

Physicochemical Implications of Surface Alkylation of High-valent, Lindqvist-type Polyoxovanadate-alkoxide Clusters

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Experimental.

General Considerations. All manipulations were carried out in the absence of water and oxygen using standard Schlenk techniques, or in a UniLab MBraun inert atmosphere drybox under a nitrogen atmosphere. All glassware was oven-dried for a minimum of 3 hours and cooled in an evacuated antechamber prior to use in the drybox. All solvents were dried and deoxygenated on a Glass Contour System (Pure Process Technology, LLC) and stored over activated 4 Å molecular sieves purchased from Fisher Scientific prior to use. $[\text{V}_6\text{O}_{13}(\text{TRIOl}^{\text{R}})_2]^{2-}$ ($\text{R} = \text{Me}, \text{NO}_2$) clusters were prepared according to published procedures.¹ Methyl trifluoromethylsulfonate and tetrabutylammonium borohydride were purchased from Sigma Aldrich and used as received.

¹H NMR spectra were recorded at 400 MHz on a Bruker DPX-400 MHz spectrometer locked on the signal of deuterated solvents. All chemical shifts were reported relative to the peak of residual H signal in deuterated solvents. CD_3CN was purchased from Cambridge Isotope Laboratories, degassed by three freeze–pump–thaw cycles, and stored in the drybox over activated 4 Å molecular sieves. Infrared (FT-IR, ATR) spectra of complexes were recorded on a Shimadzu IRAffinity-1 Fourier Transform Infrared Spectrophotometer and are reported in wavenumbers (cm^{-1}). Electronic absorption measurements were recorded at room temperature in anhydrous acetonitrile in a sealed 1 cm quartz cuvette with an Agilent Cary 60 UV-Vis spectrophotometer. Reflectance spectra were obtained for films drop-cast onto glass microscope slides with an Agilent Cary 7000 UV-Vis spectrometer equipped with a Universal Measurement Accessory (UMA). The reflectance was measured using an incident angle of $\pm 20^\circ$ and a collection angle of $\pm 40^\circ$. A film of polycrystalline barium sulfate was used as a 100% reflectance standard. The Kubelka-Munk transformation (eq. S1) is used to approximate electronic absorption, where R is the measured reflectance.

$$f(R) = \frac{(1-R)^2}{2R} \quad (\text{S1})$$

Mass spectrometry analyses were performed on an Advion Expression^L Compact Mass Spectrometer equipped with an electrospray probe and an ion-trap mass analyser. Direct injection analysis was employed in all cases with a sample solution in acetonitrile, using a carrier solvent of methanol. Elemental analyses were performed on a PerkinElmer 2400 Series II Analyzer, at the Elemental Analysis Facility located at the University of Rochester.

Single crystals of $[\text{nBu}_4\text{P}][\text{V}_6\text{O}_{12}(\text{OMe})(\text{TRIOl}^{\text{Me}})_2]$, $[\text{nBu}_4\text{N}]_2[\text{V}_6\text{O}_{11}(\text{OMe})_2(\text{TRIOl}^{\text{Me}})_2]$, $[\text{nBu}_4\text{N}][\text{V}_6\text{O}_{12}(\text{OMe})(\text{TRIOl}^{\text{NO}_2})_2]$, and $[\text{nBu}_4\text{N}]_2[\text{V}_6\text{O}_{11}(\text{OMe})_2(\text{TRIOl}^{\text{NO}_2})_2]$ were mounted on the tip of a thin glass optical fiber (goniometer head) and mounted on a XtaLab Synergy-S Dualflex diffractometer equipped with a HyPix-6000HE HPC area detector for data collection at 100.00(10)-192.99(10) K, respectively. The structure was solved using SHELXT-2018/2² and refined using SHELXL-2018/3.³

Cyclic voltammetry experiments were recorded with a Bio-Logic SP-150 potentiostat/galvanostat and the EC-Lab software suite. All measurements were performed in a three electrode system cell configuration that consisted of a glassy-carbon ($\varnothing = 3.0$ mm) as working electrode (CH Instruments, USA), a Pt wire as the counter electrode (CH Instruments, USA), and an Ag/Ag^+ non-aqueous reference electrode with 0.01 M AgNO_3 in 0.05 M $[\text{nBu}_4\text{N}][\text{PF}_6]$ in acetonitrile (BASi, USA). The supporting electrolyte, $[\text{nBu}_4\text{N}][\text{PF}_6]$ was purchased from Sigma-Aldrich, recrystallized three times using hot methanol, and stored under dynamic vacuum for a minimum of two days prior to use. All electrochemical measurements were performed at room temperature in a nitrogen-filled drybox.

Synthesis of [¹⁸Bu₄P][V₆O₁₂(OMe)(TRIOl^{Me})₂] (1-OMe): A 20 mL scintillation vial was charged with [¹⁸Bu₄P]₂[V₆O₁₃(TRIOl^{Me})₂] (0.050 g, 0.0395 mmol) and 2 mL of DCM. Methyl trifluoromethylsulfonate (10.7 μL, 0.0978 mmol) was added to the solution with stirring. The reaction was stirred at 45 °C for 5 minutes, after which the solvent was concentrated to 0.5 mL under vacuum. Following the addition of 6 mL of diethylether (Et₂O), a red precipitate was formed. The solid was collected by filtration through filter paper and washed with 5 mL of Et₂O to give [¹⁸Bu₄P][V₆O₁₂(OMe)(TRIOl^{Me})₂] (0.036 g, 0.0351 mmol, 89%). ¹H NMR (400 MHz, CD₃CN): *d* = 0.92 (s, 6H, CH₃), 0.95 (t, 12H, CH₃), 1.48 (m, 16H, CH₂), 2.07 (m, 8H, CH₂), 4.48 (s, 3H, CH₃), 4.95-5.3 (m, 12H, CH₂). UV-Vis [ε (M⁻¹ nm⁻¹): 384 (6.20 x 10³), 458 (2.97 x 10²), 530 (1.11 x 10³). Elemental analysis: Calc. for C₂₇H₅₇O₁₉PV₆ (MW = 1022.35 g/mol): C, 31.72; H, 5.62. Found: C, 31.746; H, 5.501.

Synthesis of [¹⁸Bu₄N]₂[V₆O₁₁(OMe)₂(TRIOl^{Me})₂] (1-(OMe)₂): A 20 mL scintillation vial was charged with [¹⁸Bu₄N]₂[V₆O₁₃(TRIOl^{Me})₂] (0.050 g, 0.0395 mmol) and 2 mL DCM. Methyl trifluoromethylsulfonate (84.5 μL, 0.772 mmol) was added with stirring. The reaction was stirred at 45 °C for 3 hours, whereupon a red precipitate formed. The solid was collected by filtration through filter paper and washed with 4 mL Et₂O. A 20 mL scintillation vial was charged with the red precipitate and 2 mL of acetonitrile. Tetrabutylammonium borohydride (0.030 mg, 0.116 mmol) was added with stirring. The solution was stirred at room temperature for 2 hours to give a green solution. After it was finished stirring, the solution was concentrated to 0.5 mL under vacuum. 6 mL of Et₂O was then added, and a green precipitate crashed out. The solid is collected by filtration through filter paper and washed with 4 mL Et₂O to give [¹⁸Bu₄N]₂[V₆O₁₁(OMe)₂(TRIOl^{Me})₂] (0.043 g, 0.0340 mmol, 88%). ¹H NMR (400 MHz, CD₃CN): *d* = 16.48, 13.65, 10.39, 3.12, 1.60, 1.35, 0.96, 0.39, -6.40. UV-Vis [ε (M⁻¹ nm⁻¹): 360 (4.19 x 10³), 746 (6.51 x 10²). Elemental analysis: Calc. for C₄₄H₉₆O₁₉N₂V₆ (MW = 1262.88 g/mol): C, 38.08; H, 6.85; N, 4.23. Found: C, 38.006; H, 6.704; N, 4.255.

Synthesis of [¹⁸Bu₄N][V₆O₁₂(OMe)(TRIOl^{NO2})₂] (2-OMe): A 20 mL scintillation vial was charged with [¹⁸Bu₄N]₂[V₆O₁₃(TRIOl^{NO2})₂] (0.050 mg, 0.0386 mmol) and 2 mL of DCM. Methyl trifluoromethylsulfonate (10.6 μL, 0.0969 mmol) was added to the solution with stirring. The reaction was stirred at 45 °C for 20 minutes, after which the solvent was concentrated to 0.5 mL under vacuum. Following the addition of 6 mL of Et₂O, a red precipitate was formed. The solid was collected by filtration through filter paper and washed with 5 mL of Et₂O to give [¹⁸Bu₄N][V₆O₁₂(OMe)(TRIOl^{NO2})₂] (0.026 g, 0.0244 mmol, 65%). ¹H NMR (500 MHz, CD₃CN): *d* = 0.97 (t, 12H, CH₃), 1.35 (m, 8H, CH₂), 1.60 (m, 8H, CH₂), 3.08 (m, 8H, CH₂), 4.65 (s, 3H, CH₃), 5.57-5.87 (m, 12H, CH₂). UV-Vis [ε (M⁻¹ nm⁻¹): 378 (6.50 x 10³), 438 (3.58 x 10³), 520 (1.11 x 10³). Elemental analysis: Calc. for C₂₅H₅₁O₂₃N₃V₆ (MW = 1067.33 g/mol): C, 28.13; H, 4.82; N, 3.94. Found: C, 27.745; H, 4.553; N, 3.757.

Synthesis of [¹⁸Bu₄N]₂[V₆O₁₁(OMe)₂(TRIOl^{NO2})₂] (2-(OMe)₂): A 20 mL scintillation vial was charged with [¹⁸Bu₄N]₂[V₆O₁₃(TRIOl^{NO2})₂] (0.050 g, 0.0386 mmol) and 2 mL DCM. Methyl trifluoromethylsulfonate (84.5 μL, 0.772 mmol) was added with stirring. The reaction was stirred at 45 °C for 3 hours, whereupon an orange solid crashed out of solution. The solid was collected by filtration through filter paper and washed with 4 mL Et₂O. A 20 mL scintillation vial was charged with the orange precipitate and 2 mL of acetonitrile. Tetrabutylammonium borohydride (0.020 g, 0.077 mmol) was added with stirring. The solution was stirred at room temperature for 20 minutes to give a green solution. After it was finished stirring, the solution was concentrated to 0.5 mL under vacuum. 6 mL of Et₂O was added, where a green precipitate crashed out. The solid is collected by filtration through filter paper and washed with 4 mL Et₂O to give [¹⁸Bu₄N]₂[V₆O₁₁(OMe)₂(TRIOl^{NO2})₂] (0.0343 g, 0.026 mmol, 68%). ¹H NMR (400 MHz, CD₃CN): *d* = 14.39, 12.40, 9.62, 5.07, 3.11, 1.58, 1.34, 0.94. UV-Vis [ε (M⁻¹ nm⁻¹): 350 (4.25 x

10^3), 778 (6.78×10^2). Elemental analysis: Calc. for $C_{42}H_{90}O_{23}N_4V_6$ (MW = 1324.82 g/mol): C, 38.08; H, 6.85; N, 4.23. Found: C, 38.075; H, 6.968; N, 4.497.

Computational Details. All geometries were fully optimized without symmetry using the density functional theory (DFT) implementation in the Gaussian 16 package (Revision A.03) in conjunction with the meta-GGA M06-L exchange-correlation functional.^{4, 5} Vanadium centers were described using the def2-TZVP basis set, while light atoms were described using the def2-SVP basis set.^{6, 7} Solvent effects were taken into account using the Solvation Model based on Density (SMD) with the acetonitrile parameters.⁸ The nature of all stationary points and transition states was verified by analytic computation of vibrational frequencies. Molecular partition functions were used in the computation of 298.15 K thermal contributions to Gibbs free energy employing the usual ideal-gas, rigid-rotator, and quasi-harmonic oscillator approximations. A concentration of 1 M was considered for all species. Entropic terms for frequencies below 100 cm^{-1} are obtained from the free-rotor approximation instead of the quasi-harmonic oscillator approximation using the Goodvibes package.⁹ Free energy contributions were added to single-point M06-L/def2-TZVP and M06/def2-TZVP electronic energies including the acetonitrile solvation effects to arrive at the final composite free energies (M06-L/def2-TZVP//M06-L/def2-TZVP,def2-SVP and M06/def2-TZVP//M06-L/def2-TZVP,def2-SVP).¹⁰ Mono- and di-reduced species were considered to be in a doublet and triplet ground state respectively.

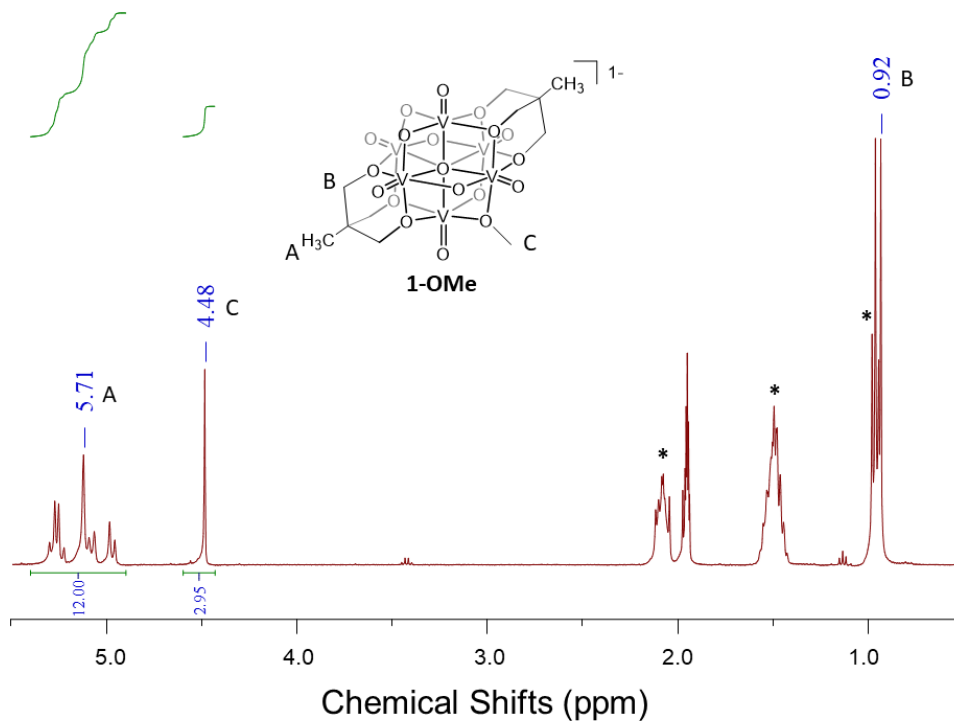


Figure S1. ^1H NMR spectrum of **1-OMe** collected in CD_3CN at 21 $^\circ\text{C}$. * indicates signals belonging to $[\text{nBu}_4\text{P}]^+$ counter ion.

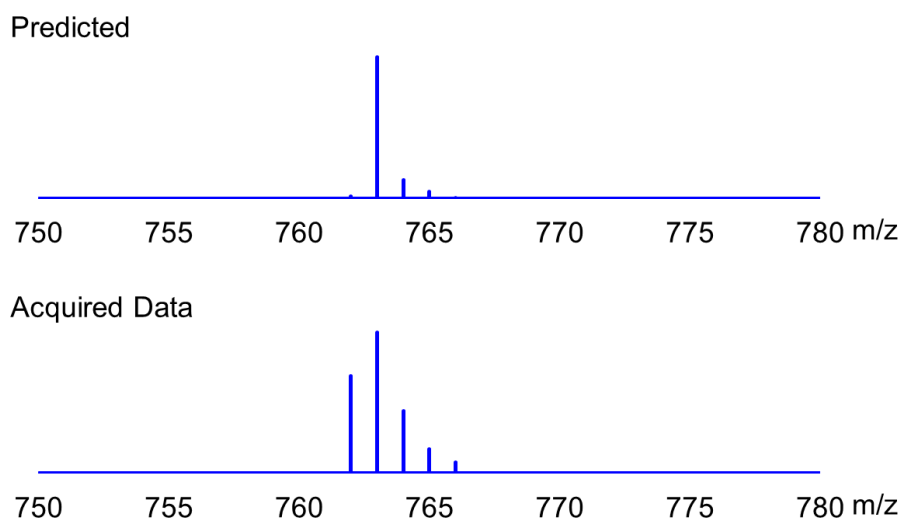


Figure S2. Predicted (top) and Experimental (bottom) data for the ESI-MS (-ve) of complex **1-OMe** ($m/z = 763$).

Table S1: Crystallographic parameters for molecular structures of complexes **1-OMe**, **1-(OMe)₂**, **2-OMe**, and **2-(OMe)₂**.

Compound	1-OMe	1-(OMe)₂	2-OMe	2-(OMe)₂
Empirical formula	C ₂₇ H ₅₇ O ₁₉ PV ₆	C ₄₆ H ₉₉ N ₃ O ₁₉ V ₆	C ₂₅ H ₅₁ N ₃ O ₂₃ V ₆	C _{48.1} H _{105.26} N ₄ O _{24.52} V ₆
Formula weight	1022.33	1303.92	1067.32	1437.92
Temperature / K	100.00(10)	100.00(11)	100.00(10)	100.00(10)
Wavelength / Å	1.54184	1.54184	1.54184	1.54184
Crystal group	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	<i>C2/c</i>	<i>P2₁/n</i>	<i>P2₁/n</i>	<i>P2₁/c</i>
Unit cell dimensions	<i>a</i> = 13.0905(4) Å <i>b</i> = 16.6569(5) Å <i>c</i> = 18.2558(5) Å <i>α</i> = 90° <i>β</i> = 92.394(3)° <i>γ</i> = 90°	<i>a</i> = 18.13612(16) Å <i>b</i> = 16.90558(16) Å <i>c</i> = 19.59064(19) Å <i>α</i> = 90° <i>β</i> = 100.8308(9)° <i>γ</i> = 90°	<i>a</i> = 13.85930(10) Å <i>b</i> = 17.31290(10) Å <i>c</i> = 17.69540(10) Å <i>α</i> = 90° <i>β</i> = 100.6180(10)° <i>γ</i> = 90°	<i>a</i> = 12.6947(4) Å <i>b</i> = 15.5293(5) Å <i>c</i> = 18.1049(6) Å <i>α</i> = 90° <i>β</i> = 109.990(4)° <i>γ</i> = 90°
Volume / Å ³	3977.1(2)	5899.53(10)	4173.22(5)	3354.2(2)
<i>Z</i>	4	4	4	2
Reflections collected	23900	76396	71313	41431
Independent reflections	4147	12405	8801	7044
Completeness (theta)	99.2% (74.504°)	99.8% (74.504°)	99.8% (74.504°)	99.9% (74.504°)
Goodness-of-fit on <i>F</i> ²	1.072	1.063	1.136	1.044
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0472	<i>R</i> 1 = 0.0544	<i>R</i> 1 = 0.0645	<i>R</i> 1 = 0.0597
Largest diff. peak and hole	0.549 and -0.366 e.Å ⁻³	0.890 and -0.630 e.Å ⁻³	1.047 and -1.006 e.Å ⁻³	0.904 and -0.653 e.Å ⁻³

Table S2. Selected structural parameters for **1**, **1-OMe**, **m-1-OMe₂**, **2**, **2-OMe**, and **p-2-OMe₂**. Mean unsigned error with the experimental crystal structure in parenthesis. All distances in Angstroms and angles in degrees.

Bond	1	1-OMe	m-1-OMe₂	2	2-OMe	p-2-OMe₂
V=O _t (avg.)	1.603 (0.008)	1.594 (0.005)	1.586 (0.024)	1.600 (0.003)	1.591 (0.005)	1.582 (0.020)
V-O _b (avg)	1.815 (0.016)	1.812 (0.007)	1.840 (0.034)	1.812 (0.010)	1.808 (0.018)	1.806 (0.029)
V-OMe (avg)	-	1.985 (0.091)	1.977 (0.006)	-	1.976 (0.097)	1.958 (0.018)
V-O _c (avg)	2.264 (0.024)	2.268 (0.029)	2.264 (0.007)	2.269 (0.028)	2.270 (0.034)	2.273 (0.010)
V-O _b -V (avg) ^a	114.05 (3.6)	114.73 (2.37)	115.03 (2.15)	114.02 (2.28)	114.84 (2.91)	115.43 (2.90)
V-OMe-V (avg) ^a	-	108.44 (1.95)	110.31 (2.14)	-	108.50 (2.52)	110.09 (2.65)

^a Larger errors are expected in angles due to crystal packing.

Table S3. Root mean square displacement of **1**, **1-OMe**, and **1-(OMe)₂** species at M06-L/def2-TZVP//M06-L/def2-TZVP,def2-SVP level of theory in acetonitrile. Only the core vanadium and oxygen centers were used to compute the RMSD.

	RMSD
1	0.00
1-OMe	0.05
<i>para-1-(OMe)₂</i>	0.06
<i>ortho-1-(OMe)₂</i>	0.07
<i>meta-1-(OMe)₂</i>	0.07

Table S4. Root mean square displacement of **2**, **2-OMe**, and **2-(OMe)₂** species at M06-L/def2-TZVP//M06-L/def2-TZVP,def2-SVP level of theory in acetonitrile. Only the core vanadium and oxygen centers were used to compute the RMSD.

	RMSD
2	0.00
2-OMe	0.05
<i>para-2-(OMe)₂</i>	0.06
<i>ortho-2-(OMe)₂</i>	0.07
<i>meta-2-(OMe)₂</i>	0.06

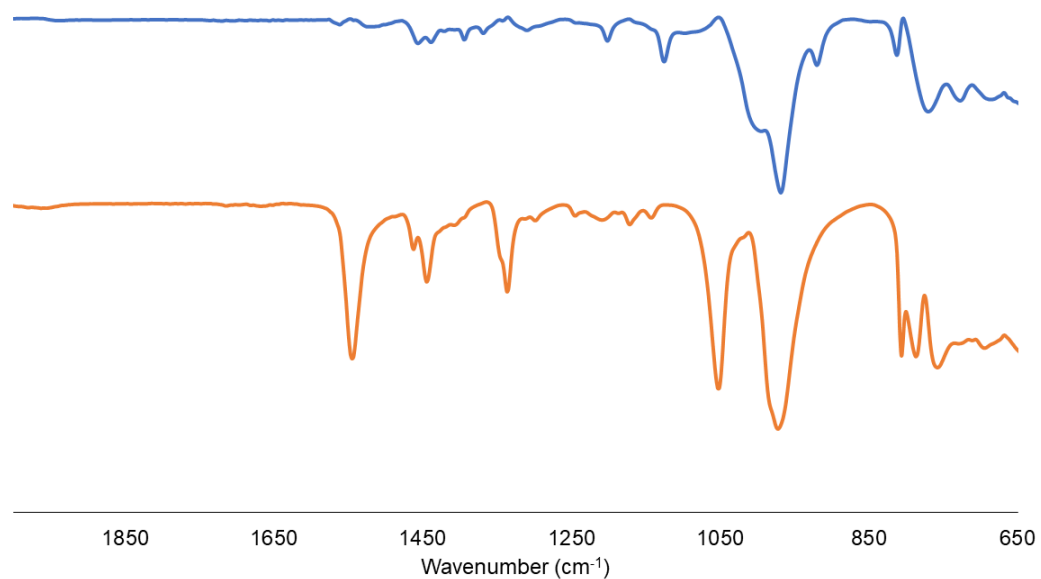


Figure S3. Infrared spectra of complexes $[\text{V}_6\text{O}_{11}(\text{OMe})_2(\text{TRIOL}^{\text{Me}})_2]$ (top, blue) and $[\text{V}_6\text{O}_{11}(\text{OMe})_2(\text{TRIOL}^{\text{NO}_2})_2]$ (bottom, orange).

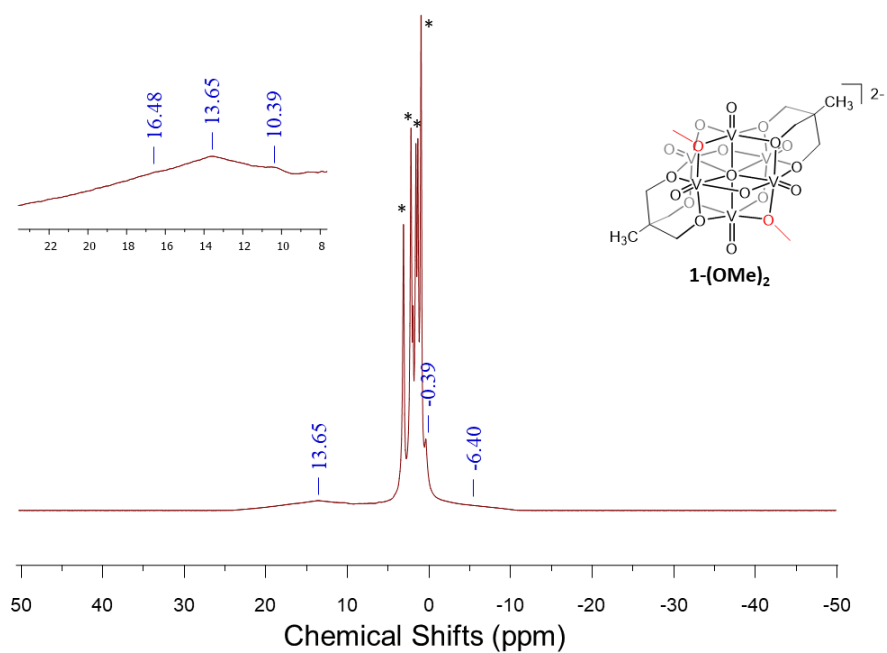


Figure S4. ^1H NMR spectrum of **1-(OMe)₂** collected in CD_3CN at 21 °C. * indicates signals belonging to $[\text{nBu}_4\text{N}]^+$ counter ions.

