

Supporting Information

DFT Calculation-Assisted Prediction of the Copolymerization Between Cyclic Ketene Acetals with Traditional Vinyl Monomers

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Table of contents

I – Figure S1

II – Figure S2

III – Figure S3

IV – Table S1

V – Table S2

VI – Table S3

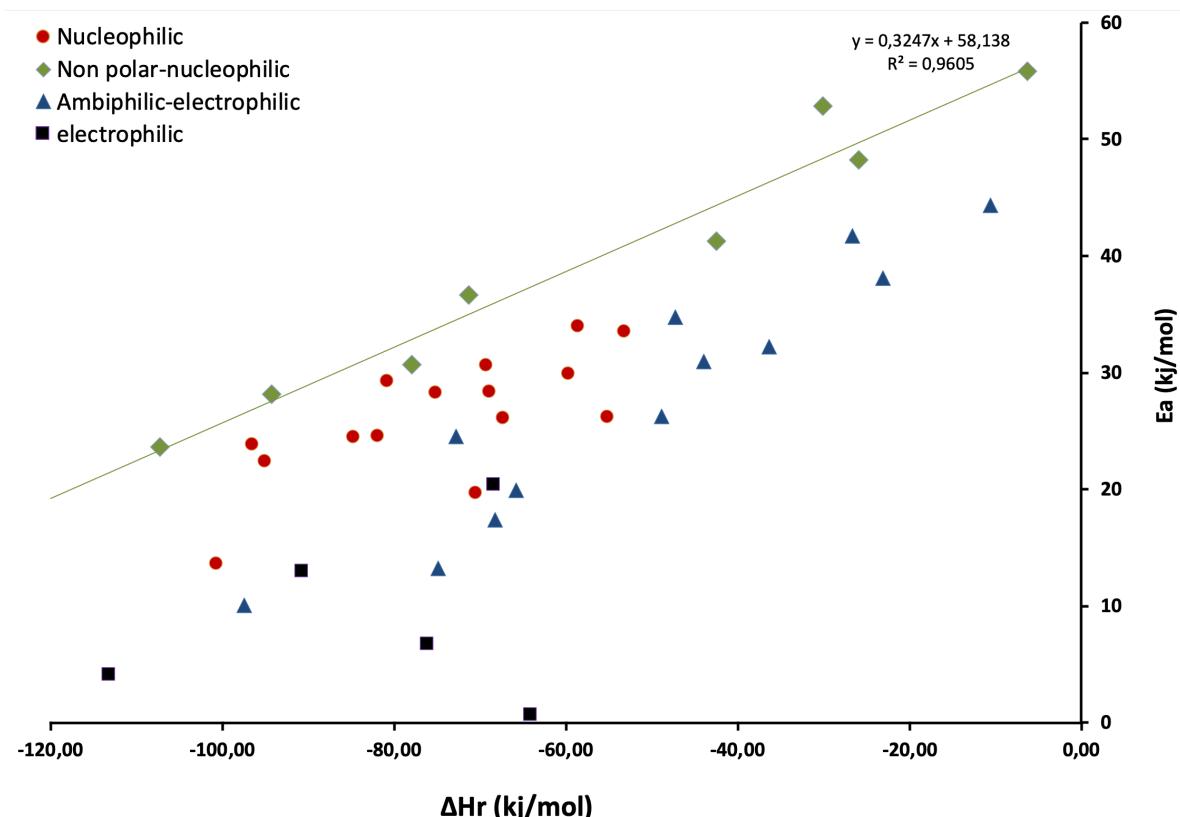
VII – Table S4

VIII – Isoprene polymerization

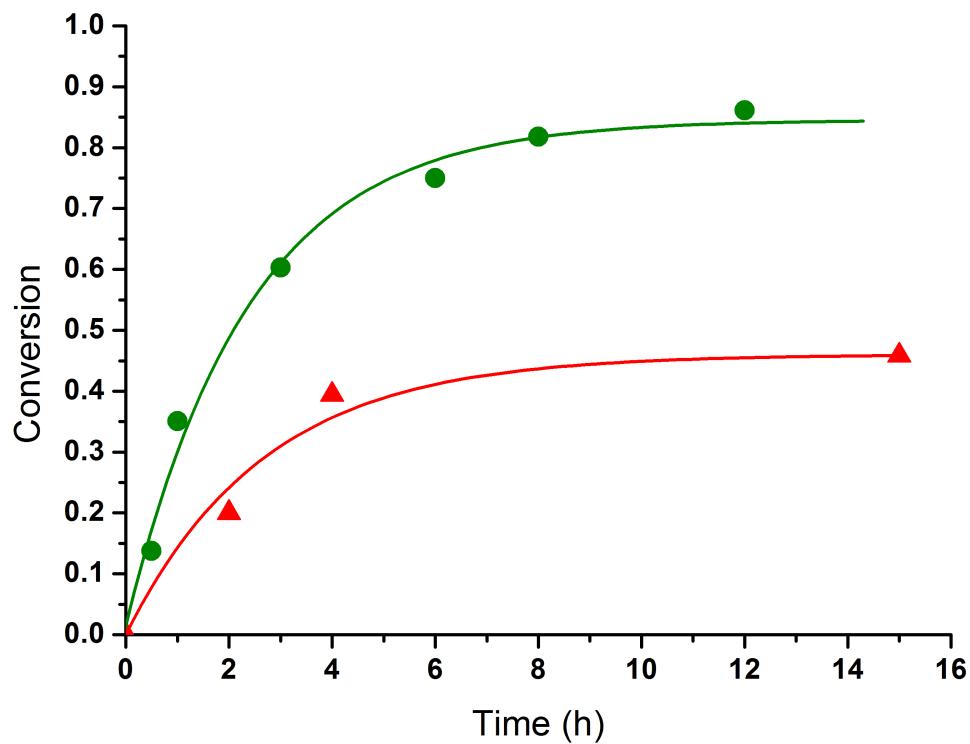
XI – Poly(MDO-*alt*-CF₃VAc) degradation and formulation in nanoparticles

X – DFT calculations

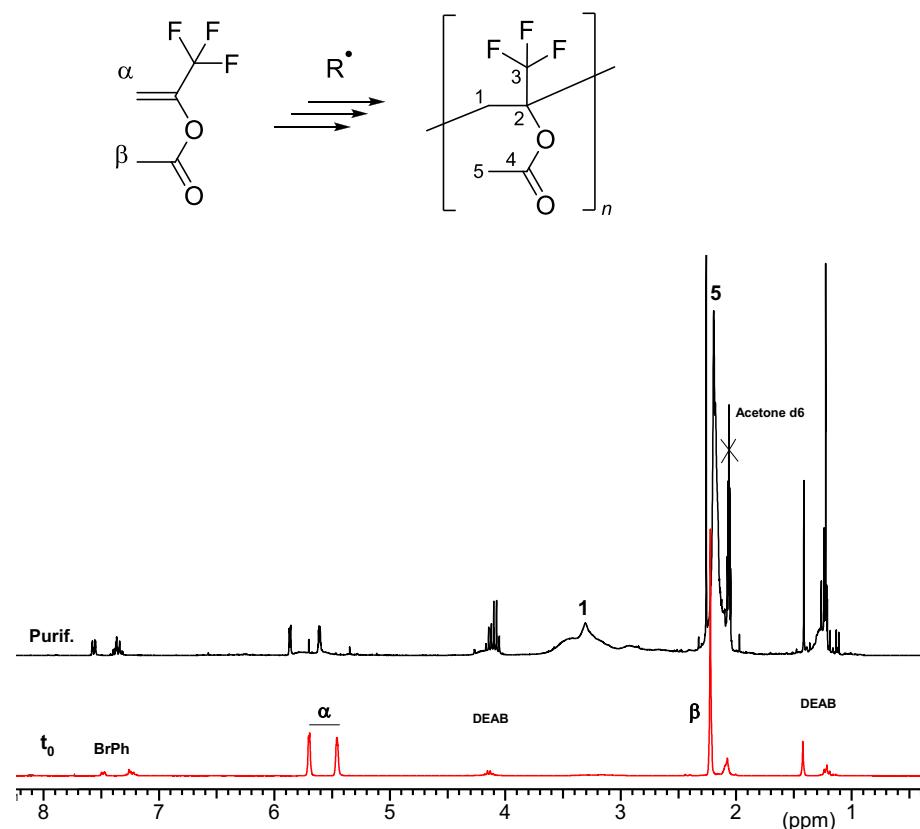
I- Figure S1. Activation energies for the full set of addition reactions versus the reaction enthalpy



II- Figure S2. Conversion vs Time plot for the homopolymerization of MDO (●) and CF₃VAc (▲) at 70 °C initiated with 3 mol% of DEAB



III- Figure S3. Radical homopolymerization of CF₃VAc



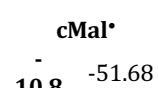
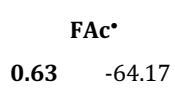
Conversion determined using:

$$\chi_{CF_3VAc} = \frac{(I_{2,6-3,82})_t}{2(I_{5,8})_t + (I_{2,6-3,82})_t}$$

IV- Table S1: Activation enthalpies ΔH^\ddagger and reaction enthalpies ΔH_r of the addition reactions on the C7B monomer calculated at the UB3-LYP/6-31G(d) level

