.653916	-3.573266	-1.549168
H	3.352171	-3.579585	0.196773
H	3.918626	-1.090206	-1.497098
O	0.495298	-0.500316	0.403013

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A

38

E= -3094.27498262 A.U.

Si	1.224605	-0.359615	-0.160775
O	1.879959	-1.146376	1.165954
O	1.598124	1.261620	0.076156
O	2.175768	-0.835419	-1.454178
Si	3.506288	-0.925493	1.474112
O	4.303077	-1.370610	0.068091
Si	3.823521	-0.592636	-1.338071
Si	3.207012	1.654051	0.302744
O	3.722540	0.733079	1.605085
O	4.020676	1.044329	-1.028756
H	3.976386	-1.654478	2.652006
H	4.561077	-1.041732	-2.518504
H	3.426289	3.087675	0.497879
O	-2.332946	0.862107	-1.790740
C	-4.410616	2.566651	1.380028
C	-3.126819	2.749309	0.650381

H	-2.248704	2.913464	1.261256
H	-4.293896	1.925768	2.251136
H	-4.742282	3.554009	1.724813
H	-5.188672	2.166582	0.729088
C	-3.068350	3.106748	-0.705868
O	-2.548427	0.734014	0.774047
H	-2.728470	2.039591	-1.314976
H	-4.016542	3.345503	-1.183372
H	-2.236446	3.742947	-0.999174
C	-3.876216	-2.632046	1.396678
C	-4.169848	-2.356804	-0.073679
O	-3.104391	-1.620427	-0.670473
H	-2.924085	-3.152995	1.506087
H	-3.827193	-1.697992	1.960260
H	-4.661280	-3.256298	1.829613
C	-5.491249	-1.628044	-0.293066
V	-2.097007	-0.181439	-0.512679
H	-5.646010	-1.427327	-1.353779
H	-6.324037	-2.234571	0.069929
H	-5.497320	-0.678648	0.247191
H	-4.196441	-3.307558	-0.617420
O	-0.339703	-0.644070	-0.366356

=====  
C  
38

E= -3094.22923072 A.U.

Si	1.205146	-0.404551	0.119971
O	1.621091	1.093831	-0.513559
O	2.005569	-1.521294	-0.834104
O	1.973110	-0.469515	1.605958
Si	3.251786	1.441577	-0.648669
O	3.881931	1.254970	0.893080
Si	3.627380	-0.230472	1.629335
Si	3.661502	-1.359219	-0.988588
O	3.911460	0.198542	-1.557562
O	4.266402	-1.365824	0.574982
H	3.511195	2.765241	-1.214972
H	4.202316	-0.307770	2.971856
H	4.266509	-2.382318	-1.840394
O	-2.463038	0.212748	-1.860335
C	-2.966983	3.539968	1.078543
C	-2.434985	2.498488	0.096711
H	-1.362697	2.667194	-0.055467
H	-2.432521	3.464108	2.026309
H	-2.827061	4.547478	0.681269
H	-4.030346	3.380019	1.265043
C	-3.141345	2.554602	-1.247466
O	-2.605687	1.196526	0.660035
H	-2.827816	1.518064	-1.791945
H	-4.227687	2.494419	-1.172924
H	-2.823493	3.370119	-1.896425
C	-5.134226	-1.305238	1.559871
C	-4.565861	-2.073155	0.372767
O	-3.201230	-1.706252	0.144305
H	-4.525046	-1.466460	2.450363
H	-5.162682	-0.233558	1.352163
H	-6.150534	-1.643270	1.773448
C	-5.371070	-1.887438	-0.907876
V	-2.137940	-0.335705	-0.144790
H	-4.915316	-2.437725	-1.731498
H	-6.389543	-2.255946	-0.766815
H	-5.419583	-0.833038	-1.187255
H	-4.531253	-3.139452	0.620278
O	-0.381660	-0.645224	0.207590

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C'  
38

E= -3094.23060286 A.U.

Si	1.058009	0.032867	0.251842
O	1.564733	-1.228716	-0.727956
O	1.988218	-0.084591	1.634820
O	1.582501	1.423026	-0.517901
Si	3.197867	-1.306435	-1.089244
O	3.579047	0.176031	-1.772052

Si	3.216206	1.536886	-0.863096
Si	3.650364	-0.080706	1.446158
O	3.986696	-1.337580	0.388490
O	4.004913	1.321999	0.599271
H	3.542016	-2.438862	-1.948155
H	3.576488	2.786067	-1.532529
H	4.375817	-0.186338	2.711027
O	-2.701125	-1.109357	2.106603
C	-4.399025	-2.717718	-1.092526
C	-3.077836	-1.966339	-1.116534
H	-2.660460	-1.995741	-2.129561
H	-5.116198	-2.256726	-1.773294
H	-4.245589	-3.754785	-1.400957
H	-4.826860	-2.715504	-0.087110
C	-2.065908	-2.430008	-0.068198
O	-3.298019	-0.584299	-0.788314
H	-2.398305	-1.955145	1.383393
H	-2.336916	-3.384778	0.393572
H	-1.036294	-2.482664	-0.410932
C	-2.632133	2.748224	-1.195250
C	-3.432375	2.517628	0.081611
O	-2.929964	1.378826	0.789981
H	-1.567246	2.832228	-0.975036
H	-2.783473	1.924975	-1.894357
H	-2.958059	3.675804	-1.670839
C	-4.927902	2.339162	-0.158335
V	-2.300973	-0.245370	0.701850
H	-5.449681	2.168887	0.784048
H	-5.336363	3.240565	-0.620598
H	-5.107560	1.490384	-0.818015
H	-3.274140	3.358531	0.765598
O	-0.524244	0.023956	0.529226

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