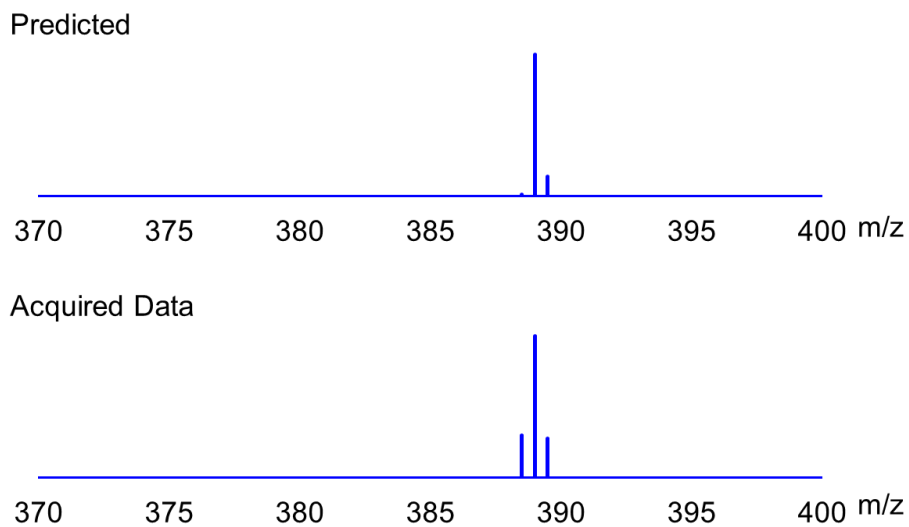


Figure S5. Predicted (top) and experimental (bottom) data for the ESI-MS (-ve) of complex **1-(OMe)₂** ($m/z = 389$).

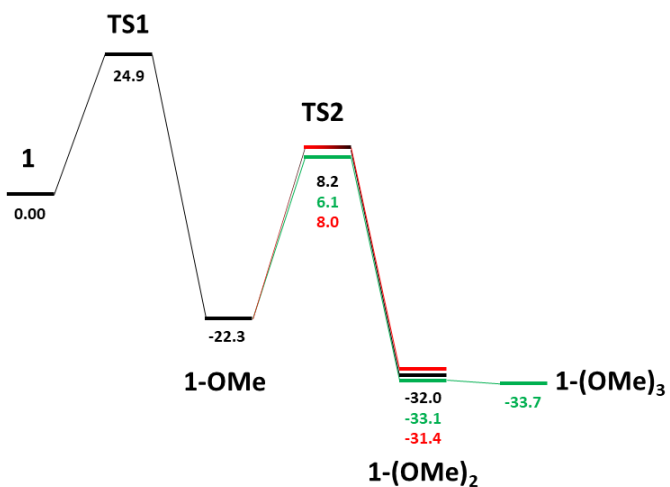


Figure S6. Energy profile for the alkylation of **1** at M06/def2-TZVP//M06-L/def2-TZVP,def2-SVP level of theory in acetonitrile. Isomers: ortho (black), meta (green), and para (red). Gibbs free energy in kcal/mol.

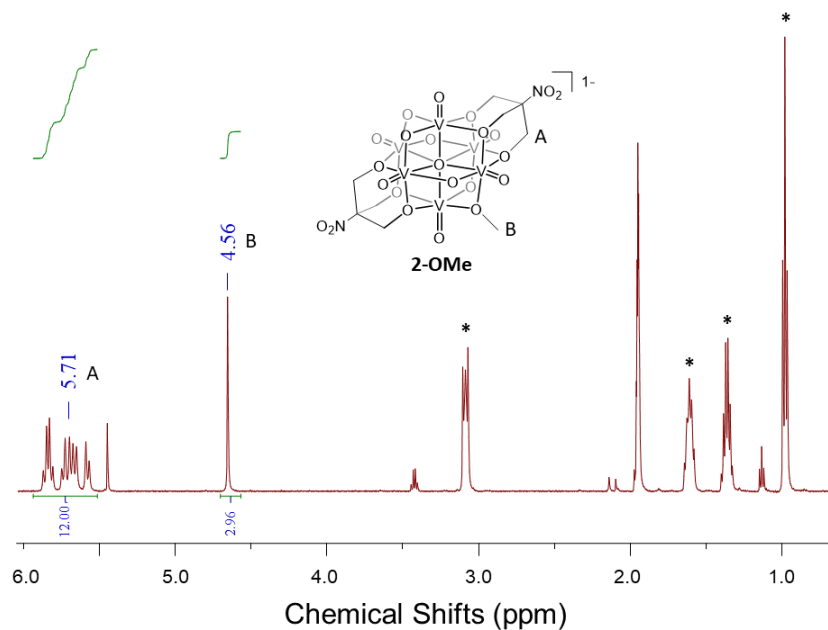
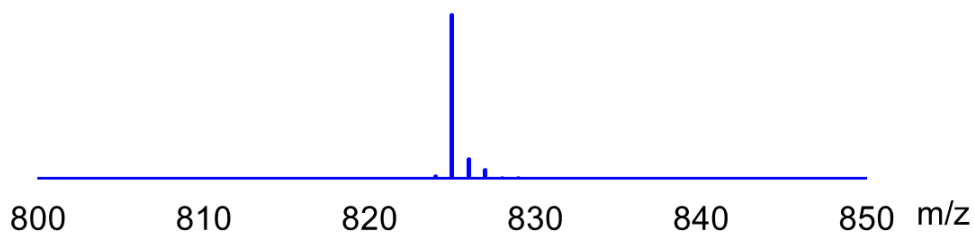


Figure S7. ^1H NMR spectrum of **2-OMe** collected in CD_3CN at 21 $^\circ\text{C}$. * indicates signals belonging to $[\text{nBu}_4\text{N}]^+$ counter ion.

Predicted



Acquired Data

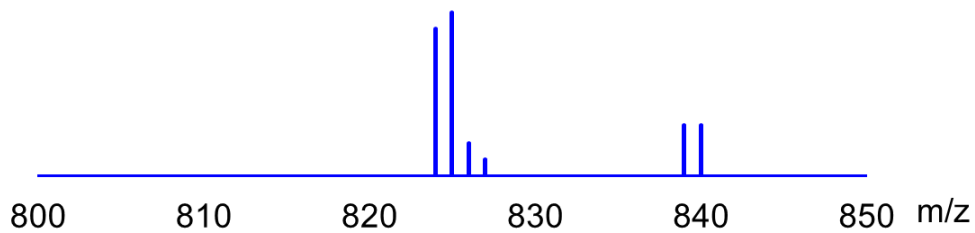


Figure S8. Predicted (top) and experimental (bottom) data for the ESI-MS (-ve) of complex **2-OMe** ($m/z = 824$).

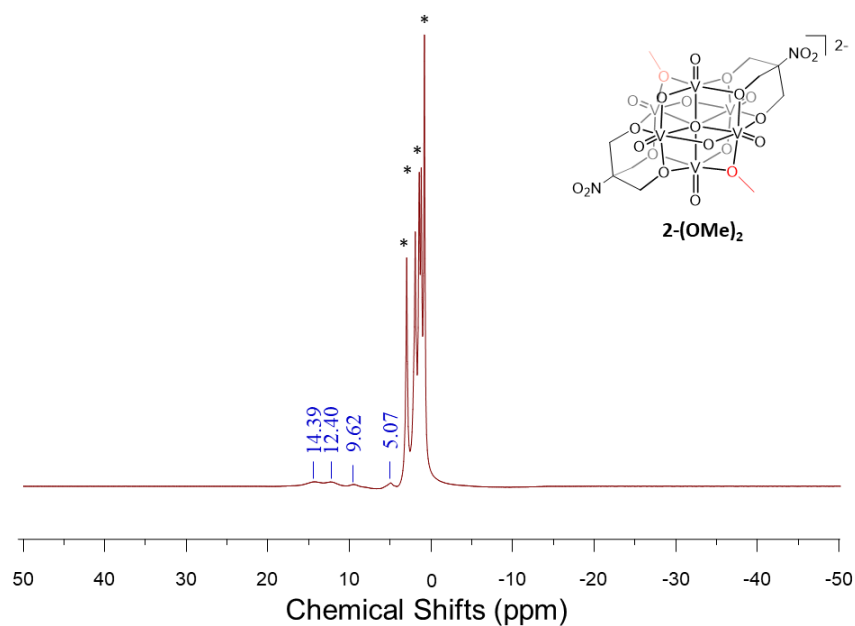


Figure S9. ^1H NMR spectrum of **2-(OMe)₂** collected in CD_3CN at 21 °C. * indicates signals belonging to $[\text{nBu}_4\text{N}]^+$ counter ions.

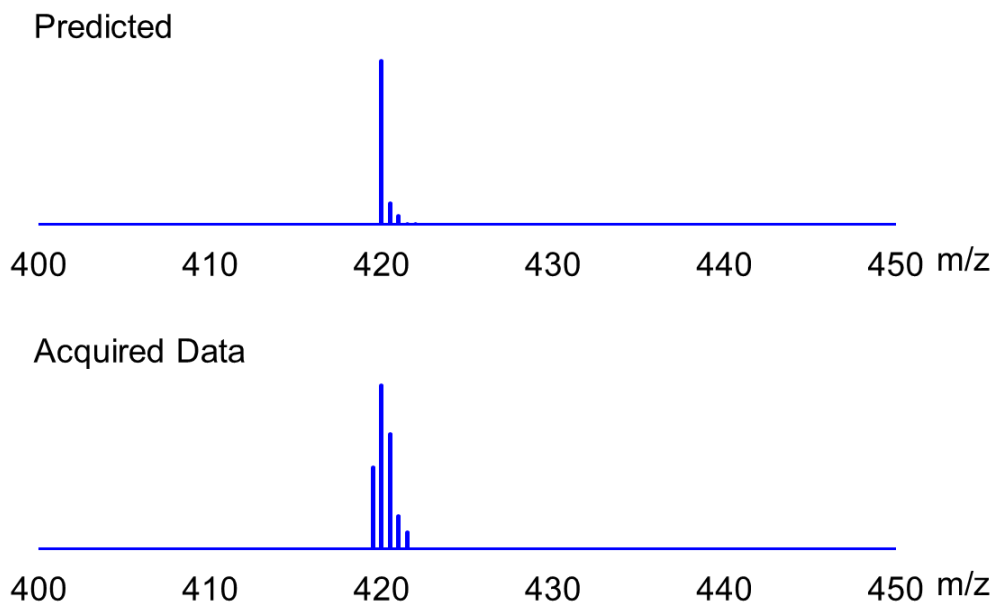


Figure S10. Predicted (top) and experimental (bottom) data for the ESI-MS (-ve) of complex **2-(OMe)₂** ($m/z = 419.5$).

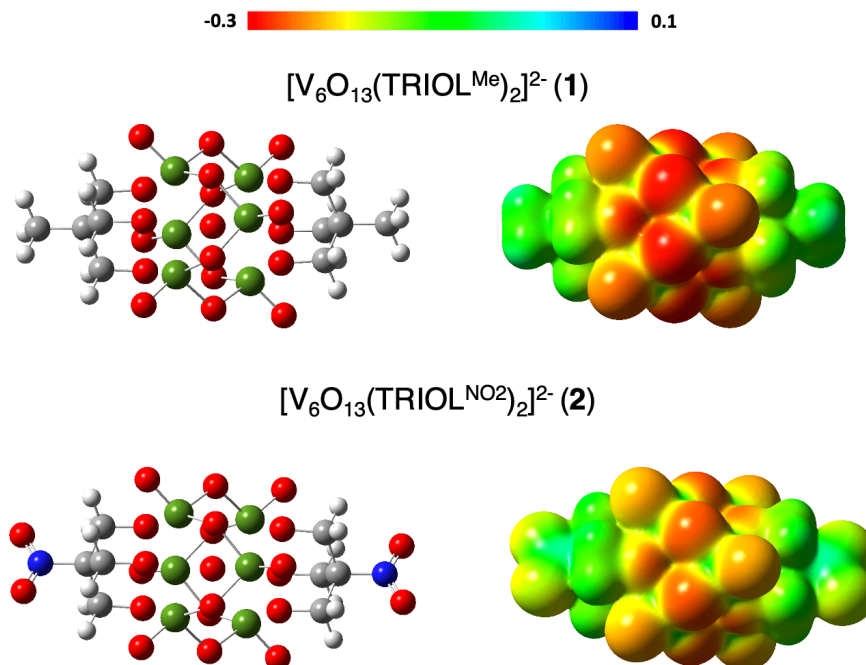


Figure S11. Electrostatic potential of complexes **1** (top) and **2** (bottom). Structure for reference (left) and electrostatic potential map (right). Density isovalue = 0.01.

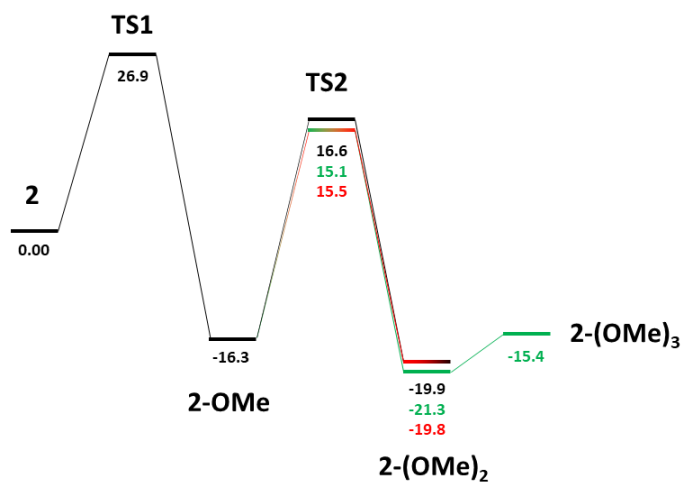


Figure S12. Energy profile for the alkylation of **2** at M06/def2-TZVP//M06-L/def2-TZVP,def2-SVP level of theory in acetonitrile. Isomers: ortho (black), meta (green), and para (red). Gibbs free energy in kcal/mol.

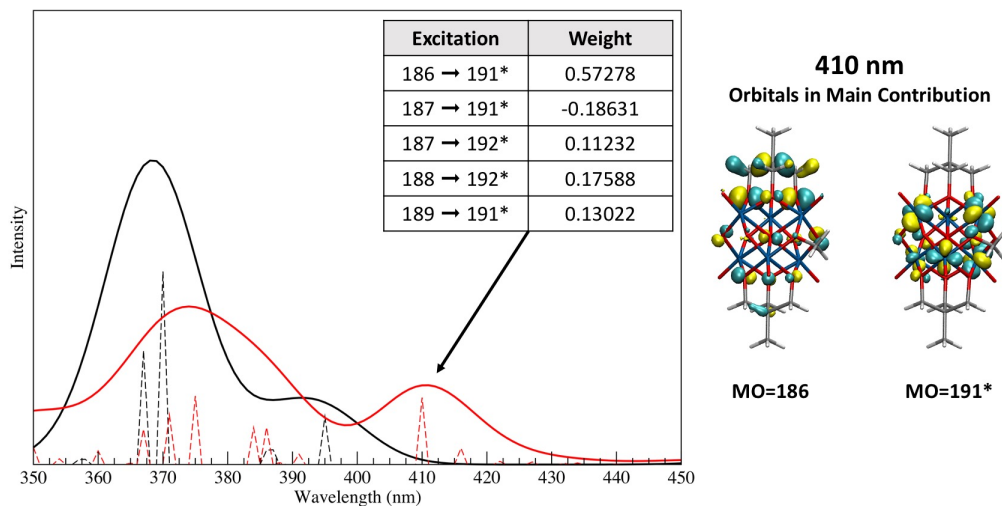


Figure S13. Calculated electronic spectra of complex **1** (black) and **1-OMe** (red) at M06/def2-TZVP//M06-L/def2-TZVP,def2-SVP level of theory in acetonitrile. Dashed lines are unwidened excitations. Inset: Excitations contributing to the 410 nm peak in **1-OMe**. Orbitals are plotted (isovalue=0.5) and an asterisk indicates a virtual orbital.

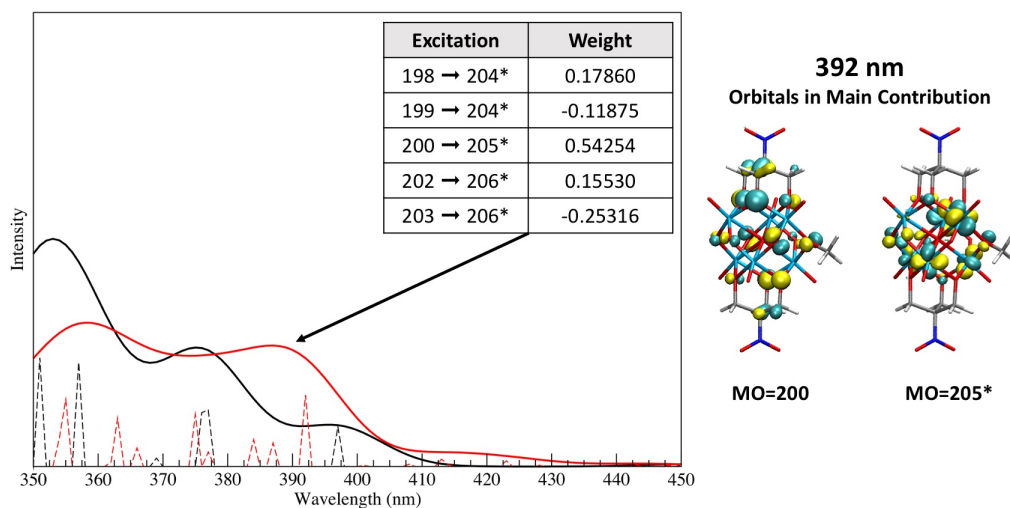


Figure S14. Calculated electronic spectra of complex **2** (black) and **2-OMe** (red) at M06/def2-TZVP//M06-L/def2-TZVP,def2-SVP level of theory in acetonitrile. Dashed lines are unwidened excitations. Inset: Excitations contributing to the 392 nm peak in **2-OMe**. Orbitals are plotted (isovalue=0.5) and an asterisk indicates a virtual orbital.

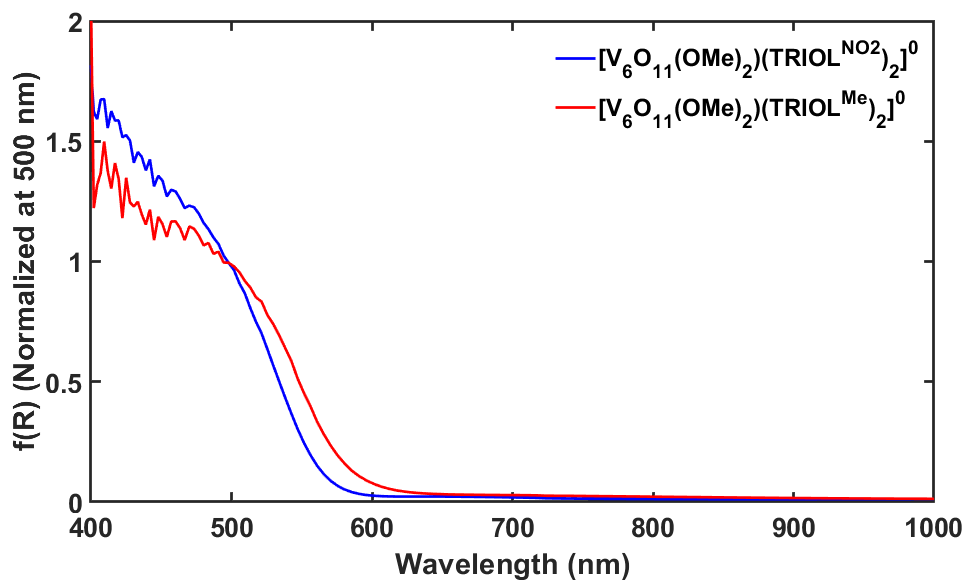


Figure S15. Kubelka-Munk transformed reflectance spectra of complexes $[\text{V}_6\text{O}_{11}(\text{OMe})_2(\text{TRIOL}^{\text{NO}_2})_2]^0$ and $[\text{V}_6\text{O}_{11}(\text{OMe})_2(\text{TRIOL}^{\text{Me}})_2]^0$. Spectra are normalized at 500 nm.

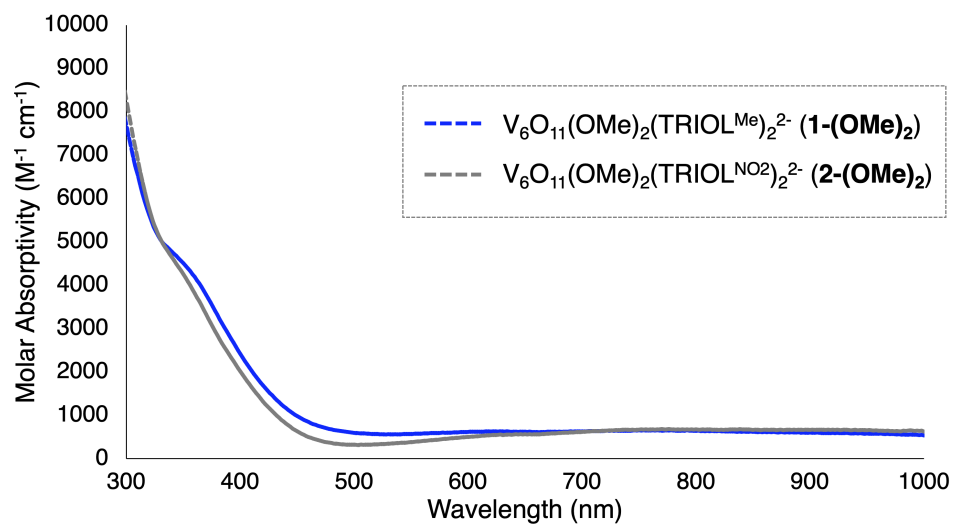


Figure S16. Electronic absorption spectra of complexes **1-(OMe)₂** and **2-(OMe)₂** collected in MeCN at 21 °C.

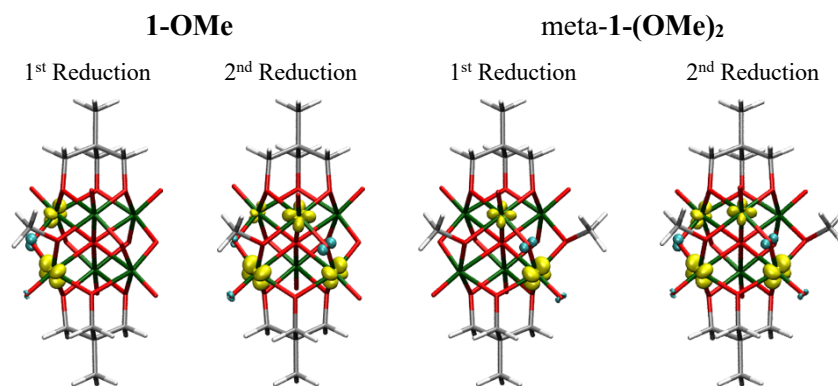


Figure S17. Spin density of reduced **1-OMe**, **m-1-(OMe)₂**, **2-OMe**, and **p-2-(OMe)₂** at M06/def2-TZVP//M06-L/def2-TZVP,def2-SVP level of theory. Vanadium in dark green, oxygen in red, nitrogen in blue, carbon in grey, and hydrogen in white. Alpha spin density in yellow and beta spin density in cyan. Isosurface=0.04.