Radicals	$\Delta H^\ddagger \quad \Delta H_r$			
	I	II	III	
Transition state				
G=				
Me [•]		23.55 -107.4		
Aromatic		41.25 Bn [•] -42.58	 48.23 Sty [•] -25.96	 55.78 MSty [•] -6.36
Alkyl		28.11 Et [•] -94.38	 30.68 iPr [•] -78.03	 33.91 tBu [•] -58.67
Methoxyalkyl		29.17 MEt [•] -80.84	 30.58 EEt [•] -69.36	 33.45 PEt [•] -53.24
Hydroxyalkyl		13.54 MOH [•] -100.74	 28.23 EOH [•] -75.15	 29.81 POH [•] -59.77
Acetylalkyl		22.27 MAC [•] -95.06	 24.48 EAc [•] -81.89	 26.03 PAc [•] -67.30
Chloroalkyl		23.77 MCl [•] -96.52	 24.35 ECl [•] -84.77	 28.3 PCl [•] -68.94
Phophonoalkyl		10.04 MP [•] -97.51	 24.52 EP [•] -72.88	 34.75 PP [•] -47.31
Methoxycarbonylalkyl		13.17 MEst [•] -74.98	 26.18 EEst [•] -48.91	 38.1 PEst [•] -23.20
Methylcarbonylalkyl		17.35 MCO [•] -68.35	 24.99 ECO [•] -36.39	 44.3 PCO [•] -10.68
Cyanoalkyl		19.84 MCN [•] -65.88	 30.89 ECN [•] -44.05	 41.68 PCN [•] -26.69
Trifluoromethylalkyl		4.01 MF [•] -113.27	 12.8 EF [•] -90.77	 20.33 PF [•] -68.39

Electrophilic



V- Table S2. Addition activation enthalpies calculated at the UB3-LYP/6-31G(d) level of theory (ΔH^\ddagger in $\text{kJ}\cdot\text{mol}^{-1}$), and corresponding addition rate at 70°C (in brackets, $\text{L}\cdot\text{mol}^{-1}\cdot\text{s}^{-1}$) as well as calculated reactivity ratios

MONOMER	1	2												
		CKA	STY	VE	VAc	VC	VDC	VP	MA	MMA	AN	CF_3VAc	Iso	
RAD														
1	ET [•]	$\text{H}_3\text{C}-\dot{\text{C}}\text{H}_2$	28.11 (2.2×10^3)	15.77 (1.7×10^5)	28.02 (7.6×10^2)	23.97 (9.6×10^3)	20.46 (3.3×10^4)	15.65 (1.8×10^5)	13.8 (3.4×10^5)	11.23 (8.4×10^5)	13.32 (4.0×10^5)	9.21 (1.7×10^6)	13.45 (3.8×10^5)	17.16 (1.1×10^5)
	STY [•]		48.23 (6.2×10^{-1})	35.32 (5.7×10^1)										
	VE [•]			30.6 (2.9×10^2)		30.72 (2.8×10^2)								
	VAc [•]				24.48 (2.5×10^3)		20.27 (1.1×10^4)							
	VC [•]					24.35 (2.7×10^3)		20.81 (9.2×10^3)						
2	VDC [•]					19.61 (4.4×10^3)		22.08 (1.9×10^3)						
	VP [•]						24.52 (2.5×10^3)		20.04 (1.2×10^4)					
	MA [•]						26.18 (9.2×10^2)			20.68 (9.6×10^3)				
	MMA [•]							38.1 (6.8)			30.02 (1.1×10^2)			
	AN [•]							30.89 (2.7×10^2)			29.78 (4.0×10^2)			
	$\text{CF}_3\text{VAc}^{\bullet}$							6.67 (4.1×10^5)				12.05 (6.3×10^4)		
	Iso [•]							46.79 (1.02)					40.39 (9.6)	
Reactivity ratio	r calc. 70°C	$r_1 = \frac{k_{11}}{k_{12}}$	0.013	0.97	0.23	0.068	0.013	0.007	0.003	0.006	0.001	0.006	0.022	
		$r_2 = \frac{k_{22}}{k_{21}}$	92	0.99	4.3	3.4	0.42	4.8	10	17	1.48	0.16	9.42	
	r litt.	r_1	0.021	-	~0.7	-	-	-	0.023	~0.045	-	-	-	
		r_2	22.6	-	~1.6	-	-	-	26.5	3.5-34.1	-	-	-	

VI- Table S3. Addition activation enthalpies calculated at the UB3-LYP/6-31G(d) level of theory (ΔH^\ddagger in $\text{kJ}\cdot\text{mol}^{-1}$) for the isoprene BMDO system, and corresponding addition rate at 70°C (in brackets, $\text{L}\cdot\text{mol}^{-1}\cdot\text{s}^{-1}$) as well as calculated reactivity ratios

MONO		1	2
RAD		BMDO	Iso
1	BMDO [•]	50.34 (2.9×10^{-1})	35.94 (4.6×10^1)
2	Iso [•]	54.72 (6.3×10^{-2})	40.3 (9×9)
Reactivity ratio	r calc. 70°C	$r_1 = \frac{k_{11}}{k_{12}}$ 0.006	$r_2 = \frac{k_{22}}{k_{21}}$ 157

VII- Table S4. Bulk polymerization of MDO and CF₃VAc – experimental results

Initial MDO:CF ₃ VAc	Time (h)	M _n (g.mol ⁻¹)	M _w (g.mol ⁻¹)	D
0 : 100	5	19600	29800	1.5
		21900	30600	1.40
18 : 82	0.5	12900	21000	1.62
	1	12500	20400	1.63
	3	10900	18200	1.68
45 : 55	0.5	37700	73100	1.9
	1	36700	79700	2.2
	3	15200	41900	2.8
	4	14500	44900	3.1
82 : 18	10	24000	52700	2.19
	0.5	18400	49700	2.71
	1	11900	54400	4.58
	3	22700	52600	2.31
	6	11100	20300	1.82

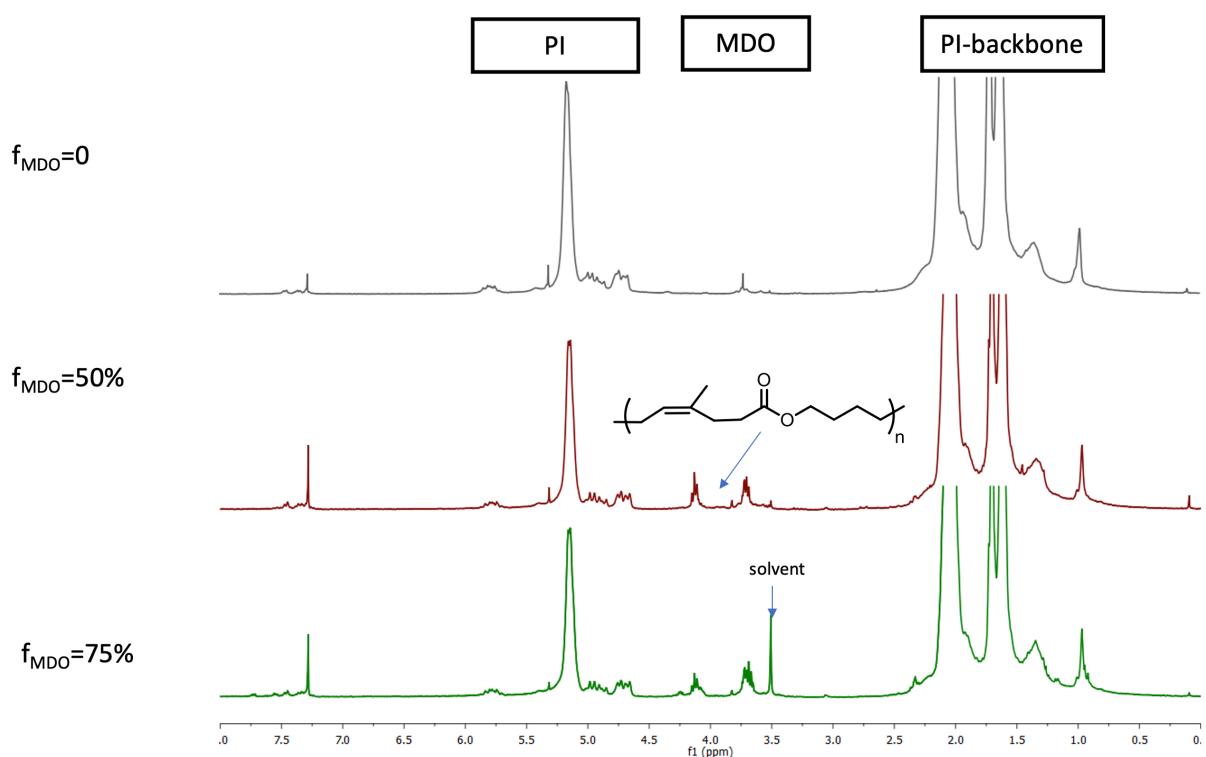
VIII- Isoprene Polymerization

- Polymerization:

Dicumyl peroxide (25 mg, 9.246×10^{-2} mmol) was placed in a 15 mL-capacity pressure tube (Ace Glass 8648) with a stir bar and fitted with a plunger valve, a thermowell. After the addition of isoprene (4 mL, 40.0 mmol) and dioxane (5 mL) under the fumehood, the tube underwent three to five freeze-pump-thaw degassing cycles and was then backfilled with argon. The tube was then sealed and placed in a preheated oil bath at 115 °C for 30 h. After the reaction, the tube was cooled in an ice bath to room temperature. The reaction solution was then transferred into a vial. Unreacted dioxane and isoprene were then removed via rotary evaporation and the resulting polymer was further dried under vacuum overnight. The conversion was determined by gravimetry using the dried polymer, which was then precipitated in cold methanol to give the purified polymer as a colorless viscous oil.

For $f_{MDO} = 0.50$, dicumyl peroxide (12.5 mg, 4.623×10^{-2} mmol); isoprene (2 mL, 20.0 mmol); dioxane (5 mL) and MDO (2.279 g, 20.0 mmol) were placed in a 15 mL-capacity pressure tube (Ace Glass 8648) with a stir bar inside. For $f_{MDO} = 0.75$, dicumyl peroxide (12.5 mg, 4.623×10^{-2} mmol); isoprene (2 mL, 20.0 mmol); dioxane (5 mL) and MDO (6.838 g, 60.0 mmol) were placed in a 38 mL-capacity pressure tube (Ace Glass 8648) with a stir bar inside. All reactions were fitted with plunger valves, thermowells. All polymers were characterized by SEC (chloroform), ^1H and ^{13}C NMR in CDCl_3 .

Target MDO	M_n	\bar{D}	F_{MDO}	M_n after degradation 1h	M_n after degradation 24h	M_n loss
0%	10600	1,52	0	--	10100	0%
75%	10200	1,36	7%	5090	5080	-50%
50%	6900	1,41	5%	4090	4400	-41%



- Characterization:

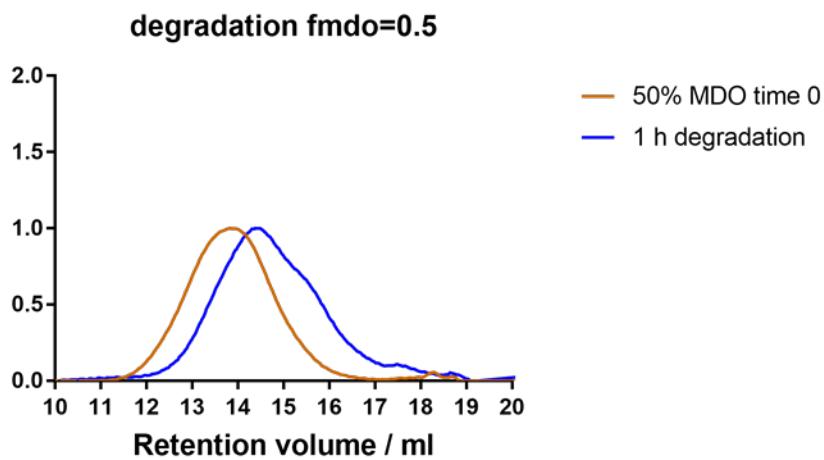
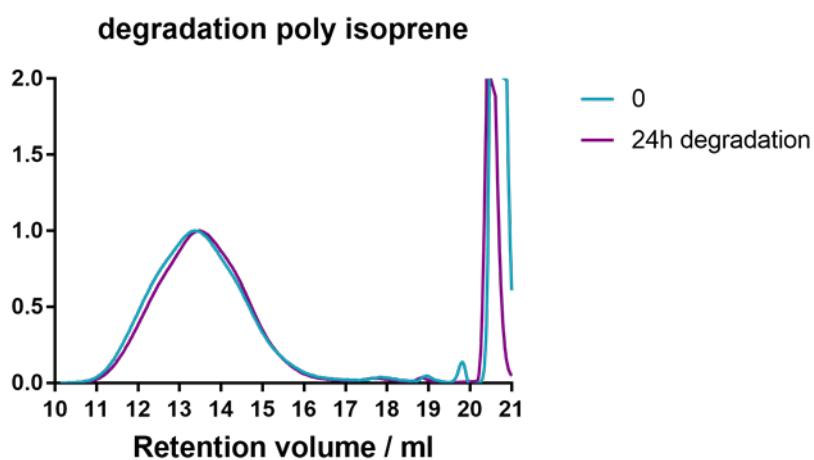
Size exclusion chromatography (SEC): SEC was performed at 30 °C with two columns from Polymer Laboratories (PL-gel MIXED-D; 300 × 7.5 mm; bead diameter, 5 µm; linear part, 400–400 000 g·mol⁻¹) and a differential refractive index detector (Spectrasystem RI-150 from Thermo Electron Corp.), using chloroform (CHCl₃) as eluent at a flow rate of 1 mL·min⁻¹ and toluene as a flow-rate marker. A conventional calibration curve was based on polystyrene (PS) standards (peak molar masses, $M_p = 162\text{--}523,000 \text{ g}\cdot\text{mol}^{-1}$) from Polymer Laboratories. A polyisoprene (PI) calibration curve was constructed by converting the PS standard peak molecular weights (MPS) to PI molecular weights (MPI) using Mark-Houwink-Sakurada (MHS) constants determined for both polymers in CCl₄ at 25 °C. For PI, the MHS constants used were $K_{PI} = 2.44 \times 10^4$ and $\alpha_{PI} = 0.712$. For PS, $K_{PS} = 7.1 \times 10^4$ and $\alpha_{PS} = 0.54$ ($M_w < 16,700 \text{ g}\cdot\text{mol}^{-1}$) or $K_{PS} = 1.44 \times 10^4$ and $\alpha_{PS} = 0.713$ ($M_w > 16,700 \text{ g}\cdot\text{mol}^{-1}$).¹ This technique allowed the M_n (the number-average molar mass), M_w (the weight-average molar mass), and M_w/M_n (the dispersity, D) to be determined.

The SEC of the degraded copolymers was performed in the presence of 0.1 % (v/v) of trifluoroacetic acid (TFA, 99%) in chloroform (in both the mobile phase and the sample) to avoid the formation of aggregates and/or interaction with the columns because of carboxylic acid chain ends.

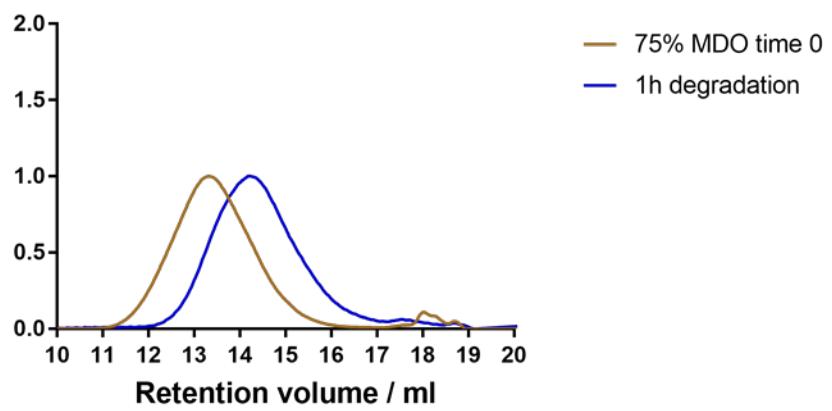
¹ Harrisson, S., Nicolas, J., Maksimenko, A., Bui, D.T., Mougin, J. and Couvreur, P. (2013), Nanoparticles with In Vivo Anticancer Activity from Polymer Prodrug Amphiphiles Prepared by Living Radical Polymerization. *Angew. Chem. Int. Ed.*, 52: 1678-1682.

- Degradation:

In a 5-mL vial, 20 mg of purified copolymer was dissolved in 1 mL of THF. After solubilization, 1 mL of potassium hydroxide solution (KOH, 5 wt% in MeOH) was added and the cloudy mixture then stirred at room temperature. Samples (1 mL) were periodically taken, immediately dried under vacuum, and mixed with 2 mL of chloroform, followed by filtration with a 0.2 μ m PTFE filter to remove salts. After filtration, a HCl solution (1ml, 1 mol.L⁻¹) was added into the solution to wash the organic medium three times. The solvent was then removed under reduced pressure and the degradation products analyzed by SEC in CHCl₃.



degradation fmdo=0.75



IX- Poly(MDO-*alt*-CF₃VAc) degradation and formulation in nanoparticles

- Degradation:

15 mg of poly(MDO-*alt*-CF₃VAc) was dissolved in 750 µL of THF. After solubilization, 750 µL of potassium hydroxide solution (KOH, 5 wt% in MeOH) was added and the cloudy mixture stirred at room temperature for 15 minutes. At the end of the degradation, the mixture was dried under reduced pressure. Next, 1.5mL of chloroform was added followed by filtration with a 0.2 µm PTFE filter to remove salts. The solvent was then removed under reduced pressure and the isolated degradation products were analyzed by SEC in THF.

- Nanoparticles preparation:

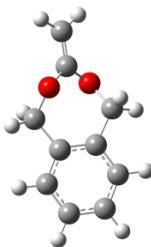
4 mg of copolymer was dissolved in 1.34 mL of THF and the solution was added dropwise to 20 mL of a solution of Pluronic F127 (1 wt% in Milli-Q water) with stirring. The THF was then evaporated at room temperature using rotary evaporation. The resulting nanoparticles were analyzed by DLS (Zetasizer Nano Series Malvern Instruments).

X- DFT Calculations

All the calculations were performed using the Gaussian 16 package.² The geometry of all species was optimized at the (U)B3LYP/6-31G(d) level of theory.³ Vibrational frequencies were calculated to insure, that the obtained geometries were minima or transition states (0 or 1 imaginary frequency respectively) and to determine enthalpy values (standard frequency scale factor value 0.9603 was used). Intrinsic reaction coordinate (IRC) calculations, at the same level of theory, were performed to insure that the transition states led to the expected reactants and products.