Table S5. Calculated redox potentials at M06/def2-TZVP//M06-L/def2-TZVP,def2-SVP level of theory in acetonitrile. Reference electrode Fc^+/Fc in acetonitrile. The absolute potential of the Fc^+/Fc in acetonitrile can be obtained from E_{SHE} (4.28 V) in aqueous solution and the conversion constant between aqueous SHE and Fc^+/Fc in acetonitrile (0.624 V).^{8, 11, 12}

	X=1		X=2	
	1st Reduction	2nd Reduction	1st Reduction	2nd Reduction
X	-1.39	-1.87	-1.09	-1.85
X-OMe	-0.66	-1.36	-0.37	-1.08
p-X-(OMe)₂	-0.26	-0.56	0.04	-0.28
o-X-(OMe)₂	0.01	-0.66	0.33	-0.38
m-X-(OMe)₂	-0.14	-0.66	0.23	-0.47

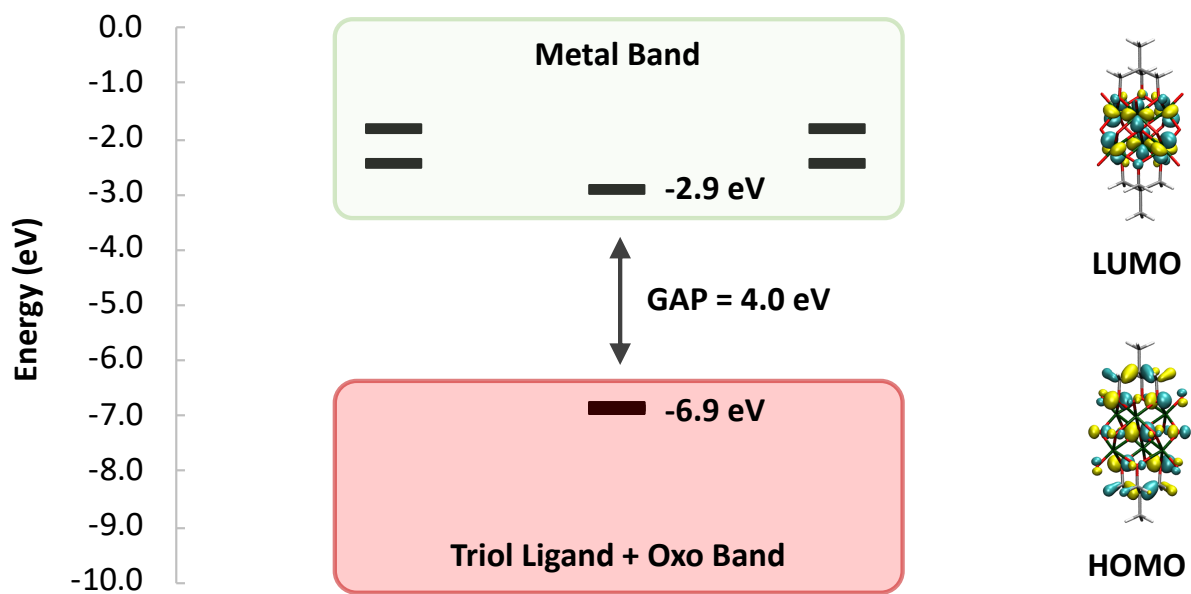


Figure S18. Frontier orbitals for complex **1** at M06/def2-TZVP//M06-L/def2-TZVP,def2-SVP level of theory in acetonitrile. HOMO and LUMO orbitals are plotted (isovalue=0.4). Only HOMO-4 to LUMO+4 are shown for clarity. All energies in eV.

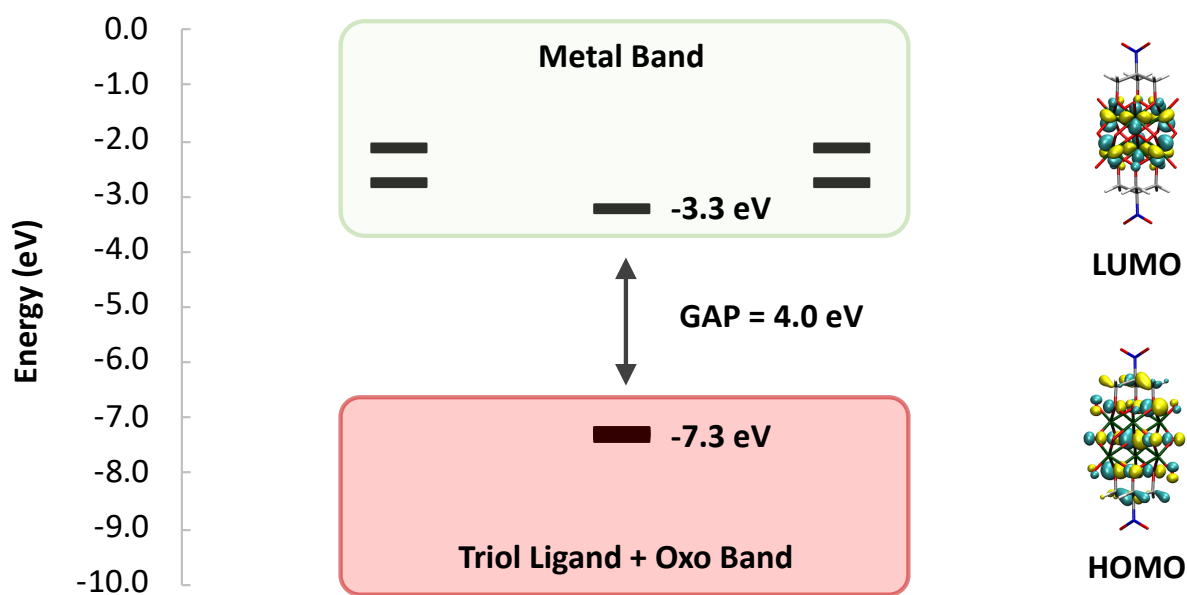


Figure S19. Frontier orbitals for complex **2** at M06/def2-TZVP//M06-L/def2-TZVP,def2-SVP level of theory in acetonitrile. HOMO and LUMO orbitals are plotted (isovalue=0.4). Only HOMO-4 to LUMO+4 are shown for clarity. All energies in eV.

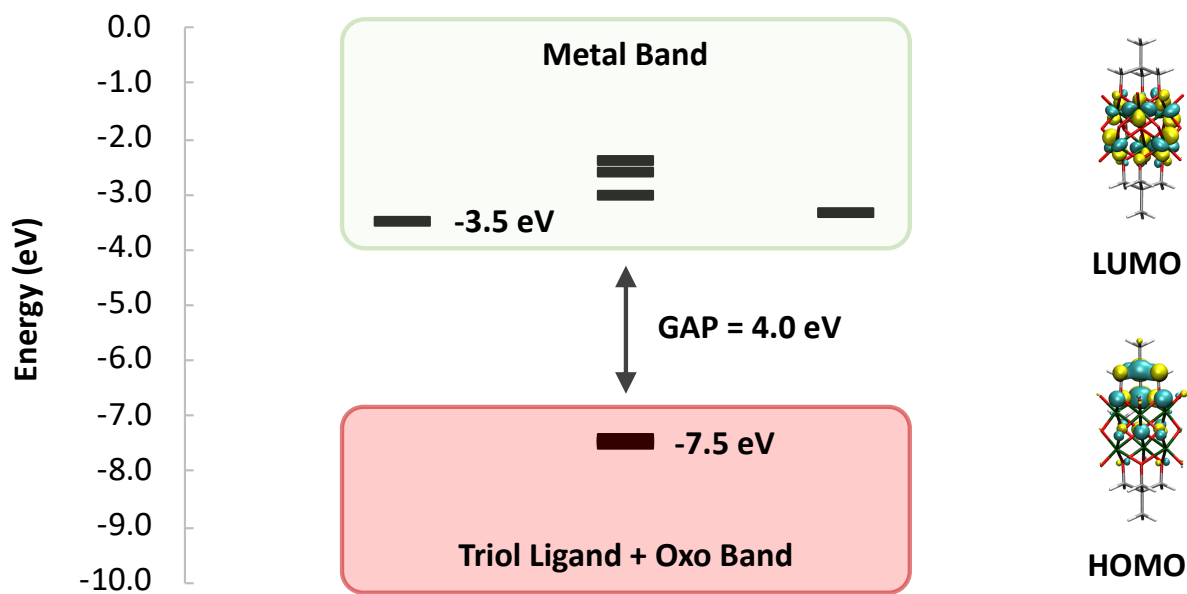


Figure S20. Frontier orbitals for complex **1-OMe** at M06/def2-TZVP//M06-L/def2-TZVP,def2-SVP level of theory in acetonitrile. HOMO and LUMO orbitals are plotted (isovalue=0.4). Only HOMO-4 to LUMO+4 are shown for clarity. All energies in eV.

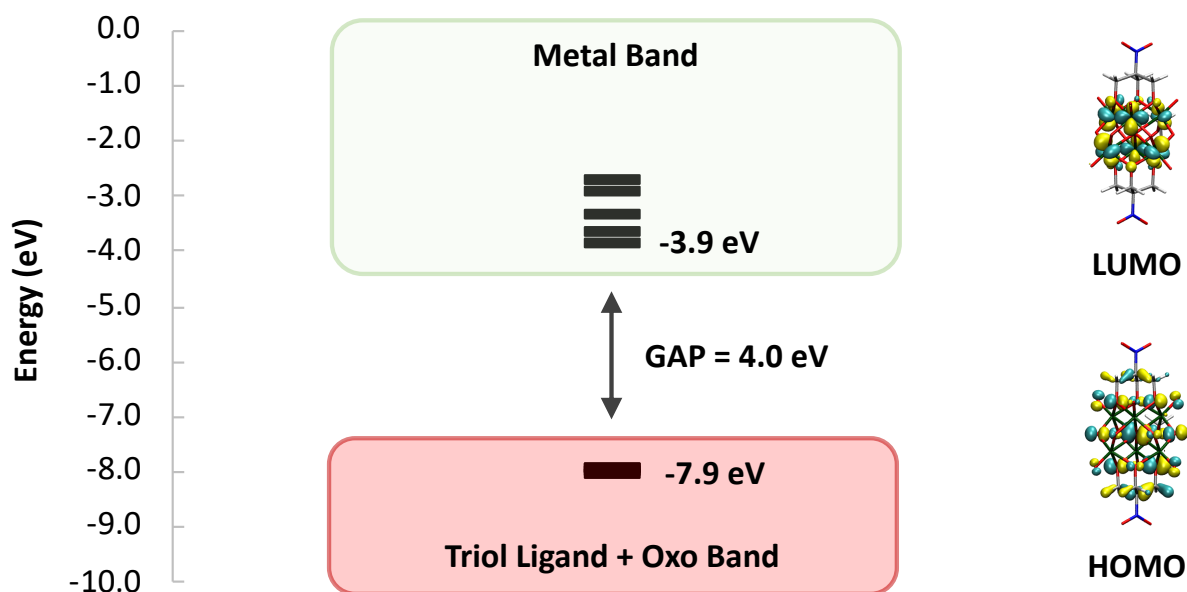


Figure S21. Frontier orbitals for complex **2-OMe** at M06/def2-TZVP//M06-L/def2-TZVP,def2-SVP level of theory in acetonitrile. HOMO and LUMO orbitals are plotted (isovalue=0.4). Only HOMO-4 to LUMO+4 are shown for clarity. All energies in eV.

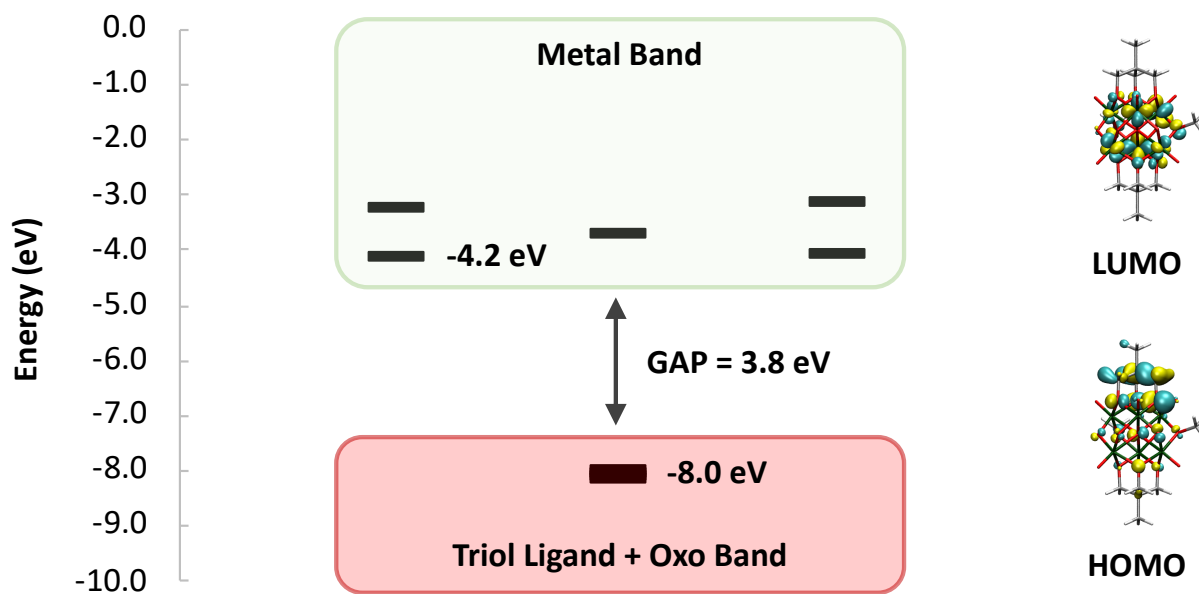


Figure S22. Frontier orbitals for complex **m-1-(OMe)₂** at M06/def2-TZVP//M06-L/def2-TZVP,def2-SVP level of theory in acetonitrile. HOMO and LUMO orbitals are plotted (isovalue=0.4). Only HOMO-4 to LUMO+4 are shown for clarity. All energies in eV.

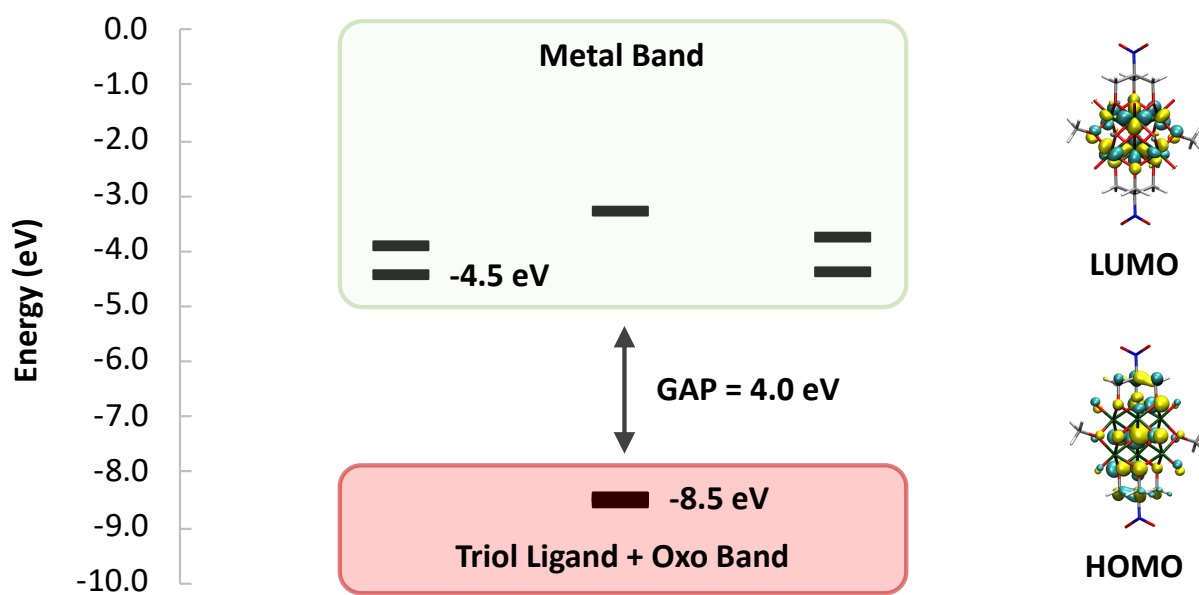


Figure S23. Frontier orbitals for complex **p-2-(OMe)₂** at M06/def2-TZVP//M06-L/def2-TZVP,def2-SVP level of theory in acetonitrile. HOMO and LUMO orbitals are plotted (isovalue=0.4). Only HOMO-4 to LUMO+4 are shown for clarity. All energies in eV.

Cartesian coordinates 1, 1-OMe, and 1-(OMe)₂ species at M06-L/def2-TZVP,def2-SVP level of theory.

1

V	-1.676659404450	0.968275324541	-1.175495741106
V	-0.000940693810	-1.934238520408	-1.175154227083
V	1.675227584324	0.966982779678	-1.176805000764
V	0.000135781533	1.934677850958	1.175467336976
V	-1.675993305878	-0.966244423646	1.176908408228
V	1.678106240915	-0.968632208636	1.176169471111
O	-2.720496743892	1.571014278058	-2.232916225197
O	-0.001615767534	-3.139262399395	-2.232804455982
O	2.717600110592	1.569013680853	-2.236048840388
O	0.001634068983	3.139323105847	2.233677348979
O	-2.717784421286	-1.568598131669	2.236711341179
O	2.722578460344	-1.571965013010	2.232313506312
O	-1.325551429436	-0.764109783937	-2.188442853255
O	-0.000275798525	1.527547620625	-2.188217187476
O	-1.332252462847	2.307926095647	-0.000055903702
O	-2.664298361872	0.000714210469	0.000867110808
O	1.323162297895	-0.764405712046	-2.188002285495
O	1.331119180881	2.306119349492	-0.000890428092
O	-1.323660863812	0.764936361751	2.188665835902
O	-1.331605137589	-2.305752179616	0.000843960488
O	1.331582771627	-2.306907432448	0.000643278056
O	2.663386823697	-0.000473815570	-0.000577489576
O	1.325195657029	0.763737328351	2.187826726365

O	0.000330972871	-1.526857903567	2.187300137903
O	-0.001942007576	0.001231365785	0.000102720487
C	-1.249664024525	-0.721637024262	-3.596548914472
H	-2.151137916784	-0.211617263146	-3.984385209715
H	-1.258040826457	-1.757887839566	-3.983006561395
C	-0.000112069276	1.442023702091	-3.596238966398
H	0.892738138695	1.968088078921	-3.982559493486
H	-0.892767063243	1.967887715517	-3.983144483207
C	1.249374538496	-0.721490432826	-3.596212545177
H	1.259731489369	-1.757653407279	-3.982792818590
H	2.150700404025	-0.210294342934	-3.982676259922
C	0.000032107186	-0.000508576446	-4.101827151365
C	1.249591320817	0.721580938038	3.596071381373
H	1.258108135558	1.757890103090	3.982337217505
H	2.151155254168	0.211669060490	3.983853795659
C	0.000009898166	-1.441905393483	3.595429156422
H	0.892534035722	-1.968038321533	3.982304314387
H	-0.892881405136	-1.968075215328	3.981504652914
C	-1.249495678922	0.721661077241	3.596800731159
H	-2.150698847841	0.210388230854	3.983462888810
H	-1.259656342708	1.757696883726	3.983747296739
C	0.000039331844	0.000420156623	4.101647215938
C	-0.000293778308	-0.000775706052	5.620511769732
H	0.888382437231	-0.511769178196	6.020566505177
H	-0.003136318399	1.024007392523	6.021438690551
H	-0.887193214204	-0.515853411028	6.019396454047

C	0.001043092867	0.000075427933	-5.620721099964
H	0.004097436426	-1.024855767714	-6.021269171557
H	-0.887505839102	0.510864196504	-6.021311689387
H	0.888062152153	0.515057078131	-6.019464250455

1-OMe

V	-1.661948842751	0.983407287179	-1.190377046847
V	-0.139753882451	-1.931410291910	-1.197787495441
V	1.670916743966	0.897051460156	-1.174697389251
V	0.003655453728	1.934416053039	1.186291618271
V	-1.695775368383	-0.929287591149	1.203123233937
V	1.663542774170	-0.899522170424	1.271203906270
O	-2.695392266202	1.592415373798	-2.239459947084
O	-0.076071973448	-3.164301435702	-2.207639305140
O	2.733868506746	1.469812966642	-2.216795651280
O	0.034394225862	3.149678688020	2.217293952140
O	-2.747526649881	-1.511442056734	2.252010882727
O	2.686812815975	-1.600719991479	2.272343237908
O	-1.352387848503	-0.780753785826	-2.213196347611
O	0.024495161116	1.471420464861	-2.184176739261
O	-1.296676847867	2.305325938313	-0.007510100833
O	-2.647728464786	0.008728672945	-0.011175264597
O	1.292716694026	-0.832141372065	-2.154951509461
O	1.368455297165	2.219893168611	0.019725864809
O	-1.304097192800	0.777249603534	2.194918572732
O	-1.354511458385	-2.318779812339	0.023685192195
O	1.345423758882	-2.420593848306	0.001272276367
O	2.656459127229	-0.111045580590	0.034839762375
O	1.333911529431	0.745805126137	2.245808287495
O	-0.026028266421	-1.520660419995	2.201162784361
O	0.009626137183	-0.064607627734	0.017377153387

C	-1.255317200493	-0.737568797038	-3.629618748669
H	-2.137973592574	-0.200452946290	-4.017549915491
H	-1.291752721129	-1.773698911835	-4.010206435195
C	0.042161733728	1.393546291783	-3.601427218715
H	0.948585132459	1.907443673082	-3.966088431406
H	-0.836155443182	1.936949420264	-3.991523489880
C	1.247424410732	-0.800835003873	-3.571352410643
H	1.237299355981	-1.840155044166	-3.945831893682
H	2.168635061740	-0.318767528603	-3.943652710678
C	0.024801822423	-0.050290751356	-4.102101783035
C	1.235181482759	0.707165792563	3.663245818902
H	1.244685720309	1.745797843234	4.035470615779
H	2.129409786921	0.193186065093	4.058066249872
C	-0.039925819920	-1.448823655787	3.618256746128
H	0.842977667934	-1.986556767939	4.007238323443
H	-0.940409734150	-1.969445062356	3.988128117287
C	-1.258068477990	0.740975596222	3.613059801121
H	-2.178850219192	0.254068186183	3.978427844281
H	-1.250772193425	1.779122780779	3.988509207832
C	-0.031139320521	-0.007475100100	4.132406659114
C	2.480881400668	-3.098786359209	-0.491127000527
H	2.166238296386	-3.970302884740	-1.083814778593
H	3.089050560599	-2.434041144425	-1.127089485345
H	3.100991118531	-3.443041179859	0.350083392978
C	-0.058839809137	-0.019453276138	5.652284595549
H	-0.050058447643	1.002418698979	6.057856329804

H	-0.962377045747	-0.521112870153	6.027200887039
H	0.813038063904	-0.549931860101	6.061062086636
C	0.057153413471	-0.052307446467	-5.621828808345
H	-0.810191537752	0.479312556589	-6.038915424398
H	0.964865600397	0.440255300717	-5.998897826065
H	0.043621010313	-1.077969524032	-6.017637313268

p-1-(OMe)₂

V	-1.647672027148	0.919751996299	-1.280295719020
V	-0.141473519768	-1.930086286962	-1.200818420720
V	1.698064624468	0.856543740361	-1.202956983999
V	0.141473519820	1.930086286962	1.200818420824
V	-1.698064624416	-0.856543740361	1.202956984103
V	1.647672027200	-0.919751996299	1.280295719123
O	-2.666488585024	1.611827327458	-2.277516211908
O	-0.107439384236	-3.170421772305	-2.189348690259
O	2.766085665530	1.419975366180	-2.233631875273
O	0.107439384288	3.170421772305	2.189348690363
O	-2.766085665478	-1.419975366180	2.233631875377
O	2.666488585076	-1.611827327458	2.277516212012
O	-1.351315167634	-0.762547181710	-2.259729918791
O	0.046926341998	1.472354430774	-2.194801323944
O	-1.322048313903	2.400614849837	-0.000451858410
O	-2.643600935863	0.098548870288	-0.049560283786
O	1.283787918034	-0.833753861911	-2.166270577917
O	1.384499215789	2.241862547983	-0.007670100795
O	-1.283787917982	0.833753861911	2.166270578021
O	-1.384499215737	-2.241862547983	0.007670100899
O	1.322048313955	-2.400614849837	0.000451858514
O	2.643600935915	-0.098548870288	0.049560283890
O	1.351315167686	0.762547181710	2.259729918895
O	-0.046926341946	-1.472354430774	2.194801324048
O	0.000000000026	0.000000000000	0.000000000052

C	-1.235691069901	-0.726003247649	-3.684917480256
H	-2.116621059482	-0.193478029901	-4.080080576594
H	-1.265248439580	-1.765276825183	-4.051110122786
C	0.075895393875	1.405891298327	-3.620993220059
H	0.987483092171	1.916682096180	-3.972133111916
H	-0.794904609676	1.957789323999	-4.012882255987
C	1.258844409503	-0.808388169463	-3.591651754652
H	1.234024133745	-1.849457825045	-3.955423044233
H	2.194321794706	-0.345363558395	-3.947272771588
C	0.052602508866	-0.036852769715	-4.129288138738
C	1.235691069953	0.726003247649	3.684917480360
H	1.265248439631	1.765276825183	4.051110122890
H	2.116621059534	0.193478029901	4.080080576698
C	-0.075895393823	-1.405891298327	3.620993220163
H	0.794904609728	-1.957789323999	4.012882256090
H	-0.987483092119	-1.916682096180	3.972133112020
C	-1.258844409451	0.808388169463	3.591651754755
H	-2.194321794655	0.345363558395	3.947272771691
H	-1.234024133693	1.849457825045	3.955423044336
C	-0.052602508814	0.036852769715	4.129288138842
C	2.436481128191	-3.163132392697	-0.441126960203
H	2.083767133693	-4.020419314663	-1.029997830715
H	3.103594552606	-2.544072111142	-1.061579234020
H	2.996792307706	-3.526758829345	0.431345991811
C	-2.436481128140	3.163132392697	0.441126960306
H	-3.103594552554	2.544072111142	1.061579234124