UB3LYP/6-31G(d)

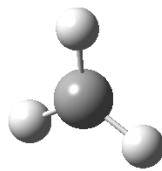
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C	0.008612	-0.000436	2.377477
C	2.329122	-0.042791	1.936427
H	-0.328757	0.997993	0.118024
H	-0.644879	-0.533169	-0.713134
H	3.181442	0.440512	2.421798
O	-0.229122	-0.737469	1.253436
C	2.526506	-0.045876	0.434760
C	1.443660	-0.099764	-0.459360
C	1.696023	-0.158448	-1.834317
C	2.998993	-0.157524	-2.330938
C	4.073417	-0.102219	-1.443842
C	3.830698	-0.044427	-0.071947
H	5.094329	-0.099758	-1.815625
H	3.172079	-0.203904	-3.402563
H	0.857161	-0.207407	-2.525601
H	4.668429	0.004611	0.620701
O	1.178723	0.702497	2.374554
H	2.260806	-1.068691	2.322332
C	-0.841100	0.030778	3.404465
H	-0.564837	0.529203	4.324428
H	-1.810912	-0.442393	3.322909

Sum of electronic and thermal Enthalpies = - 537.308006 Hartree

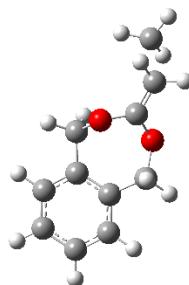
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C	0.126019	0.218271	0.089109
H	-0.054428	-0.094273	1.109950
H	1.028328	-0.094273	-0.421299
H	-0.595807	0.843422	-0.421299

Sum of electronic and thermal Enthalpies = -39.805573 Hartree
 $\langle S^2 \rangle = 0.753765$

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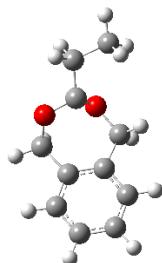


C	0.002817	-0.000009	-0.003525
C	0.000132	0.002626	2.362284
C	2.322512	0.000481	1.931773
H	-0.344928	1.035093	0.111860
H	-0.637688	-0.488357	-0.743048
H	3.167819	0.487822	2.425416
O	-0.234443	-0.713841	1.225512
C	2.522083	0.024199	0.430317
C	1.443588	-0.032924	-0.469287
C	1.703079	-0.068860	-1.843858
C	3.007693	-0.042240	-2.335234
C	4.077493	0.016744	-1.442909
C	3.828041	0.051631	-0.071503
H	5.099860	0.039612	-1.809988
H	3.185587	-0.071218	-3.406679
H	0.867885	-0.119912	-2.539421
H	4.662335	0.102923	0.625150
O	1.161192	0.719685	2.382160
H	2.268860	-1.033078	2.299810
C	-2.215862	2.059707	3.093237
H	-2.727557	1.857584	2.157602
H	-2.814425	2.001910	3.997697
H	-1.431625	2.808995	3.071567
C	-0.914060	0.100509	3.358436
H	-1.813049	-0.497821	3.297733
H	-0.595621	0.459481	4.327929

Sum of electronic and thermal Enthalpies = -577.104609 Hartree
 $\langle S^2 \rangle = 0.774228$

Imaginary frequency = i386 cm⁻¹

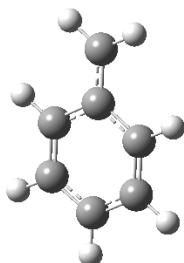
AT_A0-MEadd_8



C	0.250386	-0.532247	-0.009337
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C	2.476757	0.022839	1.987632
H	-0.715453	-0.070755	-0.259203
H	0.372308	-1.410343	-0.655120
H	3.332919	0.394271	2.555320
O	0.191956	-1.064641	1.315712
C	2.399884	0.726985	0.647539
C	1.364247	0.468696	-0.268765
C	1.349749	1.148788	-1.492131
C	2.349984	2.060080	-1.825866
C	3.379652	2.315775	-0.920505
C	3.391058	1.655910	0.307104
H	4.161308	3.030506	-1.162601
H	2.319375	2.572826	-2.783484
H	0.540638	0.959318	-2.195378
H	4.184736	1.863060	1.021415
O	1.349039	0.259056	2.838792
H	2.598287	-1.058645	1.850273
C	-2.325304	-0.448070	2.867899
H	-2.430573	-1.212862	2.091336
H	-3.031245	-0.682870	3.671836
H	-2.611752	0.516815	2.434347
C	-0.888531	-0.409429	3.398691
H	-0.647576	-1.372145	3.884146
H	-0.781149	0.360058	4.171551

Sum of electronic and thermal Enthalpies = -577.154604 Hartree
 $\langle S^2 \rangle = 0.752568$

AT_BZ1

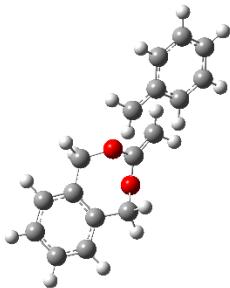


C	0.007692	0.000000	0.004483
C	0.007263	0.000000	1.407065
C	1.201511	0.000000	2.110146
C	2.457252	0.000000	1.432029

C	2.428234	0.000000	0.005185
C	1.227807	0.000000	-0.687295
H	-0.930868	0.000000	-0.542488
H	-0.935911	0.000000	1.947532
H	1.194484	0.000000	3.197455
H	3.370791	0.000000	-0.536919
H	1.233106	0.000000	-1.774334
C	3.672547	0.000000	2.140275
H	3.690593	0.000000	3.225439
H	4.625598	0.000000	1.621043

Sum of electronic and thermal Enthalpies = -270.797928 Hartree
 $\langle S^2 \rangle = 0.783706$

AT_A0-BZts



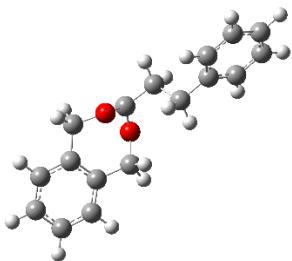
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C	0.005237	-0.012677	2.381913
C	2.326290	-0.005379	1.939699
H	-0.318111	1.041466	0.126086
H	-0.661883	-0.473679	-0.725783
H	3.169699	0.503992	2.413878
O	-0.264533	-0.709312	1.242607
C	2.516074	-0.024184	0.436983
C	1.433069	-0.083383	-0.456978
C	1.686766	-0.162886	-1.830928
C	2.989748	-0.177551	-2.327002
C	4.063886	-0.116535	-1.440044
C	3.820524	-0.038246	-0.069454
H	5.085069	-0.125687	-1.810878
H	3.162858	-0.240132	-3.397753
H	0.848120	-0.215356	-2.522103
H	4.658387	0.014225	0.622794
O	1.159795	0.713296	2.380896
H	2.284329	-1.028273	2.338365
C	-0.906902	0.108501	3.396640
H	-0.542045	0.399554	4.374037
H	-1.778648	-0.533433	3.366699
C	-2.098896	1.954286	3.180654
C	-2.955735	2.016734	4.335362
H	-1.252372	2.632617	3.129196
C	-4.236218	1.409945	4.336928
C	-2.528612	2.637660	5.535464
C	-5.042591	1.431178	5.468972
H	-4.590098	0.925820	3.429047
C	-3.338647	2.656193	6.665057
H	-1.550001	3.112382	5.562592
C	-4.601669	2.053540	6.642569

H	-6.023598	0.962952	5.439210
H	-2.987585	3.145932	7.570277
H	-5.233829	2.070210	7.526067
H	-2.547619	1.706114	2.222809

Sum of electronic and thermal Enthalpies = -808.090223 Hartree
 $\langle S^2 \rangle = 0.783852$

Imaginary frequency = 1500 cm⁻¹

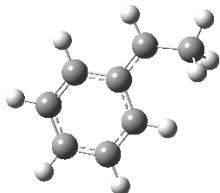
AT_A0-BZpro



C	-0.087831	0.040296	0.239805
C	0.102789	-0.324483	2.605075
C	2.374706	-0.089731	2.009701
H	-0.360788	1.070624	0.501352
H	-0.796552	-0.314246	-0.513698
H	3.218175	0.442025	2.460484
O	-0.302854	-0.812408	1.383097
C	2.458011	0.004056	0.499256
C	1.317749	-0.001752	-0.323052
C	1.482128	0.017087	-1.713211
C	2.748826	0.049377	-2.294585
C	3.878977	0.059502	-1.477849
C	3.726087	0.038809	-0.092330
H	4.873628	0.086456	-1.914441
H	2.850827	0.063018	-3.376228
H	0.599445	0.006143	-2.349267
H	4.607966	0.050592	0.545239
O	1.199633	0.501693	2.580458
H	2.427445	-1.139593	2.331180
C	-0.960654	0.083297	3.578001
H	-0.510631	0.172196	4.573119
H	-1.707018	-0.717540	3.627061
C	-1.677503	1.423093	3.227705
C	-2.720658	1.801296	4.253949
H	-0.920523	2.211923	3.149984
C	-4.039001	1.336895	4.144806
C	-2.384634	2.590187	5.363126
C	-4.993527	1.650243	5.112991
H	-4.320010	0.727501	3.288061
C	-3.335380	2.906267	6.334281
H	-1.367464	2.964063	5.462044
C	-4.644485	2.436579	6.212640
H	-6.011455	1.283830	5.006191
H	-3.054600	3.523633	7.183909
H	-5.387289	2.684388	6.966251
H	-2.145943	1.321132	2.241264

Sum of electronic and thermal Enthalpies = -808.122153 Hartree
 $\langle S^2 \rangle = 0.752871$

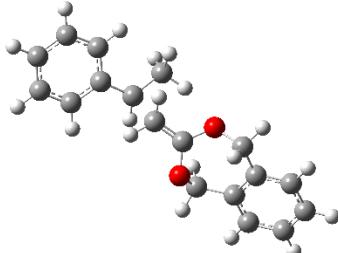
AT_STY



C	0.002009	0.103967	0.032611
C	0.150474	-0.496005	1.289834
C	1.409140	-0.663236	1.850304
C	2.582222	-0.231271	1.166009
C	2.401821	0.375810	-0.111339
C	1.140436	0.537960	-0.661848
H	-0.986081	0.231830	-0.400362
H	-0.727923	-0.834802	1.833725
H	1.503362	-1.130653	2.826025
H	3.280480	0.714801	-0.655600
H	1.034571	1.004599	-1.638026
C	3.881174	-0.385752	1.707277
H	4.715933	-0.025097	1.110750
C	4.185244	-1.007064	3.035132
H	3.834978	-2.048720	3.095113
H	5.261265	-1.011065	3.231213
H	3.700584	-0.470019	3.864581

Sum of electronic and thermal Enthalpies = -310.087199 Hartree
 $\langle S^2 \rangle = 0.779926$

AT_A0-STYts



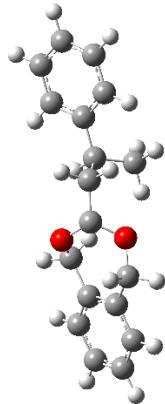
C	0.002491	0.003586	-0.007531
C	-0.004312	0.007563	2.365699
C	2.319914	0.001973	1.939001
H	-0.315578	1.049564	0.095989
H	-0.646745	-0.472636	-0.747136
H	3.163546	0.504370	2.420278
O	-0.265568	-0.692985	1.225528
C	2.520873	-0.016423	0.437748
C	1.444290	-0.074138	-0.464034
C	1.707437	-0.152434	-1.836323
C	3.013660	-0.167336	-2.323582
C	4.081508	-0.107493	-1.429010
C	3.828708	-0.030284	-0.060028
H	5.105308	-0.116767	-1.792591
H	3.194255	-0.229412	-3.393117
H	0.873236	-0.204005	-2.532946
H	4.662035	0.021782	0.637707

O	1.154972	0.729064	2.371391
H	2.266164	-1.020823	2.336272
C	-0.930884	0.126776	3.373107
H	-0.568373	0.404798	4.356508
H	-1.780062	-0.545228	3.339208
C	-2.176167	1.908268	3.180922
C	-3.208189	1.702208	4.181840
C	-1.181349	3.034566	3.291363
C	-4.343054	0.912160	3.874722
C	-3.116406	2.215714	5.497128
H	-0.658465	3.035379	4.255075
H	-0.416492	2.956581	2.513025
H	-1.669947	4.015805	3.187880
C	-5.326333	0.652798	4.821802
H	-4.442270	0.506719	2.869564
C	-4.104138	1.954960	6.443127
H	-2.265757	2.830620	5.775974
C	-5.215372	1.172533	6.116522
H	-6.187715	0.046770	4.551190
H	-4.008102	2.368490	7.444356
H	-5.984570	0.972702	6.857445
H	-2.496690	1.685622	2.163964

Sum of electronic and thermal Enthalpies = -847.376834 Hartree
 $\langle S^2 \rangle = 0.781729$

Imaginary frequency = i517 cm⁻¹

AT_A0-STYpro

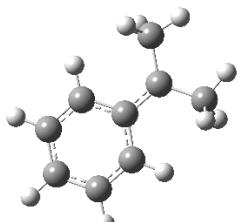


C	-0.045860	-0.025328	0.289707
C	0.204568	-0.169317	2.674396
C	2.452459	0.103741	2.013430
H	-0.380633	1.005782	0.462366
H	-0.741545	-0.488874	-0.415272
H	3.283403	0.697331	2.406383
O	-0.190631	-0.783223	1.507300
C	2.504048	0.089865	0.499025
C	1.351255	-0.032516	-0.296407
C	1.490088	-0.104336	-1.687684
C	2.742887	-0.050452	-2.296780
C	3.885345	0.073841	-1.507009
C	3.758009	0.145075	-0.120641
H	4.869480	0.118985	-1.965353
H	2.824799	-0.108904	-3.378634
H	0.598168	-0.205358	-2.302612

H	4.649193	0.246997	0.495578
O	1.266370	0.694789	2.563445
H	2.548528	-0.916619	2.410635
C	-0.864632	0.213245	3.651667
H	-0.385303	0.489575	4.598138
H	-1.464637	-0.684069	3.843469
C	-1.840258	1.354575	3.209194
C	-3.044123	1.411124	4.138679
C	-1.133555	2.716846	3.094046
C	-4.318712	1.060048	3.674664
C	-2.914821	1.794129	5.482764
H	-0.736218	3.041722	4.062686
H	-0.290272	2.668074	2.399026
H	-1.831552	3.486510	2.746057
C	-5.430636	1.093076	4.518453
H	-4.441345	0.757534	2.636689
C	-4.021767	1.827409	6.330716
H	-1.938695	2.070800	5.873970
C	-5.286057	1.477671	5.851521
H	-6.409151	0.818509	4.132412
H	-3.896728	2.127912	7.368038
H	-6.149021	1.504891	6.511587
H	-2.215093	1.078414	2.214659

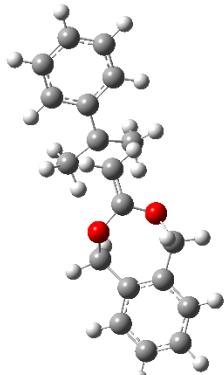
Sum of electronic and thermal Enthalpies = -847.405093 Hartree
 $\langle S^2 \rangle = 0.752923$

AT_MSTY



C	0.098596	0.298772	0.052279
C	0.051874	0.162077	1.475072
C	1.346844	-0.054841	-0.710940
C	1.171762	-0.308969	2.219823
C	-1.116990	0.489864	2.221397
H	1.635393	-1.107497	-0.570839
H	1.214714	0.106832	-1.784498
H	2.212482	0.545580	-0.392920
C	1.121513	-0.439928	3.600716
H	2.086619	-0.572357	1.699128
C	-1.157450	0.355491	3.602283
H	-1.997682	0.853179	1.701934
C	-0.041152	-0.110032	4.307392
H	1.996006	-0.802718	4.135445
H	-2.067109	0.615419	4.138237
H	-0.076649	-0.213866	5.388211
C	-1.099594	0.798902	-0.709226
H	-1.980350	0.154462	-0.568034
H	-1.403102	1.807536	-0.390608
H	-0.897020	0.843420	-1.783053

Sum of electronic and thermal Enthalpies = -349.374372 Hartree
 $\langle S^2 \rangle = 0.775865$

AT_A0-MSTYts

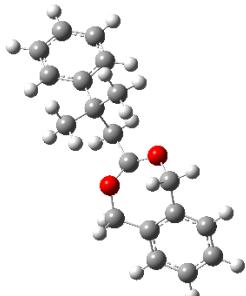
C	-0.000620	0.003877	-0.001191
C	-0.000910	-0.000089	2.376709
C	2.321604	0.002989	1.943837
H	-0.668484	-0.445697	-0.740736
H	-0.270486	1.063519	0.096676
H	3.162311	0.534804	2.398248
O	-0.304999	-0.675038	1.231543
C	2.516701	-0.080653	0.443810
C	1.437179	-0.139335	-0.454251
C	1.696321	-0.278383	-1.822694
C	3.000657	-0.353198	-2.309384
C	4.071200	-0.292994	-1.418020
C	3.822873	-0.155325	-0.053044
H	5.093675	-0.348648	-1.781215
H	3.177607	-0.461821	-3.375809
H	0.860099	-0.330016	-2.516803
H	4.658328	-0.102904	0.642202
O	1.150094	0.734518	2.351382
H	2.281186	-1.002088	2.386292
C	-0.868979	0.054159	3.445332
H	-0.436701	0.270840	4.416206
H	-1.694506	-0.648870	3.433326
C	-2.163582	1.784913	3.487506
C	-2.955030	1.491938	4.691495
C	-1.159906	2.918274	3.553935
C	-2.526881	1.888465	5.981809
C	-4.161675	0.753297	4.626993
H	-0.476210	2.836985	4.404289
H	-0.541859	2.936147	2.651036
H	-1.666304	3.893311	3.632229
C	-3.254753	1.569321	7.124523
H	-1.613280	2.462473	6.094467
C	-4.887984	0.435589	5.771165
H	-4.543452	0.428158	3.664957
C	-4.442545	0.839865	7.031901
H	-2.892706	1.897497	8.096075
H	-5.812491	-0.129126	5.676206
H	-5.011124	0.593620	7.924486
C	-2.863315	1.683550	2.146922
H	-3.317220	0.702631	1.972793
H	-3.661957	2.436063	2.054333
H	-2.153708	1.861953	1.332179

Sum of electronic and thermal Enthalpies = -886.66113 Hartree

$\langle S^2 \rangle = 0.779102$

Imaginary frequency = i518 cm⁻¹

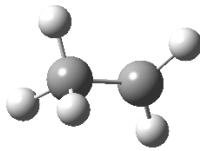
AT_A0-MSTYpro



C	0.073273	0.867506	-0.407482
C	-0.073593	0.567906	1.942608
C	2.258074	0.939873	1.707482
H	-0.573801	0.685851	-1.268431
H	0.271136	1.944629	-0.347584
H	2.919020	1.813918	1.659033
O	-0.713562	0.474829	0.725446
C	2.368286	0.120671	0.432338
C	1.366250	0.091110	-0.555679
C	1.571549	-0.677484	-1.707897
C	2.749032	-1.397759	-1.902306
C	3.739044	-1.369276	-0.920549
C	3.539192	-0.621272	0.238475
H	4.658637	-1.933521	-1.050119
H	2.886239	-1.984359	-2.806430
H	0.790301	-0.710243	-2.463939
H	4.307787	-0.611287	1.009227
O	0.961876	1.482009	1.980022
H	2.583400	0.327518	2.560499
C	-0.967429	0.448641	3.136129
H	-0.337311	0.222118	4.005066
H	-1.601652	-0.428894	2.969370
C	-1.897455	1.664035	3.530298
C	-2.740047	1.205441	4.736469
C	-1.029831	2.891807	3.864716
C	-2.598473	1.761120	6.016284
C	-3.685883	0.175449	4.584619
H	-0.296415	2.676070	4.649776
H	-0.470627	3.210742	2.982064
H	-1.650589	3.732070	4.197326
C	-3.367731	1.314160	7.094309
H	-1.883553	2.558040	6.187541
C	-4.455035	-0.275206	5.655709
H	-3.829773	-0.285730	3.611386
C	-4.300373	0.293922	6.921302
H	-3.232994	1.770395	8.072034
H	-5.177867	-1.072284	5.499946
H	-4.899248	-0.054071	7.758806
C	-2.833612	2.043062	2.360062
H	-3.429256	1.193584	2.012399
H	-3.524582	2.835209	2.671168
H	-2.256594	2.405414	1.504603

Sum of electronic and thermal Enthalpies = -886.684802 Hartree
 $\langle S^2 \rangle = 0.752983$