H	-2.083767133641	4.020419314663	1.029997830819
H	-2.996792307654	3.526758829345	-0.431345991707
C	-0.103630309186	0.026661954477	5.649436605759
H	0.755552128450	-0.514561413289	6.069436244294
H	-0.088160114429	1.049297366320	6.051332225604
H	-1.019579873859	-0.463512483489	6.007393779417
C	0.103630309238	-0.026661954477	-5.649436605655
H	0.088160114481	-1.049297366320	-6.051332225501
H	-0.755552128398	0.514561413289	-6.069436244191
H	1.019579873911	0.463512483489	-6.007393779314

o-1-(OMe)₂

V	-1.647324744071	1.035605686123	-1.207310810407
V	-0.099551517198	-1.851921109853	-1.312482580864
V	1.679258953608	0.916950803227	-1.188473675869
V	0.023046385915	1.944461919775	1.204641947395
V	-1.739624118210	-0.829406453115	1.217344950241
V	1.610868681130	-0.929707150414	1.240402895535
O	-2.685678977918	1.645301535004	-2.242115282723
O	-0.052946829174	-3.111613730419	-2.270938276167
O	2.749132468313	1.501145681196	-2.204346195431
O	0.041005382016	3.158063004306	2.224155587652
O	-2.788247920923	-1.513143081929	2.196266715329
O	2.626022405912	-1.644090208149	2.229191163783
O	-1.336416906145	-0.761336411334	-2.264177570846
O	0.021520136936	1.480602764005	-2.192995628063
O	-1.318253198822	2.290964387744	0.013937624572
O	-2.651415094501	-0.021831663293	-0.060061635911
O	1.297280363861	-0.807584258517	-2.220015711407
O	1.339889758417	2.230486074187	0.015744548052
O	-1.348092448703	0.783376228473	2.209143154892
O	-1.379593941966	-2.404362700547	0.012100576977
O	1.280552764264	-2.419196305965	-0.039539116485
O	2.611971500714	-0.106516568130	0.011486208310
O	1.286211626970	0.724582718480	2.224502095060
O	-0.076720698669	-1.521125157894	2.164974697061
O	-0.033815876120	-0.106883094903	-0.021631914650

C	-1.265526178596	-0.694102709057	-3.689442754271
H	-2.153481925961	-0.150434414359	-4.049307056983
H	-1.305609710004	-1.722609462848	-4.087168417424
C	0.034937553617	1.439624958834	-3.618818687451
H	0.942398776823	1.959936038860	-3.967196911329
H	-0.842193068888	1.995952904899	-3.988572543736
C	1.245350778800	-0.749150003885	-3.645886557094
H	1.242349486276	-1.783243852271	-4.031874988055
H	2.164537910837	-0.255547973258	-4.000830760225
C	0.014092053919	0.005664110463	-4.148574581062
C	1.207318527429	0.672411294349	3.650630868193
H	1.231467796825	1.706651749346	4.030898061105
H	2.104309401185	0.148446753364	4.020982870821
C	-0.087020679846	-1.474397521037	3.589524482789
H	0.789139530777	-2.030671400390	3.963960833440
H	-0.993372489575	-1.991508248056	3.947952433815
C	-1.286014425513	0.728235137666	3.635753800971
H	-2.209766130301	0.246954428325	3.998399397932
H	-1.266101826787	1.763345266521	4.014055936846
C	-0.058660278910	-0.040087847962	4.122523904990
C	2.302199101794	-3.342898233245	-0.369535013376
H	1.863738146025	-4.213695340240	-0.876969914099
H	3.044471029040	-2.872824850180	-1.035078531893
H	2.808944537692	-3.675814323230	0.546838312240
C	-1.421202088364	-3.734187029508	0.499325479264
H	-0.575897425332	-3.909462408708	1.184487445263

H	-2.363194203551	-3.896573649292	1.040315943133
H	-1.354211312142	-4.439503280820	-0.340990280616
C	-0.067412752727	-0.073923621332	5.643194532479
H	-0.048605564745	0.942307896559	6.060920362482
H	-0.968521603095	-0.577341776174	6.020062679285
H	0.807985499621	-0.614107833349	6.029562259703
C	0.039293055170	0.033714668705	-5.669287647251
H	-0.833667324281	0.569650529938	-6.066889961775
H	0.943098077503	0.538342653973	-6.037809807909
H	0.028176879650	-0.984190800658	-6.082887696237

m-1-(OMe)₂

V	-1.597343057607	1.085538626947	-1.202648330043
V	-0.196810585043	-1.883691786116	-1.204432986621
V	1.681872299004	0.891020571557	-1.195372102969
V	0.037440909412	1.938938707082	1.209849632340
V	-1.611025036056	-0.976105464986	1.300346431821
V	1.674071401563	-0.895468010648	1.261602805633
O	-2.686400937605	1.650885646347	-2.207084911924
O	-0.139677608716	-3.120614636775	-2.196997532229
O	2.741179126899	1.467140712262	-2.225389201915
O	0.083760214675	3.153952769355	2.229265100021
O	-2.744011084168	-1.486814992890	2.286392997176
O	2.692257162711	-1.612807590763	2.242669082346
O	-1.380815440823	-0.732845695055	-2.202006374099
O	0.018213259450	1.507186128795	-2.204479764143
O	-1.302561891721	2.329225717698	0.013329511929
O	-2.732821716842	0.030249355264	-0.016788682855
O	1.248269655935	-0.807989433425	-2.156256330812
O	1.356007204792	2.213237023176	0.006664953375
O	-1.290742121496	0.789043851237	2.204215070097
O	-1.429820061177	-2.272736975644	0.049724030825
O	1.265770614020	-2.385030521256	0.018280785158
O	2.649303641509	-0.106794444804	0.023586703983
O	1.327742069593	0.733090873570	2.243685014073
O	-0.039466564395	-1.521293302120	2.264726975216
O	-0.048614500302	-0.046608896043	0.030419382066

C	-1.304131850253	-0.697242110567	-3.625966824310
H	-2.183737056190	-0.147446108769	-4.000127062342
H	-1.361791052718	-1.733430945910	-4.000352660303
C	0.026903974698	1.418269171846	-3.629809309944
H	0.940172931563	1.916507501978	-3.994036546824
H	-0.844384925832	1.975792231810	-4.012632544133
C	1.201051591476	-0.791465221656	-3.581414777089
H	1.179115782752	-1.835414733845	-3.937566365792
H	2.128138279873	-0.325537599240	-3.955078826792
C	-0.016331388910	-0.031147522347	-4.110062873551
C	1.253014635149	0.719998033986	3.670363873558
H	1.283415305630	1.764852344126	4.019175694290
H	2.145953171815	0.199742093336	4.055261083613
C	-0.030546996082	-1.424435906007	3.690451883443
H	0.861741278037	-1.954271933767	4.062034879910
H	-0.923943919721	-1.943715653520	4.075955915653
C	-1.247198375677	0.772998205253	3.630804524868
H	-2.168553862625	0.292364383453	4.000510510276
H	-1.241326755499	1.815486296959	3.989248582135
C	-0.019053203616	0.030396720245	4.160821340564
C	2.335353793889	-3.221503240750	-0.393635961662
H	1.940462550482	-4.065929582772	-0.974054683269
H	3.048733780759	-2.655865786173	-1.014332403920
H	2.862465491523	-3.605528544683	0.491028890333
C	-3.965967022522	-0.535493094321	-0.430615571310
H	-4.502574323735	0.175994673930	-1.072441412525

H	-3.794590564718	-1.469951606103	-0.988160571381
H	-4.579211990919	-0.758842011889	0.453868919923
C	-0.041112398852	0.055441743238	5.681617356146
H	0.828945375037	-0.471422318217	6.097290011656
H	-0.022843794426	1.087668660647	6.057729619782
H	-0.947312501953	-0.429868976707	6.069507704845
C	0.007988560224	-0.048932872368	-5.630671304947
H	-0.857129120654	0.486907458179	-6.045450315171
H	0.918636979022	0.430905776998	-6.015263803329
H	-0.018125370638	-1.078948979139	-6.012574900849

TS1 (1 → 1-OMe)

V	-2.424589991780	-0.438970451755	1.821381368233
V	-0.054570868739	-1.804629078968	-0.076545983458
V	-2.772277727634	-0.436110494829	-1.502225766485
V	-2.341914154788	2.101013341469	0.138851092442
V	0.380105425926	0.744278008074	1.534415622506
V	-0.000885447195	0.758908056753	-1.806470187312
O	-3.342018280557	-1.087175851397	2.960621139230
O	0.540446597020	-3.286883030064	-0.150540115756
O	-3.889461128132	-1.090455919293	-2.442933602413
O	-2.910397172210	3.595606251717	0.184724641818
O	1.488681959643	1.393741589793	2.485101469628
O	0.959656431694	1.384702007233	-2.925490327985
O	-1.412183470891	-2.148982613834	1.364930152435
O	-3.551220023196	-1.074813962209	0.245267381119
O	-3.093362242034	1.229453568467	1.528823874458
O	-0.931270383444	0.148817663181	2.649109724250
O	-1.662289820566	-2.138602770193	-1.263920767846
O	-3.337820481498	1.229685269387	-1.124689971392
O	-0.711675016267	2.443148777797	1.286346211772
O	0.969772027942	-0.934766880969	1.130185251389
O	0.742802249551	-0.924997436972	-1.511663837213
O	-1.444596657644	0.136404859741	-2.645662493739
O	-0.969248615679	2.448450075984	-1.343631177275
O	1.169790402056	1.363184059201	-0.215667519236
O	-1.186760063263	0.145264710166	-0.001749285688

C	-2.113352739249	-3.377118126332	1.357912677770
H	-2.655153636802	-3.476960007398	2.315740067966
H	-1.378391705878	-4.200563625450	1.297841181487
C	-4.134851178514	-2.361351879174	0.300601349978
H	-4.865730118206	-2.452682821001	-0.523375953412
H	-4.687141974064	-2.455720056339	1.253220390694
C	-2.347620897155	-3.367717200733	-1.131314631622
H	-1.615751399224	-4.192282711348	-1.212657610265
H	-3.060450147558	-3.467523091381	-1.970029127217
C	-3.099803723043	-3.481375817692	0.195302070503
C	-0.259730071975	3.671162600285	-1.339055704186
H	-0.989526149389	4.498633585886	-1.274984451543
H	0.278255110167	3.769716450126	-2.299595553443
C	1.761919986874	2.643995182179	-0.277286405418
H	2.319884787055	2.728798270938	-1.228735225965
H	2.490582528087	2.741827060436	0.547724219149
C	-0.019452290129	3.668252164517	1.146281797150
H	0.693525016016	3.766394028974	1.985005533307
H	-0.748357911320	4.495338314383	1.224887188808
C	0.732440948623	3.771277485360	-0.181040041114
C	2.732616326547	-0.976618924144	-1.521029092974
H	2.691306076839	-0.506375719017	-0.543838667213
H	2.724171708958	-0.365143808769	-2.418277111796
H	2.712132936873	-2.058665713322	-1.606851914366
O	4.676632054675	-0.935972323236	-1.578682358872
S	5.398605492251	-1.369546107499	-0.316879014322

O	4.625336003079	-2.282732941333	0.525689438444
O	6.806880627892	-1.663622239452	-0.569783657327
C	5.435586441811	0.213615238620	0.650136132516
F	4.195611540699	0.661386376086	0.868703788594
F	6.108476786152	1.155790347455	-0.008319039950
F	6.023991365854	0.020825816987	1.829650370121
C	1.447048278673	5.110605049210	-0.249088696078
H	2.000206300102	5.219314759268	-1.193568621065
H	0.735697935176	5.946777947813	-0.181191428953
H	2.168615922148	5.219040903587	0.573915687493
C	-3.806888665856	-4.824975287934	0.258119252486
H	-3.090154762462	-5.656237563965	0.187659009342
H	-4.359949616160	-4.940634611515	1.201799991223
H	-4.526965365883	-4.934728383550	-0.565983523412

TS2 (1-OMe → p-1-(OMe)₂)

V	2.328168550572	-0.518713778024	-1.735566115185
V	-0.070428739529	-1.853933641161	0.017253267712
V	2.614983246503	-0.662456818665	1.599148146356
V	2.276671839868	2.030153039845	0.234083654180
V	-0.380942331988	0.836767284164	-1.429317220684
V	-0.143778755124	0.616452516398	1.898832025380
O	3.311374863158	-1.022464473144	-2.880147603907
O	-0.715984089773	-3.305795391445	-0.030490301754
O	3.685119093612	-1.392812047376	2.524397053712
O	2.908920823596	3.490159934864	0.213907278689
O	-1.441986457672	1.559178784886	-2.368422554917
O	-1.104822763201	1.183289302546	3.033683795905
O	1.332894182643	-2.166447237804	-1.422966124290
O	3.435740197305	-1.176031583375	-0.170117885157
O	3.123377883526	1.277370662284	-1.366641511009
O	0.974823404574	0.268351712944	-2.561420802722
O	1.495731808073	-2.291417149904	1.202434271988
O	3.265353460011	1.042705203177	1.323553122974
O	0.742646889575	2.463240666578	-1.037408664277
O	-0.993107471131	-0.862986818956	-1.171911021581
O	-0.891584388382	-1.030448230026	1.472284616698
O	1.292317051699	-0.079101121040	2.716042781904
O	0.894994464398	2.329845986333	1.597127399166
O	-1.206242390571	1.350742633981	0.324739476710
O	1.148918752234	0.097950254283	0.074232912351

C	2.016688273481	-3.416115936783	-1.459703927788
H	2.577516682872	-3.470821115065	-2.408431504788
H	1.259361339968	-4.217904366339	-1.459833552449
C	4.015402354775	-2.469780973263	-0.286229026381
H	4.721816458559	-2.612735981059	0.549138147393
H	4.591240000994	-2.511550432555	-1.227045089122
C	2.163774216901	-3.535742788772	1.028834235287
H	1.408427777313	-4.340183209967	1.034129191643
H	2.834323260771	-3.692668551289	1.890609514341
C	2.964170765380	-3.581585340446	-0.273116807153
C	0.202377039919	3.573467377298	1.637787008410
H	0.953220605110	4.381994571732	1.658769120249
H	-0.370790324645	3.613058683355	2.579388623658
C	-1.786145489209	2.644027075368	0.439320631070
H	-2.376041994741	2.678468876968	1.372289208541
H	-2.478573598648	2.792436783659	-0.406360992556
C	0.074588942650	3.704779067612	-0.857745853829
H	-0.596454972892	3.869188439626	-1.718419375638
H	0.829420692554	4.510489456515	-0.859288041564
C	-0.730942794683	3.750529990920	0.442126754876
C	-2.830472968830	-1.086230119058	1.440464990286
H	-2.808526352875	-0.548104336960	0.498770249028
H	-2.884274431639	-0.541931414720	2.378666783757
H	-2.842377633102	-2.172037129943	1.448170163155
O	-4.831186505206	-1.045336145325	1.431700774191
S	-5.485316048678	-1.355448130058	0.102720424316

O	-4.675813513144	-2.202114524740	-0.776101415299
O	-6.909652274515	-1.649799893210	0.244557285957
C	-5.453235036180	0.304777125694	-0.727091621964
F	-4.194785285232	0.743312980797	-0.859822780851
F	-6.132438545803	1.204623990243	-0.018490149319
F	-5.995603861758	0.226866219200	-1.940982831750
C	3.453978912208	2.090310047139	-2.476290443226
H	2.544143129349	2.400377996484	-3.015834232336
H	3.990780366631	2.985759142573	-2.132400277158
H	4.098450032148	1.526908778680	-3.166546339592
C	-1.423777880251	5.099375991793	0.552556599723
H	-2.011446315093	5.168242651642	1.479019742495
H	-0.693416457164	5.920938651284	0.555765992132
H	-2.108197204680	5.261414732614	-0.292153077316
C	3.661701431925	-4.928170948883	-0.383399732656
H	2.934286505770	-5.752240388936	-0.382714765133
H	4.246092896600	-4.995975655243	-1.311894858841
H	4.349505869116	-5.085771779946	0.459286297962

TS2 (1-OMe → o-1-(OMe)₂)

V	-2.376919552479	-0.330663559958	1.956000343269
V	-0.041786138818	-1.773203550556	0.097596874509
V	-2.817683759813	-0.502789308285	-1.295658004523
V	-2.301343131576	2.132371105009	0.132581646655
V	0.419611093296	0.871586086186	1.581134051322
V	0.104448762337	0.742094930169	-1.695274868697
O	-3.281742502967	-0.896038171018	3.135138515501
O	0.564472400857	-3.244387233613	0.088057303328
O	-3.869947872759	-1.200648331114	-2.267184682236
O	-2.880809610243	3.615218322067	0.093236604982
O	1.539373008321	1.554961484763	2.479295684692
O	0.989371014174	1.270545179334	-2.905732787763
O	-1.376796407454	-2.035385140644	1.557305472018
O	-3.544650561089	-1.060957606444	0.413997876346
O	-3.056844520007	1.313534406234	1.535435395129
O	-0.883263594611	0.327590826628	2.716281053851
O	-1.643413566639	-2.163652776158	-1.053287424821
O	-3.298173269293	1.182678787244	-1.118705863195
O	-0.664807942619	2.533377198075	1.212816127176
O	1.000209837102	-0.815123081088	1.215782822041
O	0.761672239921	-0.952005327604	-1.415425654384
O	-1.423357110199	-0.036777157350	-2.643557210092
O	-0.935397515473	2.390226755556	-1.392996954400
O	1.227553800485	1.411828160672	-0.232356854143
O	-1.160530972898	0.179647058201	0.025774043679

C	-2.061270132689	-3.281267841048	1.629394410124
H	-2.590813723857	-3.329251337530	2.595987810227
H	-1.308670944534	-4.088042498026	1.611569205088
C	-4.110940416681	-2.360842275933	0.545311569944
H	-4.851412551705	-2.496426260191	-0.261981550110
H	-4.644331603987	-2.404123627562	1.509803649008
C	-2.314958277845	-3.400732064062	-0.860363548938
H	-1.572836730651	-4.216226541413	-0.913379707027
H	-3.031774355116	-3.542448490437	-1.688140944709
C	-3.051734037998	-3.459927226392	0.479440820062
C	-0.248997991977	3.634444740653	-1.470476332690
H	-0.996915156737	4.444728859626	-1.448008297900
H	0.278091081755	3.684733935794	-2.439120925211
C	1.804621826431	2.707196570355	-0.362375195634
H	2.359867056320	2.742194967320	-1.316699374449
H	2.527955782822	2.846092531129	0.458081628787
C	0.011396821380	3.768745569386	1.014139539707
H	0.726063503382	3.908972347860	1.843000093700
H	-0.732210634317	4.582355708819	1.062789507134
C	0.748743548108	3.812283027556	-0.324425694794
C	2.699046172128	-1.083182312167	-1.449014360976
H	2.718377354714	-0.505502117216	-0.530508932253
H	2.743883768342	-0.581365302364	-2.411121474853
H	2.671268496694	-2.168074584260	-1.410763343141
O	4.695584273793	-1.111091980323	-1.492619966557
S	5.378283514876	-1.455547915273	-0.185865218829

O	4.564484966613	-2.277554893526	0.711656785931
O	6.784783225201	-1.803527402089	-0.375428997142
C	5.439646388706	0.199405361580	0.653854135263
F	4.206255250538	0.691179819556	0.824935894447
F	6.137075963631	1.073268311399	-0.069505507944
F	6.011978834658	0.090669054662	1.851412833999
C	-1.193727436923	-0.848135035698	-3.778286503833
H	-0.688379357000	-1.783242798202	-3.485946567050
H	-2.151627338927	-1.091466408859	-4.258982960523
H	-0.555236597801	-0.310776455589	-4.494676678798
C	1.438543102807	5.159375276866	-0.471551976307
H	0.709225327569	5.981259144771	-0.444294272995
H	2.161424602784	5.323688610437	0.340027471341
H	1.982470538055	5.223598244884	-1.424529694397
C	-3.732680382545	-4.812638472141	0.615185486312
H	-2.998140327185	-5.629562393368	0.580163951249
H	-4.275752559773	-4.889366884063	1.567827380094
H	-4.454762640619	-4.974714131226	-0.197589595602

TS2 (1-OMe → m-1-(OMe)₂)

V	-2.334217230754	-0.630660903152	1.875907746999
V	0.077547347443	-1.848389651391	-0.030671477699
V	-2.605544791654	-0.605508359474	-1.466762746460
V	-2.271747632974	2.013768241725	0.395891161118
V	0.451671003990	0.666302746626	1.657391782871
V	0.049496073431	0.819042279581	-1.662479183726
O	-3.231817912200	-1.338131706578	2.984207613617
O	0.725174789519	-3.292574114654	-0.183315482837
O	-3.755995751926	-1.153192014562	-2.419004984786
O	-2.923814235726	3.465223013281	0.427888186681
O	1.538278636350	1.287642953575	2.637219261992
O	0.986053640784	1.501649850480	-2.754995935526
O	-1.287852711134	-2.277502782772	1.343506957182
O	-3.430762534228	-1.212204026144	0.265142765377
O	-3.066400939696	1.050993458188	1.643340028404
O	-0.868289966805	-0.004394074877	2.717496517005
O	-1.539696980904	-2.211328717102	-1.278753338897
O	-3.340890848636	1.205867373002	-1.044112197340
O	-0.693327861042	2.363146762328	1.490045362390
O	1.069739711621	-0.983902685800	1.180767864167
O	0.797542883799	-0.870409272485	-1.454345876205
O	-1.413665496321	0.183114436768	-2.549627022276
O	-0.967860040459	2.439301824038	-1.137089063596
O	1.191056319560	1.376709504662	-0.063099939456
O	-1.158381697451	0.092413405613	0.074752395407

C	-1.960761138523	-3.530914500476	1.308342788493
H	-2.488429309152	-3.664008075445	2.267758386821
H	-1.203124977547	-4.328286249841	1.220519543718
C	-4.004368552023	-2.513902586576	0.280251339373
H	-4.729034569242	-2.587524162449	-0.549176493222
H	-4.558993943871	-2.640122814346	1.225552991777
C	-2.198161129724	-3.470547322966	-1.175288675480
H	-1.436466886812	-4.262656844224	-1.268392294765
H	-2.897644116981	-3.564916873906	-2.023896600121
C	-2.950587480693	-3.615502576148	0.147159343603
C	-0.295950308167	3.690639389670	-1.098785233081
H	-1.053608192724	4.487568900112	-1.001846775356
H	0.227833659558	3.836576477298	-2.059374725851
C	1.759979738145	2.680020546856	-0.076392925876
H	2.321865833620	2.802350746989	-1.019078168776
H	2.475055550537	2.758407116751	0.759651249823
C	-0.028617438788	3.618337594351	1.388268970605
H	0.686459179344	3.693937571395	2.224824056537
H	-0.781587230546	4.416468264623	1.507593930292
C	0.702243771384	3.776075331522	0.055701760799
C	2.739048103410	-0.953032956284	-1.573345068319
H	2.787393836151	-0.481921482575	-0.596648188580
H	2.724018135994	-0.344847505457	-2.472770908828
H	2.726233018242	-2.035637955218	-1.654857758814
O	4.723350359347	-0.948825164100	-1.732018902373
S	5.493640264968	-1.306822113278	-0.478648810761

O	4.739264879885	-2.130323938392	0.468152577271
O	6.881963332527	-1.659552349463	-0.766310530850
C	5.614022592174	0.343052970304	0.361906525573
F	4.392873670416	0.843921691977	0.587962946343
F	6.285197874328	1.212901520902	-0.389828182839
F	6.238558556887	0.226542201013	1.532058441215
C	-3.854632018923	1.977095481767	-2.112185175278
H	-4.613876616696	1.395061969786	-2.654804454598
H	-4.317079362157	2.893817043062	-1.719743534067
H	-3.051992663490	2.251511666569	-2.816195582028
C	1.385818742218	5.133759861249	0.023914577482
H	2.111051549213	5.231129894215	0.844207630994
H	1.926390354041	5.281403882626	-0.921727912007
H	0.654060504614	5.947975445593	0.123577013014
C	-3.639734726363	-4.970554681710	0.177226997352
H	-2.910615364059	-5.787698652577	0.083310268930
H	-4.186452575077	-5.113904235328	1.119898583370
H	-4.360139570028	-5.065859648749	-0.647389535916

Cartesian coordinates 2, 2-OMe, and 2-(OMe)₂ species at M06-L/def2-TZVP,def2-SVP level of theory.