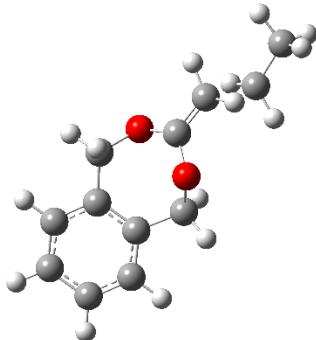
AT_ETHYL



C	-0.021991	-0.023156	-0.015663
H	-0.009822	0.016711	1.080541
H	1.016063	0.017212	-0.368110
H	-0.403039	-1.024822	-0.285862
C	-0.848312	1.069448	-0.600455
H	-0.670946	1.421791	-1.611470
H	-1.743117	1.421381	-0.097242

Sum of electronic and thermal Enthalpies = -79.095625 Hartree
 $\langle S^2 \rangle = 0.753919$

AT_A0-ETts



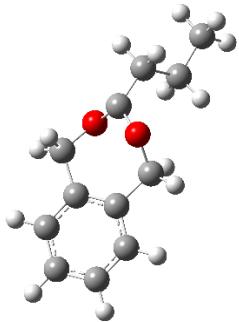
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.366484
C	2.322039	0.000000	1.934008
H	-0.639096	0.488681	-0.740691
H	-0.349736	-1.034517	0.115980
H	2.268488	1.034319	2.300188
O	-0.235033	0.715643	1.227764
C	2.520267	-0.026363	0.432219
C	1.440891	0.028966	-0.466593
C	1.699290	0.060034	-1.841524
C	3.003360	0.030533	-2.334198
C	4.073987	-0.026160	-1.442713
C	3.825683	-0.056308	-0.070982
H	5.095999	-0.051031	-1.810687
H	3.180161	0.055591	-3.405944
H	0.863445	0.109721	-2.536443
H	4.660580	-0.106168	0.625069
O	1.161588	-0.718795	2.385384
H	3.168494	-0.486035	2.427233
C	-2.217566	-2.034401	3.135016
H	-2.686486	-1.812979	2.178350
H	-1.406001	-2.756294	3.080566
C	-0.919116	-0.106741	3.360645
H	-1.810394	0.504587	3.304465
H	-0.593680	-0.449409	4.334533
C	-3.094809	-2.057686	4.349957

H	-2.505275	-2.091864	5.275088
H	-3.760983	-2.937809	4.368644
H	-3.742876	-1.173292	4.400953

Sum of electronic and thermal Enthalpies = -616.392926 Hartree
 $\langle S^2 \rangle = 0.775727$

Imaginary frequency = i406 cm⁻¹

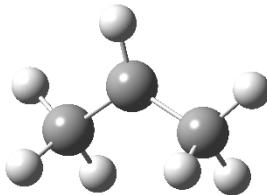
AT_A0-ETpro



C	-0.078482	-0.085383	0.159447
C	0.022866	0.189806	2.541677
C	2.315844	-0.000805	2.019781
H	-0.757235	0.300161	-0.606584
H	-0.368239	-1.121539	0.375897
H	2.339383	1.042997	2.363757
O	-0.326001	0.729883	1.323074
C	2.456038	-0.062453	0.512056
C	1.346840	-0.036541	-0.351459
C	1.562438	-0.026838	-1.734630
C	2.849762	-0.050115	-2.269549
C	3.949036	-0.080244	-1.412207
C	3.744955	-0.088028	-0.033130
H	4.959096	-0.100899	-1.812286
H	2.991502	-0.041598	-3.346792
H	0.703882	-0.000256	-2.402537
H	4.602637	-0.115469	0.636203
O	1.130986	-0.622901	2.533238
H	3.151228	-0.528255	2.490321
C	-1.775358	-1.592396	3.003915
H	-2.203967	-1.456990	2.002249
H	-1.019272	-2.383151	2.922117
C	-1.083504	-0.278314	3.439885
H	-1.832482	0.521732	3.494324
H	-0.673581	-0.407057	4.449506
C	-2.876740	-2.022982	3.977221
H	-2.472645	-2.191045	4.983159
H	-3.356193	-2.953289	3.651342
H	-3.657111	-1.256149	4.057980

Sum of electronic and thermal Enthalpies = -616.439578 Hartree
 $\langle S^2 \rangle = 0.75272$

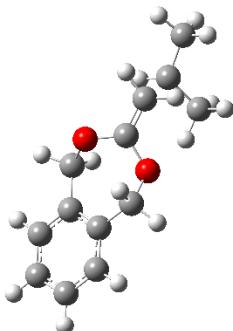
AT_PR



C	0.115955	0.128673	0.032103
C	-0.006838	0.014577	1.515393
H	0.964712	0.147926	2.012288
H	-0.702350	0.754900	1.926964
H	-0.376923	-0.979278	1.829580
C	1.218094	-0.552191	-0.709491
H	1.313874	-0.177989	-1.735164
H	2.186399	-0.417345	-0.206700
H	1.061116	-1.644650	-0.782393
H	-0.739232	0.494468	-0.531915

Sum of electronic and thermal Enthalpies = -118.386889 Hartree
 $\langle S^2 \rangle = 0.754002$

AT_A0-PRts



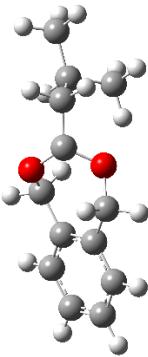
C	-0.004671	0.000550	0.006368
C	-0.000955	-0.002784	2.375342
C	2.321649	-0.000300	1.938394
H	-0.352244	1.036226	0.120449
H	-0.644503	-0.487143	-0.734456
H	3.168861	0.487253	2.428917
O	-0.241482	-0.713500	1.233896
C	2.517016	0.022724	0.436145
C	1.436100	-0.031997	-0.461026
C	1.692779	-0.066764	-1.836231
C	2.996162	-0.041003	-2.330866
C	4.068139	0.015661	-1.441043
C	3.821754	0.049402	-0.069081
H	5.089686	0.037732	-1.810503
H	3.171356	-0.069104	-3.402808
H	0.855866	-0.116514	-2.529858
H	4.657711	0.099362	0.625700
O	1.161133	0.718527	2.389760
H	2.268584	-1.033626	2.307487
C	-2.216976	1.998343	3.204461
C	-0.917379	0.099551	3.376248
H	-1.797846	-0.528537	3.324271
H	-0.578661	0.420155	4.353968
C	-3.232888	1.815763	4.295274

H	-3.826548	0.904226	4.155739
H	-2.754950	1.758491	5.283172
H	-3.945099	2.658887	4.341603
H	-2.581486	1.806625	2.194600
C	-1.234729	3.126777	3.328324
H	-0.772483	3.145835	4.324566
H	-0.428228	3.044936	2.591345
H	-1.715983	4.110545	3.184605

Sum of electronic and thermal Enthalpies = -655.683208 Hartree
 $\langle S^2 \rangle = 0.776306$

Imaginary frequency = i420 cm⁻¹

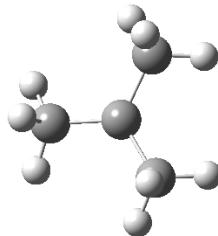
AT_A0-PRadd



C	-0.003646	-0.056773	0.355165
C	0.248349	-0.537383	2.694671
C	2.506563	-0.409603	2.025471
H	-0.245368	0.965887	0.672515
H	-0.743838	-0.358347	-0.391378
H	3.400390	0.024581	2.483539
O	-0.201532	-0.958266	1.462636
C	2.547421	-0.201801	0.525185
C	1.382274	-0.102608	-0.255529
C	1.503757	0.019824	-1.644834
C	2.751961	0.053158	-2.265047
C	3.906889	-0.040867	-1.489406
C	3.796626	-0.165305	-0.105289
H	4.887643	-0.014314	-1.956407
H	2.820222	0.148600	-3.345253
H	0.601878	0.089875	-2.249532
H	4.697734	-0.234733	0.500899
O	1.396107	0.217853	2.681434
H	2.491226	-1.482301	2.264537
C	-1.620511	1.122672	3.435008
C	-0.779890	-0.156099	3.717116
H	-1.470845	-1.004770	3.804494
H	-0.277562	-0.049683	4.687282
C	-2.801285	1.198674	4.414040
H	-3.445215	0.314491	4.336681
H	-2.446524	1.263877	5.451123
H	-3.419659	2.083224	4.219697
H	-2.033076	1.024239	2.420205
C	-0.776280	2.403173	3.498413
H	-0.370457	2.548394	4.508314
H	0.072325	2.368753	2.808952
H	-1.383536	3.283749	3.255401

Sum of electronic and thermal Enthalpies = -655.724614 Hartree
 $\langle S^2 \rangle = 0.752833$

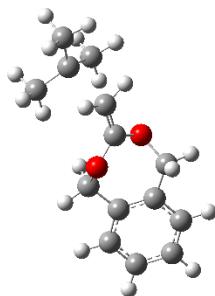
AT_TBU



C	-0.086533	0.149237	0.037162
C	-0.005638	0.009962	1.526133
H	1.034380	-0.018822	1.875844
H	-0.487693	0.856335	2.052080
H	-0.509366	-0.899600	1.877566
C	0.874935	1.064116	-0.656779
H	0.945621	0.842200	-1.729303
H	0.573019	2.126136	-0.577388
H	1.882630	0.996637	-0.226942
C	-1.359880	-0.224533	-0.656996
H	-1.202194	-0.401373	-1.728673
H	-1.808986	-1.127774	-0.224459
H	-2.125908	0.571015	-0.581830

Sum of electronic and thermal Enthalpies = -157.67824 Hartree
 $\langle S^2 \rangle = 0.75402$