2

V	-1.161201572589	0.983255883892	1.683477623544
V	-1.180862888369	-1.936071916463	0.000000000000
V	-1.161201572589	0.983255883892	-1.683477623544
V	1.180862888369	1.936071916463	0.000000000000
V	1.161201572589	-0.983255883892	1.683477623544
V	1.161201572589	-0.983255883892	-1.683477623544
O	-2.223340576954	1.585206517247	2.716933132152
O	-2.256997689379	-3.119066764778	0.000000000000
O	-2.223340576954	1.585206517247	-2.716933132152
O	2.256997689379	3.119066764778	0.000000000000
O	2.223340576954	-1.585206517247	2.716933132152
O	2.223340576954	-1.585206517247	-2.716933132152
O	-2.194719421039	-0.749004557116	1.324179896033
O	-2.175715801698	1.537655132522	0.000000000000
O	0.016435407566	2.313554513542	1.334451554035
O	0.000000000000	0.000000000000	2.666514001974
O	-2.194719421039	-0.749004557116	-1.324179896033
O	0.016435407566	2.313554513542	-1.334451554035
O	2.194719421039	0.749004557116	1.324179896033
O	-0.016435407566	-2.313554513542	1.334451554035
O	-0.016435407566	-2.313554513542	-1.334451554035
O	0.000000000000	0.000000000000	-2.666514001974

O	2.194719421039	0.749004557116	-1.324179896033
O	2.175715801698	-1.537655132522	0.000000000000
O	0.000000000000	0.000000000000	0.000000000000
O	-6.090614773958	-1.097653863359	0.000000000000
O	-6.168258425471	1.061709106333	0.000000000000
O	6.090614773958	1.097653863359	0.000000000000
O	6.168258425471	-1.061709106333	0.000000000000
N	-5.563304939494	0.003244167480	0.000000000000
N	5.563304939494	-0.003244167480	0.000000000000
C	-3.590481313761	-0.708850344156	1.263888921191
H	-3.990060887880	-0.191666917687	2.154907664323
H	-3.996298672234	-1.734678486398	1.244883465470
C	-3.579936957409	1.485409806794	0.000000000000
H	-3.969083620617	2.003921790767	-0.892507973605
H	-3.969083620617	2.003921790767	0.892507973605
C	-3.590481313761	-0.708850344156	-1.263888921191
H	-3.996298672234	-1.734678486398	-1.244883465470
H	-3.990060887880	-0.191666917687	-2.154907664323
C	-4.052587546442	0.034555231000	0.000000000000
C	3.590481313761	0.708850344156	-1.263888921191
H	3.996298672234	1.734678486398	-1.244883465470
H	3.990060887880	0.191666917687	-2.154907664323
C	3.579936957409	-1.485409806794	0.000000000000
H	3.969083620617	-2.003921790767	-0.892507973605
H	3.969083620617	-2.003921790767	0.892507973605
C	3.590481313761	0.708850344156	1.263888921191

H	3.990060887880	0.191666917687	2.154907664323
H	3.996298672234	1.734678486398	1.244883465470
C	4.052587546442	-0.034555231000	0.000000000000

2-OMe

V	-1.165631713589	0.915038630236	1.676603131532
V	-1.202256160428	-1.930742535251	-0.138826342162
V	-1.174248956817	1.001774407513	-1.669791129680
V	1.195487977239	1.937061814430	0.010329858496
V	1.244661835583	-0.917029308914	1.670454488924
V	1.192575390739	-0.941807927176	-1.701122062795
O	-2.213415752426	1.487433032960	2.728675259783
O	-2.230839392726	-3.143467297807	-0.081937740366
O	-2.219701974873	1.613270756838	-2.699662169917
O	2.238192947841	3.137249497009	0.042975060005
O	2.246052764570	-1.618498649355	2.687754010967
O	2.246439995481	-1.521556615889	-2.743642367550
O	-2.171907420942	-0.814204229381	1.288524258375
O	-2.174008639493	1.486836920554	0.018831874550
O	0.030361083584	2.226494916276	1.374112528424
O	0.024493021879	-0.109462152337	2.661884052709
O	-2.214247744831	-0.761717015101	-1.359433726092
O	0.011612373637	2.312112634372	-1.293249608951
O	2.246019964538	0.734336870450	1.340962995595
O	-0.025426497576	-2.420677110299	1.345630843260
O	0.008893540492	-2.320960858141	-1.360220060625
O	-0.001592071357	0.015520012224	-2.648631701315
O	2.205740780195	0.767040931894	-1.298713143059
O	2.191196105104	-1.529659722881	-0.022465081513
O	0.017023220140	-0.066514172186	0.014470277897

O	-6.093305537316	-1.142951345448	0.025590853926
O	-6.168328890108	1.017789768320	0.049232536563
O	6.129607566808	1.078437264009	-0.052293865133
O	6.190893525420	-1.082435818870	-0.025217880852
N	-5.570082110877	-0.042142614633	0.029757777059
N	5.599714209202	-0.018956999443	-0.033903945866
C	-3.575302217111	-0.781298210047	1.250331873061
H	-3.963167294275	-0.288672339360	2.158843708398
H	-3.972561430819	-1.809360012226	1.215864903864
C	-3.586769594760	1.440963443825	0.029376485523
H	-3.974811004537	1.978326137722	-0.850487687690
H	-3.959008501310	1.947221751484	0.934249701247
C	-3.618837967405	-0.721363185616	-1.281566518310
H	-4.018081473233	-1.748944921750	-1.291086059822
H	-4.016344096830	-0.181375181758	-2.157350955761
C	-4.054984138202	-0.011272117057	0.008291448219
C	3.611724526113	0.728887092415	-1.261422354823
H	4.009135492334	1.756172978883	-1.232034606076
H	3.990683502684	0.231730018763	-2.170548609866
C	3.602955164038	-1.489251533680	-0.029199657873
H	3.981250476943	-2.001504648640	-0.928321581932
H	3.990637515412	-2.020231355818	0.855283718601
C	3.651223828794	0.695075890100	1.261277837078
H	4.055145644852	0.174027224644	2.146371585467
H	4.044260531991	1.724192006969	1.248523160574
C	4.082646180222	-0.038525822517	-0.017007951676

C	-0.496925052009	-3.141611871001	2.468974502747
H	-1.122505157781	-2.497841624095	3.108406252126
H	-1.090571478559	-4.003013943206	2.132481287797
H	0.358334104356	-3.501085862009	3.059063536940

p-2-(OMe)₂

V	-1.200655448121	0.894100568150	1.688674714964
V	-1.211105782742	-1.927403947509	-0.131330779423
V	-1.245960750481	0.926479045352	-1.671319343709
V	1.211105782742	1.927403947509	0.131330779423
V	1.245960750481	-0.926479045352	1.671319343709
V	1.200655448121	-0.894100568150	-1.688674714964
O	-2.241910356324	1.462372800564	2.738720201013
O	-2.216257415475	-3.149328765380	-0.104313869297
O	-2.233922036804	1.614321137297	-2.696705700880
O	2.216257415475	3.149328765380	0.104313869297
O	2.233922036804	-1.614321137297	2.696705700880
O	2.241910356324	-1.462372800564	-2.738720201013
O	-2.186938856611	-0.809213676178	1.275697567648
O	-2.184365884716	1.487552876034	0.023014655308
O	0.004484735623	2.253870345575	1.377993978957
O	0.023758455394	-0.084822548676	2.647774796957
O	-2.255125561316	-0.751706715338	-1.363984913806
O	0.026628899891	2.397500833984	-1.329748721581
O	2.255125561316	0.751706715338	1.363984913806
O	-0.026628899891	-2.397500833984	1.329748721581
O	-0.004484735623	-2.253870345575	-1.377993978957
O	-0.023758455394	0.084822548676	-2.647774796957
O	2.186938856611	0.809213676178	-1.275697567648
O	2.184365884716	-1.487552876034	-0.023014655308
O	0.000000000000	0.000000000000	0.000000000000

O	-6.129108091104	-1.110822605747	0.026680259593
O	-6.186713655584	1.049698102291	0.112331082841
O	6.129108091104	1.110822605747	-0.026680259593
O	6.186713655584	-1.049698102291	-0.112331082841
N	-5.601840197536	-0.014130366813	0.055105758317
N	5.601840197536	0.014130366813	-0.055105758317
C	-3.599020839889	-0.779395454890	1.250501483918
H	-3.974456507601	-0.299733178657	2.169354617355
H	-3.987677262270	-1.809458298137	1.209532391121
C	-3.604564549286	1.455488241136	0.041513736411
H	-3.991832749844	1.997967427116	-0.835031851362
H	-3.965636724246	1.963733751367	0.948227461483
C	-3.668426839054	-0.711242560546	-1.273458533458
H	-4.057436429129	-1.741219954425	-1.277329122290
H	-4.068291090042	-0.177082493849	-2.150842374413
C	-4.080979061327	0.004075232662	0.019216815111
C	3.599020839889	0.779395454890	-1.250501483918
H	3.987677262270	1.809458298137	-1.209532391121
H	3.974456507601	0.299733178657	-2.169354617355
C	3.604564549286	-1.455488241136	-0.041513736411
H	3.965636724246	-1.963733751367	-0.948227461483
H	3.991832749844	-1.997967427116	0.835031851362
C	3.668426839054	0.711242560546	1.273458533458
H	4.068291090042	0.177082493849	2.150842374413
H	4.057436429129	1.741219954425	1.277329122290
C	4.080979061327	-0.004075232662	-0.019216815111

C	-0.431727558607	-3.224668703123	2.417193102729
H	-1.027688926975	-2.641076168573	3.135584113650
H	-1.031364219976	-4.060408150485	2.034619471810
H	0.460913687408	-3.615653441306	2.923621321595
C	0.431727558607	3.224668703123	-2.417193102729
H	1.031364219976	4.060408150485	-2.034619471810
H	1.027688926975	2.641076168573	-3.135584113650
H	-0.460913687408	3.615653441306	-2.923621321595

o-2-(OMe)₂

V	-1.186093570136	0.936007112449	1.680729216528
V	-1.307802749116	-1.855431846250	-0.097147348042
V	-1.196400159743	1.046978945123	-1.658471621624
V	1.208201188864	1.951219519861	0.025252878981
V	1.219073358227	-0.936819891621	1.625030712855
V	1.206519656923	-0.842306805008	-1.740544437910
O	-2.209674418194	1.519531522686	2.738779602623
O	-2.278876312968	-3.101248827444	-0.063540590171
O	-2.228772139723	1.660001717460	-2.692001320857
O	2.232246177844	3.156295410439	0.047378597157
O	2.207514710703	-1.648125604680	2.637759606491
O	2.196057807820	-1.518242402981	-2.779033252434
O	-2.232399025888	-0.795274790462	1.292146498011
O	-2.190104859797	1.490595211194	0.015380307786
O	0.019083400499	2.237691289850	1.342909574387
O	0.000838841355	-0.101598919656	2.616820292937
O	-2.264145703359	-0.746473145777	-1.345749786699
O	0.024061564398	2.296929980304	-1.315897906538
O	2.225519742181	0.721804734978	1.296454066802
O	-0.060460137480	-2.417904721842	1.285650074600
O	0.005275861060	-2.403115103496	-1.380517479532
O	-0.050000330907	-0.014346283460	-2.655527365735
O	2.216252529037	0.780132414773	-1.338633015246
O	2.157454552543	-1.522487690337	-0.066534068289
O	-0.023315262516	-0.106905466710	-0.031900644556

O	-6.159389800429	-1.066262293020	0.017705253166
O	-6.196223863985	1.096700790437	0.048861449027
O	6.135573661759	1.025985713511	-0.027473138443
O	6.165493472217	-1.135985435771	-0.084579716279
N	-5.622465083816	0.025749557655	0.023240075328
N	5.594399425985	-0.063954090818	-0.051835641446
C	-3.644210769191	-0.742961393904	1.245107128594
H	-4.019794261165	-0.247162022004	2.154336012695
H	-4.047679652087	-1.768344211964	1.213565385517
C	-3.610054350264	1.477160717459	0.025876075903
H	-3.982398907674	2.028293771904	-0.851052244610
H	-3.965260788986	1.987141396099	0.934274836003
C	-3.677181787788	-0.684556814057	-1.291690343560
H	-4.092487337841	-1.705285625736	-1.309750479944
H	-4.048678066514	-0.137013508523	-2.172229876109
C	-4.101312020929	0.032100595220	-0.000561216336
C	3.629861687780	0.727236169860	-1.283936512267
H	4.026570826929	1.753116826371	-1.237292283020
H	4.009786800464	0.243304537103	-2.198592630949
C	3.575117142881	-1.505951875601	-0.074167683612
H	3.940360524466	-2.014548545446	-0.980186006560
H	3.952529068707	-2.054706294341	0.802986975033
C	3.639485809891	0.668487251622	1.234894096454
H	4.018911912544	0.138113831410	2.123786341442
H	4.041414859712	1.693387393079	1.239206786684
C	4.072109699198	-0.061331372636	-0.043777870986

C	-0.375327673345	-3.370167618187	2.292250648682
H	-1.023851867517	-2.911824049295	3.055829575329
H	-0.893710660761	-4.225572772571	1.838599011504
H	0.550918444337	-3.716150159941	2.770014825707
C	0.461424378356	-3.746742215961	-1.464571555069
H	1.010516516405	-3.886667728756	-2.404575392421
H	1.127965472843	-3.966530243738	-0.615189700878
H	-0.399006533804	-4.428916638854	-1.433628776102

m-2-(OMe)₂

V	-1.251551902925	0.841784051832	1.670579328422
V	-1.205430407247	-1.931561755665	-0.119877728555
V	-1.202810353148	0.965866756200	-1.693502913035
V	1.205415442179	1.931763317283	-0.120214162199
V	1.251251116579	-0.841256702680	1.670678981448
V	1.202868459208	-0.966076190604	-1.693584453781
O	-2.235656543219	1.527369222521	2.703109249851
O	-2.208201439225	-3.153227100782	-0.041130325200
O	-2.238860645543	1.554605520266	-2.735856259463
O	2.208145144466	3.153452686584	-0.041591140242
O	2.235437734114	-1.526611354582	2.703272050320
O	2.238715816088	-1.555139246851	-2.735924700380
O	-2.234470357751	-0.788266072070	1.311699106425
O	-2.184574211443	1.484135686382	-0.003931607262
O	0.036345427821	2.326693678162	1.378411411023
O	-0.000123358605	0.000293214736	2.664591885753
O	-2.222447099970	-0.772474742465	-1.331887503465
O	-0.008009712743	2.318707646323	-1.332338368236
O	2.234218249355	0.788716638788	1.311529679673
O	-0.036580670756	-2.326324638332	1.378881950848
O	0.007960702636	-2.318661751054	-1.331965404403
O	0.000085642207	-0.000077106188	-2.633897837747
O	2.222319972237	0.772430395970	-1.332051873817
O	2.184306523488	-1.483845243729	-0.003713705029
O	-0.000283535157	0.000131979809	0.033641470751

O	-6.136843739389	-1.103342254037	-0.034297216084
O	-6.190713517761	1.058787932354	0.000229591212
O	6.136645522204	1.103521987323	-0.033908965974
O	6.190540177986	-1.058603261687	0.000038160396
N	-5.607805379848	-0.007436038867	-0.016236841889
N	5.607624657414	0.007613850435	-0.016129507462
C	-3.646721111073	-0.755848003458	1.245715565624
H	-4.044544385558	-0.258329348114	2.146110992440
H	-4.030394939671	-1.787559622480	1.213330921726
C	-3.604586442000	1.455672588679	-0.003597365765
H	-3.978487156404	1.988087752818	-0.891281230683
H	-3.977274068924	1.976144457590	0.892336859003
C	-3.635913140310	-0.734571184406	-1.280026046093
H	-4.027632540285	-1.764042101206	-1.273100491107
H	-4.014908015745	-0.218317405673	-2.176860714968
C	-4.086075938469	0.005914238119	-0.013443030254
C	3.635810989212	0.734518637697	-1.280145814543
H	4.027540248064	1.763987677162	-1.273410982986
H	4.014818758194	0.218083770335	-2.176866945688
C	3.604337460322	-1.455473104066	-0.003317421288
H	3.978233355394	-1.988059973296	-0.890895991207
H	3.976942431757	-1.975828305544	0.892717424677
C	3.646482695762	0.756255629034	1.245582378860
H	4.044242581197	0.258903743528	2.146097250595
H	4.030160796871	1.787959128712	1.213036951888
C	4.085894300509	-0.005737271298	-0.013391590097

C	-0.398926923189	-3.162329752376	2.472216483232
H	-0.945930576244	-2.581378544305	3.230527809719
H	-1.031434780545	-3.983898251183	2.112653172540
H	0.511804336700	-3.575992907066	2.926610913874
C	0.398745606995	3.162823261844	2.471660743419
H	0.945576961126	2.581894955983	3.230114070828
H	1.031425086412	3.984226842887	2.112027167374
H	-0.511959303352	3.576710984705	2.925905566979

TS1 (2 → 2-OMe)

V	-2.434286577993	-0.429265542457	1.820823032657
V	-0.037653650204	-1.794856692935	-0.071318809820
V	-2.758313644154	-0.429895272226	-1.521854270206
V	-2.357530250254	2.099941273092	0.131129752174
V	0.368591281591	0.745987665309	1.551142305378
V	0.011029307384	0.757821814165	-1.809478784773
O	-3.352446289542	-1.087777641784	2.947708784749
O	0.549537712854	-3.276152994257	-0.140910337308
O	-3.869663256566	-1.095119973062	-2.455092777428
O	-2.918217961034	3.593359404830	0.173133782473
O	1.473692873652	1.405949149740	2.492518672272
O	0.971061586539	1.394464354048	-2.916672117876
O	-1.412362213795	-2.147464925541	1.365760610814
O	-3.550122150821	-1.078340895427	0.234665469528
O	-3.104807684118	1.229611018472	1.522316912630
O	-0.941669358968	0.154086049460	2.654861303458
O	-1.650411665296	-2.134126418613	-1.261296536302
O	-3.336868920680	1.228234227833	-1.136567721972
O	-0.720692869731	2.445914172788	1.280440904953
O	0.972979227069	-0.925523479441	1.137656909164
O	0.760328698577	-0.917135003352	-1.507686221347
O	-1.429442427856	0.139121566416	-2.654109120474
O	-0.966889357489	2.454653716718	-1.346570380896
O	1.173330085432	1.375285260676	-0.209482275174
O	-1.183844576353	0.149015598038	-0.003678870553

C	-2.098764259211	-3.369959211431	1.369836455572
H	-2.670031048084	-3.472441395354	2.307267699842
H	-1.375940146584	-4.202528597180	1.306595628337
C	-4.140338485554	-2.347693887032	0.290696570272
H	-4.863781842996	-2.459631475644	-0.536106941266
H	-4.679274009372	-2.467658016174	1.245484603344
C	-2.323932669259	-3.366014400956	-1.153674064428
H	-1.597257597648	-4.192585425999	-1.223368092773
H	-3.038545706232	-3.468565115100	-1.986694232056
C	-3.065703988389	-3.440933159304	0.178251236324
C	-0.272297871714	3.671991806053	-1.354257205924
H	-0.990248292649	4.508267895439	-1.287877487470
H	0.295211499786	3.772187941784	-2.294446760418
C	1.770388083005	2.639749820279	-0.270392879375
H	2.315435429309	2.752410101408	-1.223749752494
H	2.490022038804	2.758629426117	0.558773983001
C	-0.040517599654	3.674143410870	1.165809585668
H	0.675014607202	3.774391680956	1.998184849436
H	-0.764229754348	4.503134816549	1.234215144956
C	0.699863063270	3.739693315812	-0.167011902045
C	2.722092533998	-0.989495976573	-1.524370187945
H	2.709786503126	-0.524985786661	-0.543830754467
H	2.737798067613	-0.373810201680	-2.418775609132
H	2.707164330229	-2.071338513655	-1.615283726927
O	4.694693199890	-0.967955292954	-1.578091546730
S	5.398902939354	-1.392685100268	-0.305551039375

O	4.616184427293	-2.303294576740	0.531868949392
O	6.812054809742	-1.684936767900	-0.533328443211
C	5.417787847137	0.194163408420	0.656686344827
F	4.170927869918	0.627559490320	0.876116354653
F	6.076919775607	1.144048792854	-0.004072481448
F	6.009255208828	0.012744909519	1.836178875190
O	1.365024453817	5.830149508376	0.679420058387
O	2.037495741039	5.277206840864	-1.298847344431
O	-4.407362723927	-4.983827917397	1.298785485174
O	-3.705128553359	-5.539673522992	-0.668221508044
N	1.425278040465	5.063533475024	-0.265613663026
N	-3.783840768696	-4.769759612140	0.272469582490

TS2 (2-OMe → p-2-(OMe)₂)

V	2.338483504726	0.260674652694	-1.684525065950
V	0.486406058268	-1.787987130114	0.073222082537
V	2.519123868875	0.341797175855	1.675066218157
V	1.325200032432	2.678827009815	0.161278793672
V	-0.685669213059	0.549723937727	-1.518213688849
V	-0.519250266028	0.553545553289	1.837432153978
O	3.486910883675	0.091293881652	-2.767536701999
O	0.398197318668	-3.371769957837	0.072578335930
O	3.735845461651	0.055492995112	2.655406053791
O	1.386638327506	4.263701274211	0.098861640550
O	-1.891734540776	0.824387999738	-2.512892689434
O	-1.670261082304	0.785710348912	2.907092121230
O	1.981449032957	-1.635687672327	-1.315224481267
O	3.538926570461	0.074747074785	-0.046314996551
O	2.443398411930	2.222604115582	-1.364595621209
O	0.837378156179	0.479268874667	-2.581532928299
O	2.060630210251	-1.608798329824	1.319948484534
O	2.534908480495	2.147557101145	1.344365190415
O	-0.220195948162	2.499993248863	-1.171141353394
O	-0.661330875883	-1.233931069046	-1.207429530425
O	-0.640281084215	-1.254258949817	1.441976861270
O	1.026748245702	0.434467031182	2.724102885764
O	-0.144917847387	2.511711737185	1.470761183542
O	-1.712702246922	0.821488594937	0.187527450104
O	0.946217102770	0.470375217977	0.066573557956

C	3.047824628787	-2.560335308306	-1.285068772133
H	3.649203629365	-2.452523602012	-2.203378412339
H	2.639086344598	-3.582426742863	-1.246945690292
C	4.553088913551	-0.912115236149	-0.082374461700
H	5.222372448447	-0.780345199683	0.782053469908
H	5.149417061594	-0.788239067763	-1.000416953398
C	3.116386727605	-2.539611474453	1.236960527019
H	2.708880858421	-3.563221735477	1.231300553806
H	3.774124370205	-2.428300072938	2.114952192540
C	3.921673579680	-2.302769425703	-0.049768288026
C	-1.215591066869	3.440167748496	1.451769337338
H	-0.802081000999	4.460703794217	1.448047899219
H	-1.815736977001	3.311497276900	2.366018886497
C	-2.715520566103	1.810564865206	0.221783390098
H	-3.326964226032	1.683315079755	1.132108532359
H	-3.371770950064	1.704761028456	-0.656312976388
C	-1.275902819143	3.426845910996	-1.084830067958
H	-1.949575786194	3.306148565706	-1.948632546388
H	-0.870807520648	4.453195642961	-1.099537683069
C	-2.073182490547	3.205882388603	0.212074220244
C	-2.412007054035	-2.056394438554	1.447430811642
H	-2.862125080048	-1.069716426867	1.476617614417
H	-2.197805164428	-2.580075971207	2.374279139098
H	-2.214961954734	-2.542024708302	0.496225882553
O	-4.249499837714	-2.831760499472	1.451398368318
S	-4.745906627290	-3.312023927759	0.102703942108

O	-3.685883138395	-3.831734920752	-0.766645294239
O	-5.993903986387	-4.061287772632	0.215232922539
C	-5.237534811174	-1.718795576679	-0.711646756847
F	-4.177034701256	-0.913455109323	-0.840799199881
F	-6.158933813552	-1.081230319918	0.007253607589
F	-5.733316282714	-1.953044915764	-1.924551652318
C	2.573260830007	3.076680534664	-2.490818988211
H	1.662071936253	3.037917341417	-3.108818409128
H	2.739644202661	4.108197835056	-2.152431786625
H	3.429526449268	2.751156380153	-3.097826422718
O	-3.999493196333	4.138328008838	-0.714030762688
O	-3.247109518605	5.038078231707	1.102426636596
O	4.670867298332	-4.510974791966	-0.046641091652
O	6.178657472562	-2.962325465962	-0.110671235029
N	-3.204354315701	4.216875329872	0.205281242969
N	5.025233790381	-3.345955534874	-0.072068139181

TS2 (2-OMe → o-2-(OMe)₂)

V	-2.395165411536	-0.309746188250	1.955037557855
V	-0.029910709307	-1.772797642729	0.122046013004
V	-2.804755780075	-0.498444852625	-1.312691527432
V	-2.311390866421	2.135316443294	0.112517416255
V	0.412183638189	0.873190265139	1.598574036728
V	0.116755789366	0.718131317001	-1.693432532038
O	-3.303735533227	-0.877706551407	3.125140633134
O	0.568733859814	-3.243125027176	0.123006359467
O	-3.849613425252	-1.209065578356	-2.276559366227
O	-2.880073315826	3.617814024070	0.065401214812
O	1.526049928550	1.563108986422	2.492869937153
O	1.010226027207	1.255423799481	-2.888794485993
O	-1.386850227846	-2.031552422729	1.569951319989
O	-3.540301606996	-1.058882132875	0.405342824898
O	-3.068018599670	1.324869158799	1.519153726617
O	-0.899286130870	0.339198794283	2.718968039520
O	-1.634124353092	-2.173535878584	-1.044245154899
O	-3.298183775769	1.181272542633	-1.135159169956
O	-0.671619364569	2.541956625343	1.209798711551
O	0.998650999973	-0.813631990018	1.237775787044
O	0.782853087488	-0.961718112047	-1.395359767490
O	-1.403758239943	-0.044680207542	-2.640861766476
O	-0.926627736234	2.390905916525	-1.399747790854
O	1.223446515084	1.412496518544	-0.217380364287
O	-1.158594613055	0.178122194613	0.021788584212

C	-2.058419512404	-3.268735599139	1.653869938738
H	-2.606275841179	-3.323961978464	2.609228801373
H	-1.322481922980	-4.088156078520	1.622153763810
C	-4.128409040994	-2.341785706598	0.537929851567
H	-4.856170874632	-2.489100858401	-0.275796964666
H	-4.665957423411	-2.388971076125	1.497499124728
C	-2.295197741448	-3.403292946515	-0.863406104774
H	-1.563846552427	-4.227573425760	-0.876584897839
H	-3.014176316870	-3.562376104029	-1.685320600430
C	-3.040928561298	-3.410415271412	0.481795630505
C	-0.251302096322	3.624709737678	-1.489460469694
H	-0.981300268625	4.448822854252	-1.454310616106
H	0.295241430828	3.680984921580	-2.446365467994
C	1.821421940426	2.690477092202	-0.352227378324
H	2.377360927340	2.728685469431	-1.303261766706
H	2.534336270222	2.842351244410	0.472731151377
C	-0.006962327940	3.771568007977	1.023024737101
H	0.709630665729	3.929565015994	1.846249747869
H	-0.741333603272	4.592347594899	1.034427416429
C	0.737676509849	3.765152845587	-0.320023582339
C	2.689079104590	-1.114783759580	-1.440690786037
H	2.742226916061	-0.522444150202	-0.533032508114
H	2.751037887004	-0.632719019574	-2.412240452771
H	2.664601305369	-2.198943511477	-1.382205111614
O	4.711092735024	-1.164034046482	-1.486197849266
S	5.383630856620	-1.482179310926	-0.169417982058

O	4.563455359744	-2.285980905667	0.739307765918
O	6.791931798362	-1.833748128543	-0.339236111368
C	5.438099744305	0.187652439496	0.641806547218
F	4.200122439652	0.671815257669	0.817453529629
F	6.119536277609	1.056244015618	-0.102338388417
F	6.021879144020	0.104146515925	1.835542928626
C	-1.198090776593	-0.806881066538	-3.819504963463
H	-0.704058548787	-1.760500116656	-3.573476533864
H	-2.165111676432	-1.010078406992	-4.298553298045
H	-0.558886498727	-0.243390812514	-4.513597704180
O	-4.897918715618	-4.825347191804	0.762312279392
O	-2.947164105473	-5.738876139104	0.572414817306
O	0.661874043105	6.094729634604	-0.401435378526
O	2.600050796423	5.166328352304	-0.640882367034
N	-3.690717456479	-4.775417826428	0.617678907752
N	1.396658443641	5.125791756016	-0.466776932298

TS2 (2-OMe → m-2-(OMe)₂)

V	-2.335250671016	-0.610899057273	1.883408710920
V	0.104935916155	-1.818550241049	-0.022306077835
V	-2.594835998505	-0.581918356605	-1.473909343877
V	-2.291288370676	2.021440008457	0.389414127598
V	0.444535158503	0.691985599164	1.672851001854
V	0.058465687932	0.834044104846	-1.669629835368
O	-3.225356975308	-1.331819525224	2.983590350131
O	0.753643640381	-3.258870822278	-0.167894438450
O	-3.736572802524	-1.149333162558	-2.418967500523
O	-2.938503623871	3.470760834968	0.421482429028
O	1.523657988077	1.329438915915	2.644728811552
O	0.986994575219	1.528399503847	-2.755775127291
O	-1.268957581670	-2.261852840483	1.351175747762
O	-3.413043419385	-1.212271750275	0.265928596417
O	-3.070420674303	1.061804593084	1.648231656859
O	-0.867997170084	0.015255846448	2.724309488853
O	-1.514511039252	-2.196757392070	-1.274921443810
O	-3.342088978353	1.209256130300	-1.044332449814
O	-0.702148824777	2.382726070484	1.484001045775
O	1.083414307137	-0.946491960049	1.184596626198
O	0.815823658420	-0.842684995449	-1.456121875195
O	-1.404758961205	0.197331489411	-2.555216577864
O	-0.972683054682	2.461946114863	-1.141703438903
O	1.192203748727	1.411352743789	-0.063192667602
O	-1.153048029757	0.112519708319	0.072984912134

C	-1.916723487610	-3.514308752590	1.323944339156
H	-2.456763477212	-3.665249061034	2.273162164822
H	-1.167031941955	-4.314023404260	1.213244337214
C	-3.995457989652	-2.502995431754	0.281168048638
H	-4.712080349110	-2.590481368744	-0.551081665466
H	-4.546003766045	-2.643671125753	1.224240190280
C	-2.152503798684	-3.452571372322	-1.187593322029
H	-1.395751607494	-4.249748364859	-1.255632365286
H	-2.859176916035	-3.564401230797	-2.027421438073
C	-2.903289322917	-3.563011611521	0.147554468759
C	-0.318819038214	3.708495644894	-1.115547776298
H	-1.066095798962	4.513736748228	-1.012515971235
H	0.231621204968	3.860614916980	-2.058099197405
C	1.763473063115	2.699435839386	-0.080962712986
H	2.303212938360	2.850551722041	-1.030316855239
H	2.481880289881	2.799520394568	0.749731814407
C	-0.055888991279	3.641686334427	1.404454068914
H	0.660725122600	3.727432875334	2.235867765068
H	-0.808416406839	4.438861592497	1.510962227641
C	0.664186862850	3.763317710678	0.064452573776
C	2.726270256460	-0.941621230619	-1.610255093224
H	2.814562561888	-0.364208712868	-0.696097993595
H	2.716204414296	-0.438249879555	-2.572700167141
H	2.728618614374	-2.026759257941	-1.572601076805
O	4.738105047991	-0.953695758157	-1.764606050610
S	5.459010291192	-1.388353220101	-0.507611886197

O	4.655139265362	-2.240327329135	0.371763366845
O	6.849197745472	-1.757907505623	-0.764096759236
C	5.587546881971	0.213184244951	0.422155999460
F	4.369090083703	0.720283171979	0.659548615059
F	6.280811747336	1.112643261337	-0.272318207318
F	6.192211681483	0.024943544354	1.593141876461
C	-3.921237712685	1.971790839378	-2.091371651565
H	-4.677927666248	1.365333474327	-2.608628666443
H	-4.398833307463	2.868026055444	-1.673156911428
H	-3.150411072089	2.274685965043	-2.817869912410
O	1.229067204579	5.865742777756	0.951520902741
O	1.981074767184	5.358661152683	-1.011389448661
O	-4.753299795552	-5.008572748788	0.300624971090
O	-2.794378601829	-5.890765425821	0.055716555301
N	1.349585888257	5.115402044429	0.001268582970
N	-3.546188160630	-4.939460799055	0.170246021499

Table X1. Cartesian coordinates for the monoreduced **1**, **1-OMe**, and **1-(OMe)₂** species at M06-L/def2-TZVP,def2-SVP level of theory.

1

V	-1.689034821494	0.975268933078	-1.175668088161
V	-0.000711883189	-1.949779335237	-1.174213316835
V	1.688779548891	0.974456837506	-1.176485828697
V	0.000242263579	1.950048035054	1.174245737051
V	-1.689218934715	-0.973678493974	1.176185772501
V	1.690061312747	-0.975238762307	1.176541832065
O	-2.750909066682	1.587253204267	-2.228181477907
O	-0.001106559241	-3.176306712860	-2.225228386433
O	2.751827231530	1.584615401577	-2.228678812033
O	0.001167001638	3.176143973380	2.225877915547
O	-2.751352688799	-1.584120538029	2.229256708955
O	2.752751952889	-1.588054121121	2.227446081725
O	-1.336199963125	-0.771236779939	-2.209229878233
O	0.000271308639	1.539943902757	-2.208515127615
O	-1.335551034297	2.314396787704	-0.000877274895
O	-2.671116155511	0.000314864379	-0.000059900743
O	1.334532970172	-0.771662933395	-2.208580842545
O	1.334790344123	2.313535531750	-0.001991932295
O	-1.334696178958	0.771928054607	2.208968157143
O	-1.335344067419	-2.313064401417	0.001973122500
O	1.334664242107	-2.313292479058	0.001139320947
O	2.669927706435	0.000044741260	0.000482661106

O	1.336301835530	0.770903246709	2.208991926656
O	0.000098378960	-1.539405966665	2.207789843628
O	-0.001570057428	0.001002887420	-0.000136675365
C	-1.248347089857	-0.721200214414	-3.604636309129
H	-2.146840250071	-0.209346354615	-4.006159023771
H	-1.253530484069	-1.755641523063	-4.005272685974
C	-0.000114488196	1.440692367298	-3.603906044530
H	0.892430288938	1.963286211388	-4.004920970681
H	-0.893194548832	1.962932438133	-4.004149179517
C	1.247756879719	-0.721363070420	-3.604152208603
H	1.253124938853	-1.755679211041	-4.004995762352
H	2.146596102866	-0.209456134915	-4.004877133714
C	-0.000107669694	-0.000253089004	-4.114594047734
C	1.248314774403	0.721089612436	3.604461363651
H	1.253436546495	1.755607325066	4.004855179563
H	2.146840569373	0.209416765359	4.006176805661
C	0.000156986580	-1.440625525258	3.603298493932
H	0.893122610123	-1.963023899990	4.003624600478
H	-0.892469432640	-1.963359603188	4.003904319015
C	-1.247825383908	0.721391015337	3.604486455675
H	-2.146613050777	0.209430139497	4.005253412069
H	-1.253057788810	1.755617331305	4.005564630435
C	0.000135410774	0.000117704896	4.114477519092
C	-0.000215723259	-0.001778099611	5.633176783024
H	0.886631149828	-0.515200754905	6.036171695397
H	-0.000044415152	1.022095878411	6.038311524825

H	-0.887852751896	-0.514464477022	6.035436516875
C	0.000557210299	0.001199551090	-5.633298784524
H	0.000485993870	-1.022786976548	-6.038146113524
H	-0.886230969283	0.514483611635	-6.036601407432
H	0.888249897943	0.513803094695	-6.035541166273

1-OMe

V	-1.612181029469	1.034078565102	-1.166553702991
V	-0.135308179073	-1.946984537766	-1.186433916069
V	1.735767472752	0.837933070224	-1.186105766068
V	0.115326327336	1.950083964092	1.204661680870
V	-1.695921562143	-0.894548612913	1.204926878375
V	1.675398348918	-0.943218687932	1.296618619215
O	-2.672330884788	1.621711968570	-2.219024395230
O	-0.095190789559	-3.185175365708	-2.206762103901
O	2.805731446724	1.444028627906	-2.222074924377
O	0.088291615266	3.194640298446	2.218685095221
O	-2.756698436922	-1.494900233235	2.249794219316
O	2.722277052733	-1.654545439400	2.286023468814
O	-1.344227954637	-0.796445692922	-2.201480593785
O	0.034331381255	1.474048128246	-2.196756718727
O	-1.297990396656	2.295992297120	0.006548160319
O	-2.636215876481	-0.015327203088	-0.013142132470
O	1.313868941582	-0.873018420129	-2.186146969022
O	1.370634646560	2.253325950993	0.039816837777
O	-1.303690574774	0.785334997629	2.198688145218
O	-1.321326267237	-2.331443155115	0.043976157817
O	1.379728109535	-2.456202901077	-0.035932960928
O	2.673817756412	-0.081388662996	0.051020449654
O	1.360007463321	0.778046550521	2.300184546590
O	-0.033603340087	-1.533020626809	2.231975917678
O	0.025993001747	-0.071955978508	0.020148910154

C	-1.263453451851	-0.752203876208	-3.608358114650
H	-2.148751793147	-0.211617653447	-3.991062986031
H	-1.305465229798	-1.786729549291	-3.999804157551
C	0.040036276386	1.375743055244	-3.601648379888
H	0.949626883609	1.876333899264	-3.983540686998
H	-0.834928039315	1.921530993763	-4.003757696510
C	1.235821355360	-0.824050204406	-3.590259854930
H	1.214347018018	-1.859686148868	-3.982064757744
H	2.151084554069	-0.340779026948	-3.982427427912
C	0.009490368512	-0.068044365732	-4.104573430147
C	1.211722868426	0.712294187897	3.699346373250
H	1.214194736236	1.743245845008	4.102231629701
H	2.093564233777	0.191053571326	4.119169627269
C	-0.062911830727	-1.443463230895	3.636826631924
H	0.816726685321	-1.974863564599	4.048713864216
H	-0.966771504516	-1.960764991327	4.011649513097
C	-1.275321861148	0.749120079488	3.607611747172
H	-2.203289633309	0.270503027358	3.973352449253
H	-1.263767138738	1.788432499534	3.986376426990
C	-0.061155172001	-0.001479158093	4.151845389687
C	2.523954207567	-3.051221319415	-0.586808145167
H	2.237742677333	-3.876664970761	-1.258896147941
H	3.119507892002	-2.323122406877	-1.163633992455
H	3.158632481088	-3.456933922225	0.217771407841
C	-0.115646836789	-0.011281591395	5.670352679410
H	-0.116753256301	1.010589862142	6.078396927898

H	-1.023398578611	-0.514768971431	6.034971076749
H	0.750333998129	-0.538173590945	6.098368953475
C	0.017882883147	-0.070800686853	-5.624015436271
H	-0.855134553896	0.460824993007	-6.031156450931
H	0.919448189918	0.421045369907	-6.018730464436
H	-0.002307461063	-1.095952145474	-6.022978541822

p-1-(OMe)₂

V	-1.639319024549	0.939133601603	-1.287219262513
V	-0.171606413734	-1.949702956459	-1.206703989272
V	1.703990287922	0.825197936202	-1.210303503915
V	0.171606413785	1.949702956459	1.206703989375
V	-1.703990287871	-0.825197936202	1.210303504018
V	1.639319024601	-0.939133601603	1.287219262617
O	-2.654830132382	1.642492968122	-2.295978372258
O	-0.157840077476	-3.207412135912	-2.190029014282
O	2.799820877652	1.375900690231	-2.234245562167
O	0.157840077528	3.207412135912	2.190029014385
O	-2.799820877600	-1.375900690231	2.234245562271
O	2.654830132434	-1.642492968122	2.295978372362
O	-1.381099779481	-0.777456035183	-2.282589520465
O	0.065459439783	1.462973953708	-2.207359821648
O	-1.307625289010	2.453669426159	-0.003027908826
O	-2.638695545965	0.131049252070	-0.061552133088
O	1.277223972716	-0.885687046633	-2.169990517424
O	1.400340352820	2.235025783789	0.001843632522
O	-1.277223972665	0.885687046633	2.169990517527
O	-1.400340352768	-2.235025783789	-0.001843632418
O	1.307625289062	-2.453669426159	0.003027908930
O	2.638695546017	-0.131049252070	0.061552133192
O	1.381099779532	0.777456035183	2.282589520568
O	-0.065459439731	-1.462973953708	2.207359821752
O	0.000000000026	0.000000000000	0.000000000052

C	-1.234331061118	-0.726826991603	-3.692813668242
H	-2.100209535953	-0.180073930419	-4.106734619980
H	-1.271409090681	-1.761480527242	-4.077779941885
C	0.102215003315	1.387403883694	-3.624968976570
H	1.021496708573	1.885286294184	-3.979416294097
H	-0.761003255735	1.943666031628	-4.031385416895
C	1.255096599898	-0.847511895701	-3.586706952797
H	1.212919090689	-1.884600137612	-3.965811466679
H	2.199072403209	-0.397758197035	-3.942169456550
C	0.065224412249	-0.056273738437	-4.132145715149
C	1.234331061170	0.726826991603	3.692813668345
H	1.271409090733	1.761480527242	4.077779941989
H	2.100209536005	0.180073930419	4.106734620083
C	-0.102215003263	-1.387403883694	3.624968976674
H	0.761003255787	-1.943666031628	4.031385416998
H	-1.021496708521	-1.885286294184	3.979416294201
C	-1.255096599846	0.847511895701	3.586706952901
H	-2.199072403157	0.397758197035	3.942169456654
H	-1.212919090637	1.884600137612	3.965811466783
C	-0.065224412197	0.056273738437	4.132145715252
C	2.450860245511	-3.089777992887	-0.524841825752
H	2.148143698866	-3.956472933456	-1.131894106945
H	3.034897235839	-2.400639645441	-1.157449505911
H	3.093171003061	-3.439209349181	0.297864784686
C	-2.450860245459	3.089777992887	0.524841825855
H	-3.034897235787	2.400639645441	1.157449506014

H	-2.148143698814	3.956472933456	1.131894107049
H	-3.093171003009	3.439209349181	-0.297864784582
C	-0.125992481790	0.048419587201	5.651544185943
H	0.721891861955	-0.504803513250	6.080544653950
H	-0.097276500803	1.070676907358	6.055454792203
H	-1.050978855236	-0.426893855337	6.008340764025
C	0.125992481842	-0.048419587201	-5.651544185840
H	0.097276500855	-1.070676907358	-6.055454792099
H	-0.721891861903	0.504803513250	-6.080544653847
H	1.050978855288	0.426893855337	-6.008340763922

o-1-(OMe)₂

V	-1.641211715172	1.008760746429	-1.232720131741
V	-0.062410760197	-1.885107938898	-1.344647517133
V	1.728685604405	0.859044953061	-1.197414306748
V	0.050827114692	1.919069950279	1.175846291913
V	-1.751150302383	-0.877103725270	1.181021558340
V	1.592164934346	-0.993799576205	1.245383659187
O	-2.684649501871	1.648854173427	-2.255350465809
O	-0.073530182790	-3.190986789504	-2.265963682181
O	2.795486831309	1.488534600795	-2.204981719610
O	0.049165911994	3.143103430192	2.199440753648
O	-2.799619459255	-1.519624969313	2.201528331616
O	2.637742569091	-1.680788431502	2.234341574076
O	-1.367749476502	-0.742510435284	-2.290574457357
O	0.029778104806	1.490413495411	-2.189368688410
O	-1.327069603026	2.249494978288	0.002004273124
O	-2.661507496087	-0.044484584714	-0.070834606480
O	1.342461128314	-0.808071474632	-2.291565443607
O	1.332974655370	2.222991050653	0.004111150434
O	-1.347361105406	0.758065680129	2.181690594507
O	-1.419188326755	-2.438550612822	0.044973307968
O	1.319437538858	-2.435201843683	-0.028420230846
O	2.630437567980	-0.093929179575	-0.008530118297
O	1.295925094588	0.715177414009	2.222165632487
O	-0.082159418539	-1.558370655257	2.195486082237
O	-0.020679379376	-0.142959489897	-0.024586303456

C	-1.269145958803	-0.654232195988	-3.701513211668
H	-2.155565657504	-0.114892058644	-4.080592359767
H	-1.297116278497	-1.677236719619	-4.119768820334
C	0.037445077599	1.475603264233	-3.606941525912
H	0.949186604018	1.992837628432	-3.954452663556
H	-0.834501925471	2.047793390021	-3.970888748482
C	1.240962183442	-0.706254222990	-3.699621569687
H	1.228524472115	-1.729151445045	-4.119730721560
H	2.148267385954	-0.202351031068	-4.079100616600
C	0.002029096422	0.056328031408	-4.169778214670
C	1.197060787460	0.669262696934	3.637115826686
H	1.221717145808	1.704313869365	4.020804383614
H	2.086274716673	0.142317999483	4.027322811704
C	-0.098164964234	-1.475109975840	3.607946684302
H	0.776540792864	-2.021610931085	4.005689891714
H	-1.006586471453	-1.982535487928	3.980156145817
C	-1.296565814556	0.720888969950	3.598111558874
H	-2.219288753598	0.238599024934	3.967822889887
H	-1.284277063225	1.760165209072	3.970792620520
C	-0.072875746365	-0.032377971443	4.116417506577
C	2.290309778542	-3.419296878933	-0.304518314574
H	1.814727934438	-4.297475621689	-0.765756077189
H	3.051919772526	-3.025919008662	-0.998553907427
H	2.791661661573	-3.727726702317	0.624557299523
C	-1.353298660762	-3.736462764610	0.585030459581
H	-0.467140565477	-3.853568809022	1.231674629492

H	-2.252934758087	-3.940980314368	1.185835463650
H	-1.293702668464	-4.475319391507	-0.228895258617
C	-0.094801585763	-0.035938102249	5.636238046110
H	-0.081175455606	0.987735195293	6.037491983667
H	-0.997878812484	-0.532968736823	6.018912705478
H	0.777344265151	-0.566750264120	6.044524239652
C	0.003745169574	0.119811749516	-5.688604419343
H	-0.873526839897	0.665179877320	-6.065577474027
H	0.901737023722	0.631072206168	-6.064718605776
H	-0.015278906026	-0.887986524294	-6.128396915523

m-1-(OMe)₂

V	-1.606851768366	1.107311786020	-1.197448598245
V	-0.252156551897	-1.905486126229	-1.174054262757
V	1.680117891546	0.831661437153	-1.163068793291
V	0.074846777850	1.935676502629	1.233448325492
V	-1.658431699957	-0.919252127317	1.327734753833
V	1.633997342131	-0.966100777392	1.308002002149
O	-2.671315624625	1.720947268349	-2.214926135665
O	-0.246130164277	-3.149385030772	-2.179059717226
O	2.762989617438	1.385563555356	-2.196280085999
O	0.132254490429	3.177502094462	2.233760837977
O	-2.791745665205	-1.429323988525	2.331821115185
O	2.670911666810	-1.658893509518	2.299627703022
O	-1.440314137894	-0.700790584973	-2.187609301922
O	0.029468860021	1.512806445671	-2.197666467612
O	-1.289973062613	2.324724312019	0.021338631146
O	-2.799562955830	0.072651847392	-0.031802921443
O	1.213200555653	-0.850191522737	-2.136319135729
O	1.374025752503	2.193188953200	0.023080252273
O	-1.283467455207	0.838354557066	2.238000357116
O	-1.459619170999	-2.255017146740	0.071064456956
O	1.253436849275	-2.461473601932	0.041539191980
O	2.619630276850	-0.164989539241	0.066023049822
O	1.363825483208	0.737778636638	2.275133546841
O	-0.036290976502	-1.526825437144	2.293099018444
O	-0.058249917329	-0.047683491595	0.050512116394

C	-1.335890642019	-0.676745450264	-3.600606737908
H	-2.195054628454	-0.109512918623	-4.001646773939
H	-1.412844438961	-1.713916020420	-3.973873346115
C	0.045965426652	1.402161349412	-3.611285865376
H	0.973746857507	1.872300041392	-3.981436809673
H	-0.808506900507	1.974952610163	-4.014704498631
C	1.167514740290	-0.833653676606	-3.552995187644
H	1.120094764564	-1.876874176493	-3.913350587577
H	2.103725509953	-0.387643460459	-3.933446782373
C	-0.031127301440	-0.047090555997	-4.087900290741
C	1.266126424489	0.716161346260	3.689850131393
H	1.306012153515	1.757933625969	4.053421800387
H	2.148065209316	0.184147159425	4.089726426652
C	-0.045094691215	-1.411986403187	3.710110095469
H	0.832982336431	-1.949806826931	4.108710526958
H	-0.951277820839	-1.912842608974	4.093389112143
C	-1.229561354665	0.810207583872	3.656182387691
H	-2.157394780872	0.345313384652	4.033269548417
H	-1.197587838669	1.849305359969	4.028785806534
C	-0.013614297510	0.042985110714	4.181445860713
C	2.373891372175	-3.113393325459	-0.512741418955
H	2.043314496718	-3.961254486524	-1.131771770824
H	2.968030276189	-2.428032612017	-1.140713640961
H	3.020844387006	-3.495607625826	0.292270879225
C	-3.918453891803	-0.604761439697	-0.556149320964
H	-4.479692973446	0.060273719114	-1.230206596033

H	-3.616137354798	-1.503424196285	-1.118641481286
H	-4.580013527014	-0.915027059522	0.267247663818
C	-0.032016482732	0.066334106295	5.702036347842
H	0.832601135035	-0.470401784078	6.118237589185
H	-0.000849870259	1.097145693278	6.083188543926
H	-0.942208315166	-0.408958760449	6.095087538907
C	-0.005496674638	-0.071055264937	-5.607762370424
H	-0.855805242793	0.484814827362	-6.028607888186
H	0.916776761368	0.383796777852	-5.997006799205
H	-0.057655276422	-1.100959774821	-5.989337701186

Cartesian coordinates for the monoreduced **2**, **2-OMe**, and **2-(OMe)₂** species at M06-L/def2-TZVP,def2-SVP level of theory.