AT_A0-TBUs3b



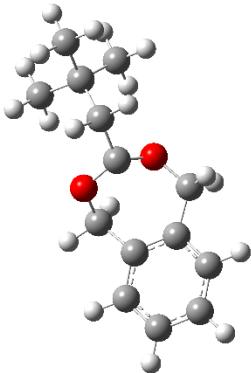
C	0.002202	-0.003915	-0.000429
C	0.002324	-0.000840	2.373970
C	2.324052	-0.002420	1.939788
H	-0.297324	1.047820	0.100851
H	-0.655202	-0.469258	-0.740042
H	3.169060	0.509723	2.408931
O	-0.274716	-0.694922	1.230492
C	2.521843	-0.047797	0.438362
C	1.442144	-0.105706	-0.459871
C	1.701793	-0.207166	-1.831382
C	3.006650	-0.245011	-2.321252
C	4.077321	-0.185061	-1.430052
C	3.828261	-0.084998	-0.061844
H	5.100142	-0.212052	-1.795664
H	3.183922	-0.324650	-3.390244
H	0.865644	-0.258858	-2.525712

H	4.663512	-0.032853	0.633690
O	1.159093	0.729245	2.359842
H	2.274932	-1.018619	2.355087
C	-2.211048	1.889834	3.457662
C	-0.867330	0.052286	3.424508
H	-1.726259	-0.607693	3.397456
H	-0.468834	0.320135	4.395917
C	-3.032127	1.608948	4.689460
H	-2.404464	1.516251	5.585055
H	-3.752155	2.422869	4.889085
H	-3.617857	0.686286	4.588747
C	-1.219865	3.018253	3.572614
H	-0.639791	2.955546	4.501565
H	-0.511426	3.019358	2.736251
H	-1.726356	4.000293	3.574939
C	-2.950621	1.805386	2.148784
H	-2.263935	1.848449	1.294295
H	-3.534596	0.880261	2.066860
H	-3.659264	2.644964	2.031192

Sum of electronic and thermal Enthalpies = -694.973332 Hartree
 $\langle S^2 \rangle = 0.776304$

Imaginary frequency = i429 cm⁻¹

AT_A0-TBUpo

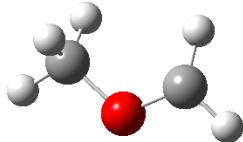


C	0.069896	0.871744	-0.428728
C	-0.065445	0.494247	1.911399
C	2.232276	1.049664	1.703213
H	0.182071	1.959025	-0.337399
H	-0.556292	0.664652	-1.299397
H	2.826329	1.971723	1.688240
O	-0.689266	0.386595	0.686342
C	2.413475	0.282695	0.403993
C	1.421200	0.204605	-0.591070
C	1.692741	-0.507777	-1.765566
C	2.925105	-1.124820	-1.974523
C	3.905448	-1.048558	-0.985608
C	3.641127	-0.356277	0.194908
H	4.868082	-1.532576	-1.126796
H	3.113038	-1.668993	-2.895919
H	0.920186	-0.578283	-2.527956
H	4.403174	-0.308721	0.970782
O	0.897999	1.483921	1.980345
H	2.597787	0.436572	2.539502
C	-1.961907	1.438661	3.499466

C	-0.962770	0.300089	3.094142
H	-1.544811	-0.611683	2.906049
H	-0.321040	0.092388	3.961045
C	-2.756540	0.932032	4.719561
H	-2.091065	0.697485	5.559974
H	-3.470405	1.691404	5.061903
H	-3.324366	0.024734	4.478057
C	-1.204011	2.720368	3.891653
H	-0.500286	2.529073	4.711433
H	-0.630521	3.123852	3.052429
H	-1.907963	3.491791	4.228979
C	-2.942703	1.744521	2.353270
H	-2.423885	2.126250	1.469254
H	-3.492726	0.845538	2.049688
H	-3.676343	2.496943	2.669559

Sum of electronic and thermal Enthalpies = -695.008592 Hartree
 $\langle S^2 \rangle = 0.75287$

AT_MET



C	-0.001929	0.027230	0.021370
O	0.020649	0.068694	1.440525
C	1.262297	0.122573	1.991748
H	1.243336	0.093651	3.075429
H	0.423062	0.944654	-0.406130
H	-1.048197	-0.064792	-0.277415
H	0.561884	-0.838128	-0.356008
H	2.082971	-0.343978	1.446092

Sum of electronic and thermal Enthalpies = -154.292685 Hartree
 $\langle S^2 \rangle = 0.752855$

AT_A0-METts



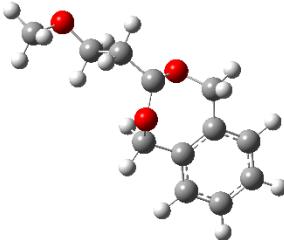
C	0.080185	-0.165184	0.095220
C	0.259882	-0.048824	2.447431
C	2.548295	-0.026836	1.836980
H	-0.296648	0.862071	0.195051
H	-0.596179	-0.705870	-0.573030
H	2.548538	-1.048861	2.239811
O	-0.030076	-0.831388	1.363533

C	2.625707	-0.049268	0.323916
C	1.480788	-0.167360	-0.483326
C	1.631004	-0.241271	-1.872673
C	2.890509	-0.193453	-2.468929
C	4.025953	-0.074140	-1.668550
C	3.885649	-0.000692	-0.283198
H	5.014514	-0.034431	-2.117711
H	2.982747	-0.253198	-3.549906
H	0.744892	-0.340127	-2.496449
H	4.770898	0.097947	0.341843
O	1.410289	0.684924	2.356419
H	3.420288	0.493347	2.243590
C	-0.470553	-0.122831	3.593614
H	-1.495163	-0.468063	3.538859
H	-0.201946	0.539653	4.406780
C	0.015923	-2.032584	4.801550
O	-0.904979	-2.231674	5.799107
C	-0.694163	-1.448719	6.960544
H	0.303666	-1.633007	7.387130
H	-1.455734	-1.742105	7.686930
H	-0.792272	-0.375786	6.746117
H	-0.113460	-2.758179	4.003834
H	1.042549	-1.850817	5.133359

Sum of electronic and thermal Enthalpies = -691.589582 Hartree
 $\langle S^2 \rangle = 0.77525$

Imaginary frequency = i390 cm⁻¹

AT_A0-METpro

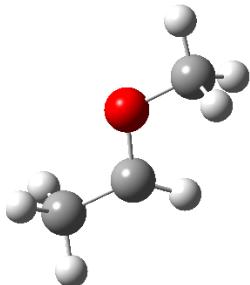


C	-0.084926	-0.017962	0.007940
C	-0.204449	0.160198	2.358347
C	2.161293	-0.104232	2.049331
H	-0.444876	1.019849	0.047362
H	-0.683350	-0.553197	-0.735431
H	2.003867	-1.146590	2.356487
O	-0.378622	-0.648512	1.262097
C	2.417968	-0.030813	0.558234
C	1.377720	-0.055540	-0.387253
C	1.694197	-0.057132	-1.750703
C	3.017699	-0.026300	-2.187477
C	4.050213	0.002981	-1.250813
C	3.743584	0.002295	0.109213
H	5.087022	0.029427	-1.574636
H	3.239127	-0.028506	-3.251238
H	0.888188	-0.083886	-2.481397
H	4.548385	0.028175	0.840963
O	1.054648	0.698484	2.508103
H	3.030893	0.277444	2.591524
C	-0.916047	-0.306186	3.593058

H	-1.987548	-0.390353	3.379942
H	-0.786941	0.463368	4.361762
C	-0.429265	-1.674763	4.127107
O	-1.184019	-2.142536	5.232237
C	-0.871984	-1.513225	6.458104
H	0.202376	-1.592865	6.691622
H	-1.441425	-2.031743	7.234320
H	-1.150710	-0.448850	6.474059
H	-0.548013	-2.429278	3.343879
H	0.639483	-1.618373	4.392962

Sum of electronic and thermal Enthalpies = -691.631482 Hartree
 $\langle S^2 \rangle = 0.752809$

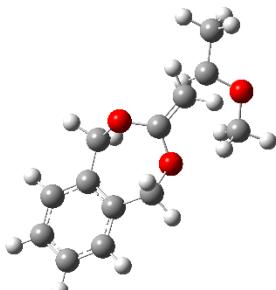
AT_VE2



C	0.040140	0.102406	0.021242
C	-0.000617	0.000629	1.505939
O	1.297248	0.048918	-0.516034
H	0.441102	0.880114	2.006971
H	-1.035923	-0.091885	1.850876
H	0.557371	-0.878235	1.852138
C	1.351289	0.197094	-1.925655
H	0.819123	-0.619699	-2.431157
H	2.406099	0.174369	-2.208239
H	0.912637	1.155481	-2.240569
H	-0.679983	0.726024	-0.514581

Sum of electronic and thermal Enthalpies = -193.586868 Hartree
 $\langle S^2 \rangle = 0.752942$

AT_A0-VEtS1



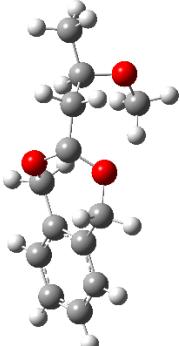
C	0.008737	-0.003739	-0.000353
C	0.019954	-0.009963	2.364007
C	2.347381	-0.001595	1.918206
H	-0.360414	1.022732	0.129779
H	-0.625767	-0.495748	-0.743180
H	2.303402	-1.042680	2.266332
O	-0.199759	-0.733784	1.219857
C	2.532722	0.052432	0.415259

C	1.447355	-0.000614	-0.477017
C	1.695984	-0.001973	-1.854196
C	2.995771	0.054748	-2.355795
C	4.072171	0.108859	-1.471159
C	3.833620	0.109874	-0.097382
H	5.090989	0.154557	-1.845995
H	3.164832	0.052571	-3.429098
H	0.855615	-0.049729	-2.543808
H	4.672982	0.158642	0.593332
O	1.185997	0.704324	2.390523
H	3.195865	0.480502	2.412164
C	-0.786652	-0.137521	3.457792
H	-1.814451	-0.447484	3.307310
H	-0.576686	0.507698	4.302549
C	-0.491783	-2.007394	4.731465
C	-0.771525	-1.536504	6.125647
O	-1.412537	-2.936004	4.307409
H	-0.725777	-2.360776	6.854911
H	-0.041289	-0.777762	6.425878
H	-1.774399	-1.096959	6.195548
C	-1.093892	-3.576351	3.080463
H	-1.031797	-2.855707	2.256715
H	-1.891889	-4.296646	2.884166
H	-0.135583	-4.112999	3.155813
H	0.545696	-2.260695	4.487916