2

V	-1.162072149314	0.990618890234	1.694808487686
V	-1.180949620207	-1.949095961351	0.000000000000
V	-1.162072149314	0.990618890234	-1.694808487686
V	1.180949620207	1.949095961351	0.000000000000
V	1.162072149314	-0.990618890234	1.694808487686
V	1.162072149314	-0.990618890234	-1.694808487686
O	-2.216022340299	1.602990752552	2.749053476516
O	-2.249141924501	-3.155035743176	0.000000000000
O	-2.216022340299	1.602990752552	-2.749053476516
O	2.249141924501	3.155035743176	0.000000000000
O	2.216022340299	-1.602990752552	2.749053476516
O	2.216022340299	-1.602990752552	-2.749053476516
O	-2.217141085033	-0.755407071011	1.335676532750
O	-2.195263976098	1.549258986694	0.000000000000
O	0.015393791300	2.318787688958	1.337396071734
O	0.000000000000	0.000000000000	2.670616902525
O	-2.217141085033	-0.755407071011	-1.335676532750
O	0.015393791300	2.318787688958	-1.337396071734
O	2.217141085033	0.755407071011	1.335676532750
O	-0.015393791300	-2.318787688958	1.337396071734
O	-0.015393791300	-2.318787688958	-1.337396071734
O	0.000000000000	0.000000000000	-2.670616902525

O	2.217141085033	0.755407071011	-1.335676532750
O	2.195263976098	-1.549258986694	0.000000000000
O	0.000000000000	0.000000000000	0.000000000000
O	-6.107622311219	-1.095515765517	0.000000000000
O	-6.184524234369	1.062790678818	0.000000000000
O	6.107622311219	1.095515765517	0.000000000000
O	6.184524234369	-1.062790678818	0.000000000000
N	-5.573455327410	0.004890723110	0.000000000000
N	5.573455327410	-0.004890723110	0.000000000000
C	-3.601225259324	-0.709862820086	1.263231657045
H	-4.014300216526	-0.190813218795	2.150494479921
H	-4.018739893926	-1.733170276942	1.237197234875
C	-3.588797613924	1.484048739691	0.000000000000
H	-3.989702263131	1.998920367763	-0.892420572185
H	-3.989702263131	1.998920367763	0.892420572185
C	-3.601225259324	-0.709862820086	-1.263231657045
H	-4.018739893926	-1.733170276942	-1.237197234875
H	-4.014300216526	-0.190813218795	-2.150494479921
C	-4.067725607958	0.035516628143	0.000000000000
C	3.601225259324	0.709862820086	-1.263231657045
H	4.018739893926	1.733170276942	-1.237197234875
H	4.014300216526	0.190813218795	-2.150494479921
C	3.588797613924	-1.484048739691	0.000000000000
H	3.989702263131	-1.998920367763	-0.892420572185
H	3.989702263131	-1.998920367763	0.892420572185
C	3.601225259324	0.709862820086	1.263231657045

H	4.014300216526	0.190813218795	2.150494479921
H	4.018739893926	1.733170276942	1.237197234875
C	4.067725607958	-0.035516628143	0.000000000000

2-OMe

V	-1.175426623832	0.852577739385	1.741336087909
V	-1.186258161084	-1.948129246418	-0.138869524973
V	-1.149736697871	1.048801265928	-1.621237267570
V	1.212653428809	1.949816018395	0.115039935623
V	1.277734789441	-0.961820825737	1.678464466299
V	1.194118564135	-0.911975939827	-1.705543521435
O	-2.213619142471	1.453960896143	2.805534906714
O	-2.230115560166	-3.161716944695	-0.104797003161
O	-2.200677187346	1.643240472712	-2.673427865500
O	2.240938502149	3.177822861888	0.100699626005
O	2.265853308244	-1.680785977504	2.715298563149
O	2.246859996735	-1.503410218285	-2.758278708338
O	-2.200134945203	-0.856105477994	1.306259680446
O	-2.183880136709	1.486010088976	0.031509825358
O	0.052052195534	2.247555050800	1.378742432546
O	0.041020024730	-0.091563343043	2.675762786575
O	-2.200837864882	-0.776463763652	-1.354692020975
O	0.025013719714	2.303633172488	-1.293425677057
O	2.301663476963	0.756092095264	1.364723170063
O	-0.061202528973	-2.456969231951	1.371478309693
O	0.031354906825	-2.337062600041	-1.336624171267
O	-0.001306568678	-0.006027815959	-2.641149259055
O	2.208512160517	0.775022071019	-1.298190535893
O	2.223669372366	-1.544091144188	-0.034830168681
O	0.020112237774	-0.078253196897	0.022244651049

O	-6.093201557542	-1.166089502033	-0.042975041177
O	-6.172925263461	0.991722141507	0.039543952686
O	6.147861729989	1.090005411630	-0.132780523986
O	6.217514753529	-1.068764925307	-0.080745777295
N	-5.566263951955	-0.065170796658	-0.005581126028
N	5.615592931157	-0.008471663721	-0.094507136669
C	-3.591576343433	-0.809748536985	1.236453386301
H	-4.000322900161	-0.317042158706	2.138207722097
H	-4.002544801804	-1.833751073919	1.185895181273
C	-3.585502186956	1.420444741914	0.028454424420
H	-3.983821944890	1.960268044309	-0.848035613511
H	-3.975491504682	1.912278870700	0.935868317435
C	-3.596266494481	-0.737814969190	-1.292550103511
H	-4.004134745118	-1.763592250471	-1.306190955245
H	-3.989184873123	-0.193515581835	-2.169869594521
C	-4.056018753860	-0.031189244896	-0.008167125787
C	3.605274231334	0.739789687016	-1.280876213221
H	4.004385135351	1.767706600834	-1.244588197889
H	3.983557568842	0.251906814858	-2.197771955321
C	3.624866234926	-1.483963710829	-0.056491879858
H	4.008447280726	-1.992214597535	-0.958217392987
H	4.034293363929	-2.007600891888	0.824860857068
C	3.690400910636	0.699694391685	1.236088575685
H	4.121880690146	0.172581697862	2.107168309432
H	4.105021818519	1.722646748983	1.211344979836
C	4.104520529971	-0.033024261944	-0.050789787314

C	-0.607268290313	-3.074323379929	2.511562006728
H	-1.205917744437	-2.360622169993	3.101876733414
H	-1.253718560603	-3.914448142944	2.213268451045
H	0.204282471043	-3.458996299316	3.148509809378

p-2-(OMe)₂

V	-1.207351806973	0.832912029756	1.709995108140
V	-1.207794966405	-1.951767755451	-0.180807091678
V	-1.263679445407	0.958920364811	-1.646218168143
V	1.207794966405	1.951767755451	0.180807091678
V	1.263679445407	-0.958920364811	1.646218168143
V	1.207351806973	-0.832912029756	-1.709995108140
O	-2.242632772900	1.382667604431	2.790201199411
O	-2.207693782460	-3.191812722825	-0.178492776035
O	-2.269576292480	1.662141794047	-2.658845575310
O	2.207693782460	3.191812722825	0.178492776035
O	2.269576292480	-1.662141794047	2.658845575310
O	2.242632772900	-1.382667604431	-2.790201199411
O	-2.187501718859	-0.875692245485	1.268516598915
O	-2.198388851651	1.473001231479	0.059712506079
O	0.008475309050	2.237719713143	1.409374731457
O	0.045088434485	-0.134481204405	2.643543404872
O	-2.278522133682	-0.760198226060	-1.390501820299
O	0.025331875950	2.455647702980	-1.304347919908
O	2.278522133682	0.760198226060	1.390501820299
O	-0.025331875950	-2.455647702980	1.304347919908
O	-0.008475309050	-2.237719713143	-1.409374731457
O	-0.045088434485	0.134481204405	-2.643543404872
O	2.187501718859	0.875692245485	-1.268516598915
O	2.198388851651	-1.473001231479	-0.059712506079
O	0.000000000000	0.000000000000	0.000000000000

O	-6.130230782203	-1.144677286012	0.053979136681
O	-6.193499185002	1.013621344422	0.155306818899
O	6.130230782203	1.144677286012	-0.053979136681
O	6.193499185002	-1.013621344422	-0.155306818899
N	-5.600044895815	-0.047239861373	0.087527187483
N	5.600044895815	0.047239861373	-0.087527187483
C	-3.591113238979	-0.840285613523	1.247965765021
H	-3.967483773792	-0.384842329251	2.180294773116
H	-3.989064090138	-1.866240452775	1.175612897134
C	-3.611259070928	1.428177441884	0.088728716773
H	-4.015133843024	1.980910742932	-0.774896923599
H	-3.974276549083	1.914378178339	1.007892382449
C	-3.677821113682	-0.712640938261	-1.269290730471
H	-4.080706567002	-1.738762183539	-1.283797190024
H	-4.097538873633	-0.158804729411	-2.126832585858
C	-4.085135866859	-0.024205701138	0.041391850708
C	3.591113238979	0.840285613523	-1.247965765021
H	3.989064090138	1.866240452775	-1.175612897134
H	3.967483773792	0.384842329251	-2.180294773116
C	3.611259070928	-1.428177441884	-0.088728716773
H	3.974276549083	-1.914378178339	-1.007892382449
H	4.015133843024	-1.980910742932	0.774896923599
C	3.677821113682	0.712640938261	1.269290730471
H	4.097538873633	0.158804729411	2.126832585858
H	4.080706567002	1.738762183539	1.283797190024
C	4.085135866859	0.024205701138	-0.041391850708

C	-0.556586587137	-3.108402788062	2.442080055835
H	-1.183662481325	-2.422470171245	3.034635177134
H	-1.166760244433	-3.966380516175	2.124457631575
H	0.267227951953	-3.469571604065	3.075065197514
C	0.556586587137	3.108402788062	-2.442080055835
H	1.166760244433	3.966380516175	-2.124457631575
H	1.183662481325	2.422470171245	-3.034635177134
H	-0.267227951953	3.469571604065	-3.075065197514

o-2-(OMe)₂

V	-1.192082699952	0.883220592720	1.726368142001
V	-1.352804829189	-1.881716575349	-0.065008509136
V	-1.215129280981	1.028441404208	-1.654804019705
V	1.182084405989	1.926913933776	0.051294921750
V	1.219820992317	-1.003551401185	1.604095352901
V	1.165449683276	-0.891933098807	-1.751191282659
O	-2.206399721938	1.507831158942	2.784367056823
O	-2.287075670526	-3.173095313450	-0.080996762033
O	-2.238956898264	1.668553302823	-2.692172622747
O	2.216710594017	3.136784799990	0.054564622174
O	2.211538098787	-1.687278660138	2.643655568796
O	2.196802745647	-1.525111468228	-2.789135847905
O	-2.304695508838	-0.791368846014	1.332803582303
O	-2.184046963332	1.502815616502	0.021829399664
O	0.011867683242	2.233518591473	1.335878912997
O	-0.018983107575	-0.089400039774	2.631051082036
O	-2.296931571114	-0.727057784829	-1.377132369565
O	0.012888724375	2.265071674213	-1.325057037641
O	2.220516029015	0.708213621888	1.303555866854
O	-0.046906784548	-2.433308221789	1.318601748989
O	0.035490813158	-2.433856384429	-1.417448591471
O	-0.065983093237	-0.033918850489	-2.665714450861
O	2.185840643716	0.756268891935	-1.340372444841
O	2.185557796534	-1.560511913332	-0.075095716970
O	-0.028309272180	-0.136658782583	-0.021965210738

O	-6.207187571373	-0.956425074932	-0.053819201109
O	-6.195466844055	1.203155532386	0.039980636484
O	6.104126221847	1.078068903640	-0.061006805687
O	6.179953785409	-1.081127575137	-0.124399361246
N	-5.638472802892	0.121346230068	-0.009774618543
N	5.580308045600	-0.022592186637	-0.083020350157
C	-3.700747992067	-0.693770646460	1.241971553308
H	-4.095636206709	-0.184161271914	2.138501563115
H	-4.138611163707	-1.705865150591	1.199138779549
C	-3.595549825323	1.518933214381	0.025336143725
H	-3.960171843458	2.082469630148	-0.848757304903
H	-3.949862132110	2.029682272962	0.935049112051
C	-3.695993568180	-0.640573907859	-1.295646194161
H	-4.133460788218	-1.653283486572	-1.298699285938
H	-4.084520058617	-0.094263162790	-2.172936719211
C	-4.123760112437	0.089451380893	-0.011430974988
C	3.589454101428	0.720460928142	-1.298509877618
H	3.982584451412	1.749472742557	-1.259739907834
H	3.974821063228	0.231555409107	-2.210367371022
C	3.593309868245	-1.505878729325	-0.087948097235
H	3.971751553666	-2.004177123942	-0.995722360024
H	3.992853271926	-2.044605753275	0.787597448151
C	3.623875760884	0.665057592510	1.223618609471
H	4.023652664231	0.130649101158	2.103195296178
H	4.025882048369	1.691230794687	1.226143331597
C	4.064234834549	-0.053735041002	-0.060134418241

C	-0.308321021792	-3.456583764481	2.259213937630
H	-1.026267537533	-3.101287171225	3.016301843232
H	-0.734032679282	-4.332167540442	1.748758867050
H	0.622574639965	-3.748672801652	2.765062204407
C	0.556075735354	-3.745403684571	-1.371764542611
H	1.175958100425	-3.933220319119	-2.260844176269
H	1.175908542687	-3.890335374953	-0.471368692968
H	-0.272064349878	-4.469220213836	-1.351714457200

m-2-(OMe)₂

V	-1.256636445778	0.840913912540	1.671108270868
V	-1.208933322557	-1.958353183625	-0.101247077668
V	-1.206680326134	0.955518864377	-1.686458209062
V	1.208220930758	1.958081438666	-0.100966798752
V	1.256597002120	-0.840931389541	1.671826197083
V	1.207740418327	-0.956092594155	-1.685851657270
O	-2.268924275912	1.514953415849	2.703947628945
O	-2.218406169827	-3.186980739464	-0.073750136514
O	-2.243558638152	1.542826009640	-2.741672383860
O	2.218575770548	3.186054975685	-0.073785177815
O	2.269729113951	-1.513933107782	2.704498027588
O	2.244042238028	-1.543779914394	-2.741323931265
O	-2.245027116688	-0.855530109173	1.297956781823
O	-2.204678460241	1.468584381612	-0.025129955071
O	0.062303911844	2.379746672901	1.398865250709
O	0.000030983697	0.000013344565	2.657090360797
O	-2.219929558792	-0.803580376376	-1.362270765245
O	-0.015272055624	2.317844848937	-1.315156203077
O	2.244404095388	0.855811906246	1.298096248374
O	-0.063311930770	-2.378411680279	1.399501204949
O	0.015700357508	-2.317869735692	-1.313991525128
O	-0.000063091056	-0.000757377804	-2.636160010899
O	2.219585725855	0.802593462793	-1.362085054044
O	2.204964994693	-1.469538251565	-0.024612582715
O	0.000228019075	0.000525361545	0.026545295505

O	-6.128927696464	-1.160167039007	-0.087157091283
O	-6.200933543543	0.999224119499	-0.020431194503
O	6.128287521448	1.161144751463	-0.086362177801
O	6.200957045741	-0.998237536155	-0.019341060705
N	-5.602691128605	-0.060810698696	-0.052073497890
N	5.602418824904	0.061608498658	-0.051195420127
C	-3.645369847614	-0.803639070509	1.214032894943
H	-4.051552004170	-0.305825379899	2.111987975454
H	-4.051803336423	-1.828016469050	1.169952855233
C	-3.616377009703	1.419959070911	-0.024754255625
H	-4.005290301391	1.949308943336	-0.909638272214
H	-3.998022335386	1.928519770527	0.875011203425
C	-3.624030471846	-0.765069621783	-1.309515804231
H	-4.021170149233	-1.793669451066	-1.305447076464
H	-4.008760198999	-0.243751068741	-2.202595025399
C	-4.087471649796	-0.033696483858	-0.041771611820
C	3.623755932973	0.764979048983	-1.309121588654
H	4.020247074911	1.793808526389	-1.305298453451
H	4.009024229414	0.243604459836	-2.201937361024
C	3.616584343420	-1.419720770296	-0.023723312142
H	4.006252371056	-1.949071308713	-0.908314046276
H	3.998382767147	-1.927827285673	0.876223957403
C	3.644850355697	0.804173861846	1.214542389750
H	4.050845502660	0.306420394941	2.112596142107
H	4.051028222620	1.828641263693	1.170508092843
C	4.087196612560	0.034149894475	-0.041076669599

C	-0.573815171850	-3.001935955486	2.560197664130
H	-1.200040938879	-2.303969198819	3.139488219297
H	-1.180204645806	-3.875826051594	2.279960440582
H	0.261613011849	-3.334580862859	3.193559045402
C	0.572948555171	3.002801550205	2.559783433193
H	1.201625715194	2.305504530379	3.137220379265
H	1.176888151080	3.878510819152	2.279902415109
H	-0.262403978396	3.332533612405	3.194742012819

Cartesian coordinates for the direduced **1**, **1-OMe**, and **1-(OMe)₂** species at M06-L/def2-TZVP,def2-SVP level of theory.

1

V	-1.728994201020	0.954678507432	-1.157437388915
V	-0.036727949008	-1.971865188378	-1.148277639698
V	1.673937479787	0.965114469468	-1.249773266592
V	0.036749570851	1.971871525314	1.148253557029
V	-1.673906397815	-0.965030817138	1.249635500978
V	1.729079424083	-0.954576824112	1.157490169217
O	-2.781324077796	1.575730128525	-2.236579328479
O	-0.015228956182	-3.188759860736	-2.231522048026
O	2.786485976899	1.612003150453	-2.245946634917
O	0.015388041946	3.188736031221	2.231518478958
O	-2.786471339299	-1.611986275435	2.245778763463
O	2.781398605889	-1.575665840637	2.236623013126
O	-1.335982439693	-0.770237327847	-2.234781867424
O	-0.006703643795	1.569331312422	-2.236039828358
O	-1.336173493963	2.324401270792	-0.006860247685
O	-2.684537970356	0.005037346944	-0.040828763920
O	1.365286401634	-0.790856672759	-2.239362324319
O	1.343336214478	2.332454454012	0.044301356828
O	-1.365246091641	0.790959172779	2.239257278443
O	-1.343324037627	-2.332449716207	-0.044410976031
O	1.336247652045	-2.324160997066	0.006838371662
O	2.684533390204	-0.004907950007	0.040776078796

O	1.336073440087	0.770245262622	2.234816747879
O	0.006689663035	-1.569249341742	2.236005774246
O	0.000008449934	-0.000029973096	0.000002500208
C	-1.239336354402	-0.716091039096	-3.618224691586
H	-2.135499009113	-0.201048924775	-4.029533358374
H	-1.243661479967	-1.750513260711	-4.027924565339
C	-0.003473847741	1.446932084500	-3.620100133001
H	0.883356524149	1.973613462048	-4.039269462976
H	-0.902412061673	1.952177521638	-4.037753865568
C	1.253250099206	-0.729623310895	-3.622636782117
H	1.236330558227	-1.761948191256	-4.037491530542
H	2.151766582198	-0.228229941093	-4.048123678710
C	0.007657170645	0.003253482387	-4.129471061642
C	1.239360663965	0.716049617498	3.618253186736
H	1.243756067716	1.750463843203	4.027975960166
H	2.135455243689	0.200906283367	4.029581438764
C	0.003447361737	-1.446913364103	3.620054380616
H	0.902376661100	-1.952152837795	4.037734399189
H	-0.883381647386	-1.973611382872	4.039219833616
C	-1.253244350990	0.729674526104	3.622541715909
H	-2.151788679795	0.228291976698	4.047976089146
H	-1.236323754419	1.761987178719	4.037426614999
C	-0.007696691806	-0.003232031901	4.129431837831
C	-0.005623315462	-0.005976076371	5.648138923745
H	0.882000098245	-0.519153452824	6.051950421920
H	-0.004681231875	1.017273697707	6.056910975583

H	-0.891879605982	-0.519237156938	6.054849317849
C	0.005504008044	0.006029074086	-5.648176060374
H	0.004582269731	-1.017214873042	-6.056962982291
H	-0.882158213345	0.519177742395	-6.051937703206
H	0.891723222626	0.519329496496	-6.054916496811

1-OMe

V	-1.695622287103	0.947963593607	-1.160495168347
V	-0.133587128293	-1.980864582637	-1.221065988018
V	1.725133013237	0.810356170114	-1.161187372548
V	0.056902241733	1.941943192595	1.163105597747
V	-1.680672225973	-0.992500466060	1.240873464358
V	1.651070714222	-0.981317269003	1.307146690717
O	-2.729119210959	1.600953103853	-2.218815181884
O	-0.115252228209	-3.250935960545	-2.221611714198
O	2.787097968192	1.411626068358	-2.224551420187
O	0.064629058174	3.180598770545	2.202250017058
O	-2.790822071761	-1.570068123979	2.265929094515
O	2.715380863159	-1.684359260931	2.301530157760
O	-1.394655032604	-0.805625050359	-2.251967454876
O	0.030704702591	1.452742186110	-2.172986071557
O	-1.279728927034	2.297969369681	0.002760113478
O	-2.661650648982	0.012389881263	-0.032334884085
O	1.307474398671	-0.895333814134	-2.205586183421
O	1.391230762560	2.223315946928	0.042805474413
O	-1.313591991208	0.784042258000	2.203436681247
O	-1.363988514288	-2.331654791825	0.023123956042
O	1.375277018087	-2.517186617312	-0.010460928837
O	2.672934674881	-0.119729154348	0.023344406854
O	1.365119372046	0.762899779459	2.287045682727
O	-0.035976114843	-1.585626206569	2.290171665067
O	0.029728955880	-0.102122008149	0.025359088141

C	-1.262307769236	-0.730436559661	-3.642653514863
H	-2.133532194547	-0.181777477191	-4.054790182712
H	-1.294526580891	-1.757740930167	-4.062152296354
C	0.049067436423	1.386726697948	-3.568617761887
H	0.960088124346	1.894224877336	-3.947428849703
H	-0.824735000931	1.937268759036	-3.975410941523
C	1.234998587584	-0.819278657686	-3.600754948366
H	1.203548167979	-1.847702444211	-4.017333253217
H	2.156563374228	-0.337821735056	-3.986849281391
C	0.019715982736	-0.043504352927	-4.111834823821
C	1.222094714447	0.719448348257	3.676930648665
H	1.224903013016	1.756618610535	4.071569018298
H	2.102243263258	0.203185129263	4.114757882811
C	-0.057475201476	-1.436646509517	3.682108194034
H	0.822923740758	-1.956039430619	4.114268577508
H	-0.961705917037	-1.936921304609	4.085638198295
C	-1.266674269988	0.757036803392	3.600125565588
H	-2.187789580129	0.274168840232	3.987216505750
H	-1.257332982480	1.797358324912	3.986548684767
C	-0.049345814856	0.018784901291	4.157379624906
C	2.526611606692	-3.065507959574	-0.575850615943
H	2.267726294113	-3.908809535244	-1.241072005711
H	3.092443795142	-2.326251768394	-1.171046148806
H	3.197659091532	-3.447130407377	0.214735519949
C	-0.093023701812	0.047223265792	5.675875373687
H	-0.087039994901	1.078983909332	6.060390348699

H	-1.000416340792	-0.442149994672	6.062604058215
H	0.773098551591	-0.471967715770	6.115040655655
C	0.045988822465	-0.011790400793	-5.630215890453
H	-0.817492661108	0.536499906495	-6.037838859242
H	0.955829324893	0.480645847897	-6.007119223351
H	0.021425996803	-1.027009142911	-6.056117051652

p-1-(OMe)₂

V	-1.641422278771	0.954202831218	-1.292019120625
V	-0.182464490254	-1.960587002255	-1.207357354064
V	1.727356613866	0.815384183691	-1.210329004170
V	0.182464490305	1.960587002255	1.207357354168
V	-1.727356613815	-0.815384183691	1.210329004273
V	1.641422278822	-0.954202831218	1.292019120729
O	-2.675110723889	1.672707103343	-2.290205568524
O	-0.158978655641	-3.229730500783	-2.192378144231
O	2.835262808016	1.382637293804	-2.231292156914
O	0.158978655693	3.229730500783	2.192378144334
O	-2.835262807964	-1.382637293804	2.231292157018
O	2.675110723940	-1.672707103343	2.290205568627
O	-1.386837515848	-0.791303716839	-2.300169490772
O	0.074869852510	1.480258953050	-2.231825536510
O	-1.309158000300	2.471144073270	0.010310674083
O	-2.644907037204	0.121121543390	-0.054416482180
O	1.287570150116	-0.902491758532	-2.188489936081
O	1.400206355468	2.250053461214	0.012525646352
O	-1.287570150064	0.902491758532	2.188489936185
O	-1.400206355416	-2.250053461214	-0.012525646249
O	1.309158000352	-2.471144073270	-0.010310673980
O	2.644907037255	-0.121121543390	0.054416482283
O	1.386837515899	0.791303716839	2.300169490876
O	-0.074869852458	-1.480258953050	2.231825536613
O	0.000000000026	0.000000000000	0.000000000052

C	-1.228536244186	-0.734912109543	-3.699037045191
H	-2.091501756502	-0.187328919051	-4.123893225230
H	-1.262746286537	-1.767730076874	-4.096381188101
C	0.110214139211	1.378413356454	-3.634936129556
H	1.031836282311	1.866438610225	-4.006329680638
H	-0.750054611290	1.932060360616	-4.059502880195
C	1.257552453457	-0.855266015099	-3.593934781922
H	1.216297781838	-1.890502537966	-3.986140838480
H	2.199328591697	-0.401516247013	-3.958100015156
C	0.069572972325	-0.065436308082	-4.144639465440
C	1.228536244238	0.734912109543	3.699037045295
H	1.262746286589	1.767730076874	4.096381188205
H	2.091501756553	0.187328919051	4.123893225333
C	-0.110214139159	-1.378413356454	3.634936129660
H	0.750054611342	-1.932060360616	4.059502880298
H	-1.031836282260	-1.866438610225	4.006329680742
C	-1.257552453406	0.855266015099	3.593934782025
H	-2.199328591646	0.401516247013	3.958100015260
H	-1.216297781787	1.890502537966	3.986140838583
C	-0.069572972273	0.065436308082	4.144639465544
C	2.450445014416	-3.077556183356	-0.557125314608
H	2.158571869241	-3.924909755756	-1.199130890768
H	3.036265250626	-2.367025598010	-1.165093698832
H	3.097382913436	-3.455895210856	0.251263942533
C	-2.450445014364	3.077556183356	0.557125314712
H	-3.036265250574	2.367025598010	1.165093698936

H	-2.158571869189	3.924909755756	1.199130890871
H	-3.097382913384	3.455895210856	-0.251263942429
C	-0.129338892454	0.061581770274	5.663260660452
H	0.717041358510	-0.491980131450	6.097043600279
H	-0.098909611626	1.083937299675	6.069143119550
H	-1.054607626615	-0.411111373152	6.025459581251
C	0.129338892506	-0.061581770274	-5.663260660349
H	0.098909611678	-1.083937299675	-6.069143119447
H	-0.717041358458	0.491980131450	-6.097043600176
H	1.054607626667	0.411111373152	-6.025459581147

o-1-(OMe)₂

V	-1.621043426088	1.031512201037	-1.229410370681
V	-0.092157714830	-1.914121561653	-1.325111539136
V	1.744352203813	0.807701434144	-1.221198057631
V	0.112962560919	1.913633943477	1.189517737015
V	-1.761037052821	-0.856756762303	1.187654733777
V	1.615679114381	-1.023304783280	1.256001874349
O	-2.664821858311	1.699315184405	-2.248692919184
O	-0.203519051158	-3.229241946546	-2.253472889638
O	2.861051358585	1.424730140349	-2.197586758590
O	0.111394301879	3.166495146914	2.194822804104
O	-2.824300848775	-1.465477425632	2.228450126486
O	2.638160611416	-1.728613224814	2.277830089387
O	-1.402646164127	-0.715222242390	-2.280323732276
O	0.061480241317	1.500331075789	-2.212382737581
O	-1.277725004222	2.258065702506	-0.013015810798
O	-2.666227705330	-0.011797147778	-0.055128626460
O	1.341667523329	-0.876574770979	-2.289358149168
O	1.389255803479	2.177589959304	0.033841568636
O	-1.343072247754	0.784891916762	2.193657903944
O	-1.478526172856	-2.443593195882	0.092949710668
O	1.298347061623	-2.543520869340	0.002464938749
O	2.628774104161	-0.186636981080	0.035619166798
O	1.319731153326	0.703354539217	2.274726916426
O	-0.113703826300	-1.561341121936	2.206982032379
O	-0.027010550294	-0.156283743082	-0.012288599950

C	-1.289723663172	-0.652041304804	-3.680995835383
H	-2.154577037962	-0.091763321400	-4.086655106319
H	-1.343700444442	-1.680527025220	-4.088931327436
C	0.069669540458	1.439339953869	-3.619306538658
H	0.992534837374	1.927632074026	-3.986411465762
H	-0.789123909486	2.020263475252	-4.007834172907
C	1.224343171985	-0.776478123425	-3.688619007356
H	1.181759646895	-1.799085343599	-4.112982381265
H	2.137717423991	-0.294678503749	-4.088711564266
C	0.001462614492	0.013147176845	-4.162329608253
C	1.180569827040	0.640018105231	3.673415313723
H	1.210226642281	1.669928380818	4.078811566916
H	2.052207300446	0.096396599114	4.086740166446
C	-0.140765723519	-1.483164033995	3.610370658875
H	0.727236083542	-2.035784390966	4.019907389913
H	-1.055952796263	-1.983375186487	3.983209567525
C	-1.305264693562	0.736281638102	3.601370327873
H	-2.241982792081	0.273455816917	3.966740533657
H	-1.271178001227	1.772130003138	3.988080164301
C	-0.105086018392	-0.044657845162	4.133935603732
C	2.432394780302	-3.196210423003	-0.495791732426
H	2.134148280236	-4.052627624198	-1.124370361647
H	3.058236734268	-2.521890334193	-1.108646589183
H	3.055173636155	-3.576302464240	0.332185747200
C	-1.421757188434	-3.722826260891	0.658455771404
H	-0.545110792192	-3.836056489328	1.317947320300

H	-2.330025369750	-3.918707957085	1.253253319021
H	-1.354252469119	-4.480925625579	-0.138902010836
C	-0.150704841850	-0.059107216669	5.652456891163
H	-0.126803285536	0.960804828589	6.064823555913
H	-1.066964876094	-0.544052341629	6.021196452417
H	0.706133804410	-0.606582753289	6.073017414281
C	0.001165483940	0.056652112179	-5.681831617572
H	-0.861209384282	0.621015334335	-6.067098395840
H	0.911614470264	0.537836493546	-6.069709221605
H	-0.047048096077	-0.955408170264	-6.111268979570

m-1-(OMe)₂

V	-1.591068705285	1.104262914872	-1.181040860973
V	-0.235692345087	-1.936351689620	-1.174484882351
V	1.719776018328	0.793283965188	-1.162891588482
V	0.126405750281	1.935941577641	1.235477891402
V	-1.660527507035	-0.933634773830	1.331017742679
V	1.641398795452	-1.005543590491	1.329764847249
O	-2.661862977420	1.719774869368	-2.206602853925
O	-0.255565000375	-3.187110685756	-2.187584902746
O	2.807854954137	1.371266486190	-2.196729878222
O	0.150469985009	3.196251875534	2.231207362007
O	-2.826718206257	-1.436861654469	2.320591467985
O	2.708552130510	-1.710501135718	2.299084604149
O	-1.444939248602	-0.710258997501	-2.189991817856
O	0.034843262983	1.508196506809	-2.197492779620
O	-1.283371797403	2.316033089539	0.028771034510
O	-2.808083777275	0.075522878488	-0.038089123423
O	1.235112034869	-0.884945740103	-2.172773530977
O	1.382185576970	2.206546686710	0.043153889601
O	-1.281787200155	0.844298901017	2.246741301277
O	-1.448214916675	-2.268637824226	0.075288137660
O	1.269850421760	-2.501712660003	0.030091363703
O	2.628272765935	-0.158835515782	0.056205104221
O	1.379626817327	0.748336512311	2.305918486286
O	-0.041201643520	-1.561049251377	2.339735267342
O	-0.052701640915	-0.056625809463	0.050383043276

C	-1.344155374099	-0.676388670707	-3.592654767115
H	-2.206151609953	-0.109771824807	-3.995481457139
H	-1.417512217314	-1.711140758488	-3.980059640472
C	0.039275560012	1.401953107662	-3.601936428422
H	0.967009736038	1.867859127998	-3.983469622796
H	-0.815622456836	1.978746580080	-4.005370266481
C	1.155768244154	-0.835656377589	-3.575632517987
H	1.099075664392	-1.871167705143	-3.964524853975
H	2.085116745424	-0.383671051560	-3.973773668976
C	-0.046232883316	-0.042128620110	-4.093560199398
C	1.258121879906	0.723291731174	3.708115732313
H	1.296342787883	1.764000734759	4.083619176101
H	2.133642516413	0.189923123321	4.126773960925
C	-0.055791223262	-1.402239553408	3.739379327475
H	0.817925106326	-1.932526884553	4.165691438572
H	-0.964515101437	-1.890671921988	4.141592227653
C	-1.232861927797	0.819097122244	3.652893800127
H	-2.161884973822	0.355051380039	4.036636673621
H	-1.202447786912	1.858940067259	4.032434347868
C	-0.024229101583	0.056574839538	4.200996844379
C	2.395011259759	-3.109801366666	-0.545266417418
H	2.085367098925	-3.938694889400	-1.203388155777
H	2.986030625489	-2.395826670594	-1.145031816656
H	3.049621081677	-3.518788264543	0.242823269842
C	-3.903046352441	-0.609527916707	-0.580757564350
H	-4.446943290638	0.036792350095	-1.289495223445

H	-3.588342138831	-1.521826820065	-1.115487105798
H	-4.594568721880	-0.905424950437	0.225370816372
C	-0.054234987311	0.095054428740	5.720194105652
H	0.806204905958	-0.437757549193	6.152326745277
H	-0.025673516584	1.128847779590	6.095934441078
H	-0.967232703165	-0.375644587539	6.114816283878
C	-0.038512255263	-0.052158651840	-5.613079317048
H	-0.891989391150	0.508681443662	-6.022751474989
H	0.879759649338	0.404080077799	-6.012358824315
H	-0.096934435661	-1.078087013950	-6.006544863347

Cartesian coordinates for the direduced **2**, **2-OMe**, and **2-(OMe)₂** species at M06-L/def2-TZVP,def2-SVP level of theory.

2

V	-1.197072574442	0.957560460670	1.705493285954
V	-1.137037637050	-1.983809545343	0.000000000000
V	-1.197072574442	0.957560460670	-1.705493285954
V	1.137037637050	1.983809545343	0.000000000000
V	1.197072574442	-0.957560460670	1.705493285954
V	1.197072574442	-0.957560460670	-1.705493285954
O	-2.233700559080	1.598670737722	2.776249682868
O	-2.244546490282	-3.174034540779	0.000000000000
O	-2.233700559080	1.598670737722	-2.776249682868
O	2.244546490282	3.174034540779	0.000000000000
O	2.233700559080	-1.598670737722	2.776249682868
O	2.233700559080	-1.598670737722	-2.776249682868
O	-2.245195388147	-0.762876234236	1.343603673571
O	-2.208443745188	1.570475352985	0.000000000000
O	0.046921795573	2.328370795130	1.348032893182
O	0.000000000000	0.000000000000	2.671283892476
O	-2.245195388147	-0.762876234236	-1.343603673571
O	0.046921795573	2.328370795130	-1.348032893182
O	2.245195388147	0.762876234236	1.343603673571
O	-0.046921795573	-2.328370795130	1.348032893182
O	-0.046921795573	-2.328370795130	-1.348032893182
O	0.000000000000	0.000000000000	-2.671283892476

O	2.245195388147	0.762876234236	-1.343603673571
O	2.208443745188	-1.570475352985	0.000000000000
O	0.000000000000	0.000000000000	0.000000000000
O	-6.128689788293	-1.082023295146	0.000000000000
O	-6.198390383029	1.081834430699	0.000000000000
O	6.128689788293	1.082023295146	0.000000000000
O	6.198390383029	-1.081834430699	0.000000000000
N	-5.582049888620	0.019528256740	0.000000000000
N	5.582049888620	-0.019528256740	0.000000000000
C	-3.618644008463	-0.714874869533	1.259065051432
H	-4.047591635640	-0.203978828620	2.147360665010
H	-4.042000117144	-1.737012535533	1.214753694581
C	-3.596185007648	1.489725673432	0.000000000000
H	-4.008386546669	2.000552215628	-0.892088188073
H	-4.008386546669	2.000552215628	0.892088188073
C	-3.618644008463	-0.714874869533	-1.259065051432
H	-4.042000117144	-1.737012535533	-1.214753694581
H	-4.047591635640	-0.203978828620	-2.147360665010
C	-4.086913389246	0.042082312818	0.000000000000
C	3.618644008463	0.714874869533	-1.259065051432
H	4.042000117144	1.737012535533	-1.214753694581
H	4.047591635640	0.203978828620	-2.147360665010
C	3.596185007648	-1.489725673432	0.000000000000
H	4.008386546669	-2.000552215628	-0.892088188073
H	4.008386546669	-2.000552215628	0.892088188073
C	3.618644008463	0.714874869533	1.259065051432

H	4.047591635640	0.203978828620	2.147360665010
H	4.042000117144	1.737012535533	1.214753694581
C	4.086913389246	-0.042082312818	0.000000000000

2-OMe

V	-1.149045037439	0.822885003317	1.732743062084
V	-1.218550657278	-1.981506987296	-0.141344839258
V	-1.145865771942	0.966586640641	-1.699596654131
V	1.170125461529	1.946630442720	0.061343864201
V	1.288347267278	-0.999639660285	1.653055524430
V	1.235833000786	-0.994594500589	-1.692164748688
O	-2.216534564116	1.421024954208	2.786703847456
O	-2.242960216645	-3.227442749006	-0.124519409931
O	-2.203205852983	1.621026658981	-2.726796235142
O	2.224817202521	3.167578239947	0.078355058295
O	2.289504444246	-1.706294698069	2.703146643977
O	2.257361167308	-1.570466531278	-2.799878458752
O	-2.217465691689	-0.878438648233	1.299184723635
O	-2.159815087924	1.467057424089	0.028711680194
O	0.055948153380	2.222920171959	1.400796889933
O	0.014100727342	-0.127504644301	2.677723535204
O	-2.251462058434	-0.786679601201	-1.397307054733
O	0.026695776197	2.307163886804	-1.277154383566
O	2.289079026026	0.744210532194	1.366038650362
O	-0.037090022835	-2.518017007463	1.370553415748
O	0.010772640723	-2.332130348171	-1.371750896714
O	-0.026168701219	0.019440918115	-2.661431712303
O	2.220272998445	0.777421522637	-1.310702679400
O	2.278718847124	-1.590999881761	-0.040987708890
O	0.026776659470	-0.101287910609	0.030767568383

O	-6.125708485268	-1.096779015220	0.002227739403
O	-6.159154430552	1.062335651729	0.055708235009
O	6.133588613328	1.157187647733	-0.079613134338
O	6.250493109465	-0.999955651615	-0.082247225783
N	-5.569311372370	-0.007098297371	0.022734474551
N	5.618568924589	0.046653008760	-0.070383623837
C	-3.600659575068	-0.806787514874	1.237487448442
H	-4.001115542920	-0.316024613845	2.146332059821
H	-4.034749953282	-1.822127241636	1.174925329434
C	-3.552825284226	1.432058583582	0.039756662468
H	-3.955871207891	1.975424060815	-0.835287408589
H	-3.938284183273	1.930794668812	0.948209913756
C	-3.632093178414	-0.716888779344	-1.289050061992
H	-4.065981181229	-1.734371920960	-1.290937909656
H	-4.049513741244	-0.161957373537	-2.151972154046
C	-4.063713690883	-0.006359160552	0.005621676120
C	3.605073854980	0.755516191680	-1.271450277622
H	4.007774952372	1.784255655613	-1.227876954429
H	4.008310483655	0.267222441714	-2.180938261434
C	3.669601619184	-1.474150334208	-0.053795399393
H	4.079885672407	-1.963641240393	-0.956370107437
H	4.096479734175	-1.988551718128	0.827095671822
C	3.668909788355	0.710827566164	1.247550653994
H	4.114181816330	0.187964637366	2.117773059919
H	4.075007915825	1.738930148816	1.221668094870
C	4.115047437225	-0.012056634108	-0.037862815333

C	-0.606376073157	-3.082271028347	2.516735325122
H	-1.223242108410	-2.355766082001	3.074349995653
H	-1.248099719288	-3.938313246933	2.245268075638
H	0.185687095717	-3.446156637060	3.193844235474

p-2-(OMe)₂

V	-1.207647123832	0.827148833973	1.729864933007
V	-1.207846685209	-1.960557322121	-0.189094522802
V	-1.270162957205	0.971544205852	-1.651646533083
V	1.207846685209	1.960557322121	0.189094522802
V	1.270162957205	-0.971544205852	1.651646533083
V	1.207647123832	-0.827148833973	-1.729864933007
O	-2.239585133764	1.391382925832	2.823558273697
O	-2.210922376680	-3.210856839773	-0.176789579225
O	-2.264897552161	1.692512855173	-2.680999827575
O	2.210922376680	3.210856839773	0.176789579225
O	2.264897552161	-1.692512855173	2.680999827575
O	2.239585133764	-1.391382925832	-2.823558273697
O	-2.206389493519	-0.889220076595	1.278395094002
O	-2.222154779171	1.489054610693	0.066498425106
O	0.020169173689	2.250174548613	1.411629570005
O	0.039652886952	-0.127061554765	2.648886838470
O	-2.297448571175	-0.770828289011	-1.396825976165
O	0.035549022935	2.472214389329	-1.304465853752
O	2.297448571175	0.770828289011	1.396825976165
O	-0.035549022935	-2.472214389329	1.304465853752
O	-0.020169173689	-2.250174548613	-1.411629570005
O	-0.039652886952	0.127061554765	-2.648886838470
O	2.206389493519	0.889220076595	-1.278395094002
O	2.222154779171	-1.489054610693	-0.066498425106
O	0.000000000000	0.000000000000	0.000000000000

O	-6.141532746141	-1.159722820616	0.055486935157
O	-6.213069901771	0.996723768397	0.163859024802
O	6.141532746141	1.159722820616	-0.055486935157
O	6.213069901771	-0.996723768397	-0.163859024802
N	-5.609164576534	-0.060640755947	0.092094548971
N	5.609164576534	0.060640755947	-0.092094548971
C	-3.599317878006	-0.847184464751	1.251902474180
H	-3.983581982001	-0.386964120036	2.181250819788
H	-4.008863527527	-1.870489725669	1.178130107410
C	-3.622489737451	1.419802766003	0.095020511504
H	-4.043489872065	1.968140359110	-0.766284468673
H	-4.000417597973	1.897554176092	1.015409574015
C	-3.686082770220	-0.721344465683	-1.263317040624
H	-4.097596138159	-1.745881387048	-1.271444977325
H	-4.118531711487	-0.167416099998	-2.116913127009
C	-4.098921899281	-0.031866316037	0.046202594931
C	3.599317878006	0.847184464751	-1.251902474180
H	4.008863527527	1.870489725669	-1.178130107410
H	3.983581982001	0.386964120036	-2.181250819788
C	3.622489737451	-1.419802766003	-0.095020511504
H	4.000417597973	-1.897554176092	-1.015409574015
H	4.043489872065	-1.968140359110	0.766284468673
C	3.686082770220	0.721344465683	1.263317040624
H	4.118531711487	0.167416099998	2.116913127009
H	4.097596138159	1.745881387048	1.271444977325
C	4.098921899281	0.031866316037	-0.046202594931

C	-0.584539879917	-3.098007191280	2.439227751369
H	-1.192921795871	-2.394768458773	3.032312667208
H	-1.223357349111	-3.940885657292	2.131606273706
H	0.225217296312	-3.482683015831	3.079078971983
C	0.584539879917	3.098007191280	-2.439227751369
H	1.223357349111	3.940885657292	-2.131606273706
H	1.192921795871	2.394768458773	-3.032312667208
H	-0.225217296312	3.482683015831	-3.079078971983

o-2-(OMe)₂

V	-1.214245961030	0.837317291990	1.739479349941
V	-1.332971412614	-1.906885777323	-0.099464622791
V	-1.213581325253	1.057021943307	-1.634606801683
V	1.198692839933	1.922584392968	0.106534472161
V	1.231506862722	-1.029389477288	1.623499834225
V	1.167726597167	-0.868344516370	-1.766799455112
O	-2.194720416309	1.450511725885	2.849017720028
O	-2.278068955964	-3.205073896282	-0.207690526138
O	-2.235237546601	1.723665849937	-2.671885762688
O	2.213901253140	3.162447968637	0.115542514728
O	2.257844763633	-1.730953115683	2.637715679261
O	2.219769572476	-1.469162372781	-2.818450467957
O	-2.297284103914	-0.854240951068	1.332119346974
O	-2.210389247443	1.510254112675	0.051652187154
O	0.039390162912	2.183695455297	1.388501023720
O	0.031374969220	-0.183199621184	2.629509869808
O	-2.288816806198	-0.699911486889	-1.414553845317
O	-0.004350912888	2.278372354433	-1.278175713897
O	2.274144090649	0.691927980463	1.321145407385
O	-0.009430390991	-2.537625156008	1.289065458850
O	0.080679194766	-2.437975366565	-1.481942653994
O	-0.053413094996	0.002423107923	-2.674120923725
O	2.199120212455	0.783790052893	-1.340581808609
O	2.193327828034	-1.562330898720	-0.109362312897
O	-0.016015516458	-0.148623903012	-0.033592948370

O	-6.184716574106	-1.038675431354	-0.075363908006
O	-6.210910190819	1.117180600023	0.061906642078
O	6.132095044345	1.042866197796	-0.126104677137
O	6.189744605274	-1.116308218338	-0.167244171420
N	-5.629484339580	0.047157374877	-0.008884934898
N	5.593244574890	-0.053195164106	-0.135033690756
C	-3.686013729163	-0.766648129310	1.228424618610
H	-4.101342037557	-0.277571422251	2.129771960720
H	-4.121689987218	-1.779412736499	1.157303122860
C	-3.612728095772	1.477724107508	0.055967480137
H	-4.001359975062	2.045983402231	-0.807116239827
H	-3.987210627435	1.961616644290	0.974477096735
C	-3.677839314260	-0.643149029015	-1.316582018848
H	-4.100607929733	-1.663485392742	-1.342538752830
H	-4.096620607786	-0.076222654898	-2.169735789439
C	-4.118163044579	0.040962361928	-0.009868107565
C	3.594535700705	0.733131005041	-1.311401189747
H	4.003831211877	1.756028129131	-1.250560508621
H	3.973256664740	0.260886135527	-2.236843973515
C	3.592945181148	-1.517800601132	-0.133594467725
H	3.970298208736	-2.010662507652	-1.047085997381
H	4.001200371880	-2.062444947791	0.735950945751
C	3.662344802109	0.632017042048	1.204421846957
H	4.082905652979	0.078452556009	2.064865426800
H	4.084677037191	1.652293465067	1.209517356823
C	4.082459783274	-0.071376825771	-0.096355445279

C	-0.497852752963	-3.233251087311	2.406269564119
H	-1.130202489715	-2.590040985649	3.044245431041
H	-1.101479849819	-4.095755660350	2.079136998912
H	0.337214777888	-3.607317112267	3.021382816747
C	0.634880789578	-3.727358773362	-1.444565192360
H	1.228920478154	-3.910994168939	-2.354576790209
H	1.289916792925	-3.856610030049	-0.567482239670
H	-0.171741788576	-4.475263839925	-1.391022234114

m-2-(OMe)₂

V	-1.251353161715	0.854743024261	1.659443334019
V	-1.205646731869	-1.966509918938	-0.126409953707
V	-1.225279944614	0.948823819658	-1.724261829334
V	1.207350115765	1.968682844662	-0.126522192273
V	1.250022584966	-0.851215649541	1.660684399954
V	1.223483560398	-0.944860140298	-1.725576789715
O	-2.268229921383	1.524190315450	2.707001333580
O	-2.204667441504	-3.217946811393	-0.078460969427
O	-2.241076304094	1.568789948991	-2.798864351059
O	2.205032238025	3.221216991564	-0.079513815322
O	2.266701760434	-1.522490513930	2.707328086287
O	2.241668832643	-1.564650965791	-2.798108804133
O	-2.249754446749	-0.856369374112	1.297501977565
O	-2.226255207048	1.484799840472	-0.031254775394
O	0.050094822295	2.396264094018	1.397740958150
O	0.000222745291	0.000825734471	2.649535438058
O	-2.253991415588	-0.816082577953	-1.382736611491
O	-0.003107554805	2.318633537886	-1.324872612557
O	2.250516116704	0.857734277690	1.297878867729
O	-0.049921587470	-2.394581282623	1.397864062645
O	0.003239918971	-2.318219062053	-1.324906723246
O	0.000846766437	0.000010900603	-2.658463079789
O	2.255052504316	0.816918042751	-1.382620497522
O	2.223391466149	-1.482525160318	-0.031035051756
O	-0.000337534247	0.000250863017	0.024005790686

O	-6.141483573913	-1.168828296549	-0.049426648448
O	-6.218882724144	0.989437399897	0.006677897858
O	6.143059857865	1.163902515787	-0.049581153976
O	6.216846040414	-0.994401994781	0.009681734969
N	-5.611817861717	-0.068147635380	-0.024823121461
N	5.611557185740	0.064129517190	-0.023674497938
C	-3.640818106932	-0.806372571614	1.221307480052
H	-4.050915351098	-0.308414627328	2.119936615555
H	-4.052852313843	-1.830187260478	1.175876846388
C	-3.626682886827	1.415384981831	-0.021867950531
H	-4.034585165115	1.934739443405	-0.906874658573
H	-4.018529281712	1.923013644335	0.876723826684
C	-3.646209042300	-0.771953634880	-1.299809754602
H	-4.053989902187	-1.798134489001	-1.284180826962
H	-4.053136392400	-0.250799121359	-2.185698805703
C	-4.101219198270	-0.037395892885	-0.029869333714
C	3.647261931453	0.770788835038	-1.299350324610
H	4.056295204029	1.796454773885	-1.283927539520
H	4.053456279973	0.248902789431	-2.185143664356
C	3.623880690575	-1.416101379482	-0.020942043219
H	4.031406666381	-1.936602454139	-0.905469501749
H	4.014423746436	-1.923902550276	0.878116849873
C	3.641509127245	0.805950889305	1.221619495631
H	4.051049717606	0.307835486868	2.120413917605
H	4.054832162568	1.829239641576	1.175799830413
C	4.100930507510	0.035869530913	-0.029329518573

C	-0.584514565138	-2.981917305631	2.557403772188
H	-1.203296985970	-2.266156876372	3.124327745314
H	-1.209441752686	-3.848735581170	2.289517614358
H	0.233285329300	-3.325854155153	3.210498448469
C	0.584787354942	2.983361510303	2.557291779692
H	1.199491971087	2.266158255227	3.126856071693
H	1.213878569115	3.847126841990	2.289276819383
H	-0.232835419295	3.331965990951	3.208195405863

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