Sum of electronic and thermal Enthalpies = -730.884274 Hartree
 $\langle S^2 \rangle = 0.776037$

Imaginary frequency = i407 cm⁻¹

AT_A0-VEpro

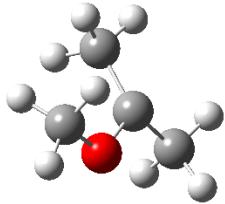


C	-0.131008	0.164475	0.083178
C	-0.100267	0.152888	2.440469
C	2.194262	-0.389960	1.965100
H	-0.354223	1.230702	0.229510
H	-0.830856	-0.227235	-0.661113
H	1.927234	-1.430564	2.189875
O	-0.436652	-0.531886	1.299888
C	2.375147	-0.207133	0.471495
C	1.292104	-0.016248	-0.404523
C	1.533707	0.069075	-1.780757
C	2.825079	-0.023549	-2.297233
C	3.900686	-0.208531	-1.429342
C	3.668457	-0.296669	-0.057601
H	4.913800	-0.280528	-1.815256
H	2.987882	0.045107	-3.369330

H	0.693602	0.209606	-2.458078
H	4.507434	-0.438102	0.620596
O	1.229142	0.490226	2.571224
H	3.135001	-0.168840	2.476806
C	-0.846015	-0.187893	3.692131
H	-1.916692	-0.239634	3.466011
H	-0.694807	0.655526	4.378389
C	-0.466575	-1.484432	4.471626
C	-0.954641	-1.398577	5.918005
O	-1.070188	-2.649481	3.919277
H	-0.706736	-2.319748	6.454070
H	-0.495412	-0.552131	6.440067
H	-2.043280	-1.273173	5.943925
C	-0.323140	-3.332934	2.931312
H	-0.233158	-2.758618	2.001628
H	-0.860316	-4.263009	2.722135
H	0.685593	-3.589928	3.296290
H	0.629961	-1.597820	4.469408

Sum of electronic and thermal Enthalpies = -730.918901 Hartree
 $\langle S^2 \rangle = 0.752911$

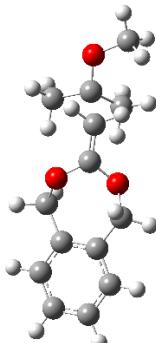
AT__PE



C	0.052771	0.129217	0.022143
C	0.000306	-0.024308	1.508642
O	1.356656	0.122141	-0.430277
H	0.289109	0.901608	2.039278
H	-1.012115	-0.284566	1.836532
H	0.686851	-0.811642	1.838763
C	1.570853	0.149875	-1.831686
H	1.036277	-0.667289	-2.335427
H	2.645512	0.019719	-1.980140
H	1.264754	1.104895	-2.279058
C	-0.969310	0.968350	-0.685839
H	-0.763123	2.051940	-0.593973
H	-1.039796	0.746003	-1.757094
H	-1.957444	0.791499	-0.248811

Sum of electronic and thermal Enthalpies = -232.877036 Hartree
 $\langle S^2 \rangle = 0.753181$

AT_A0-PEtS

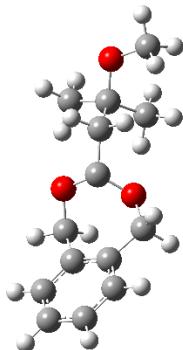


C	-0.000431	-0.000818	0.000703
C	-0.000254	-0.000318	2.362679
C	2.333881	-0.000991	1.926356
H	-0.385142	1.020768	0.127164
H	-0.624081	-0.503116	-0.744695
H	2.290380	-1.049097	2.253118
O	-0.204314	-0.731763	1.221386
C	2.521386	0.079104	0.424795
C	1.439378	0.024806	-0.471186
C	1.692145	0.043956	-1.847466
C	2.992590	0.121660	-2.344461
C	4.065839	0.177057	-1.456076
C	3.823111	0.157839	-0.083206
H	5.085165	0.238986	-1.827176
H	3.164625	0.134686	-3.417239
H	0.854462	-0.005229	-2.540325
H	4.659759	0.206772	0.610793
O	1.175708	0.696554	2.415011
H	3.183112	0.470416	2.429120
C	-0.856500	-0.079574	3.425988
H	-1.883701	-0.349938	3.210858
H	-0.682735	0.578839	4.268584
C	-0.566627	-1.869703	4.778941
C	0.828900	-1.676485	5.301647
O	-1.462935	-1.665590	5.823038
H	1.130794	-2.506114	5.962281
H	1.545978	-1.626361	4.476267
H	0.901191	-0.750273	5.881528
C	-2.832905	-1.949996	5.604133
H	-3.234086	-1.406239	4.738476
H	-3.360115	-1.619864	6.502852
H	-3.016193	-3.023422	5.460901
C	-0.794689	-3.053072	3.875176
H	-0.662166	-4.010336	4.409031
H	-1.793304	-3.058445	3.425928
H	-0.073789	-3.025238	3.052656

Sum of electronic and thermal Enthalpies = -770.172301 Hartree
 $\langle S^2 \rangle = 0.775927$

Imaginary frequency = i413 cm⁻¹

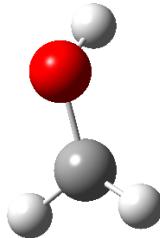
AT_A0-PEpro



C	0.190925	-1.068967	0.080120
C	0.514546	-0.562937	2.375065
C	2.755325	-0.973608	1.711094
H	-0.699396	-0.444299	-0.080998
H	0.067336	-1.977974	-0.521409
H	2.620811	-2.055186	1.589276
O	0.209434	-1.530723	1.433996
C	2.619099	-0.262379	0.380022
C	1.425226	-0.302273	-0.364460
C	1.360428	0.377877	-1.585986
C	2.459656	1.073420	-2.086808
C	3.644617	1.111633	-1.352596
C	3.710941	0.453679	-0.125427
H	4.506430	1.658129	-1.725364
H	2.386268	1.590019	-3.040000
H	0.432328	0.361012	-2.154522
H	4.628147	0.494513	0.457709
O	1.847740	-0.503443	2.718313
H	3.747918	-0.796838	2.130996
C	-0.446018	-0.372563	3.506821
H	-1.436472	-0.239795	3.056956
H	-0.197481	0.563054	4.020950
C	-0.549368	-1.485493	4.604869
C	0.708746	-1.513703	5.476880
O	-1.586328	-1.094635	5.531544
H	0.608327	-2.283142	6.249918
H	1.598842	-1.716752	4.877202
H	0.839914	-0.547147	5.974265
C	-2.933531	-1.240099	5.132449
H	-3.169706	-0.707644	4.198583
H	-3.535532	-0.802317	5.934250
H	-3.228149	-2.292389	5.012391
C	-0.816923	-2.871353	4.003632
H	-0.997640	-3.596652	4.805227
H	-1.678848	-2.872711	3.328925
H	0.045890	-3.205006	3.420909

Sum of electronic and thermal Enthalpies = -770.205321 Hartree
 $\langle S^2 \rangle = 0.752863$

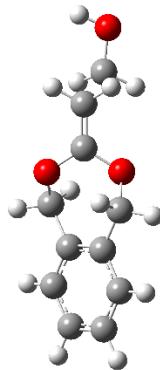
AT_OH



C	0.232615	-0.282522	0.164580
H	-0.104930	0.197714	1.081739
H	0.984948	0.197352	-0.459496
O	-0.630340	-1.157388	-0.445390
H	-0.369476	-2.074451	-0.261661

Sum of electronic and thermal Enthalpies = -115.006168 Hartree
 $\langle S^2 \rangle = 0.753352$

AT_A0-OHts1

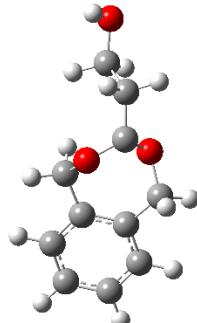


C	-0.003001	-0.000017	0.000939
C	-0.006121	0.002512	2.362181
C	2.322515	-0.000902	1.932361
H	-0.361254	1.031608	0.121293
H	-0.638081	-0.489940	-0.742664
H	3.169936	0.481650	2.427703
O	-0.227583	-0.721588	1.223069
C	2.518418	0.038265	0.430394
C	1.438040	-0.014708	-0.467633
C	1.695388	-0.033172	-1.843019
C	2.998745	0.006238	-2.336957
C	4.070181	0.060659	-1.446347
C	3.823035	0.078717	-0.074193
H	5.091673	0.092909	-1.815235
H	3.174350	-0.009729	-3.409098
H	0.859077	-0.081583	-2.537501
H	4.658453	0.126931	0.621401
O	1.161392	0.714358	2.392136
H	2.270863	-1.038596	2.289290
C	-0.824090	-0.101648	3.443469
H	-1.845753	-0.428804	3.299109
H	-0.608523	0.520399	4.303614
C	-0.483818	-2.027127	4.684316
H	-0.629570	-2.777973	3.913817
O	-1.470765	-2.111808	5.646626
H	-1.266000	-1.480828	6.353067
H	0.539699	-1.900298	5.044585

Sum of electronic and thermal Enthalpies = -652.309017 Hartree
 $\langle S^2 \rangle = 0.775271$

Imaginary frequency = i391 cm⁻¹

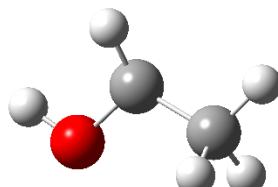
AT_A0-OHpro



C	-0.069786	-0.020195	0.021707
C	-0.133128	0.172258	2.372608
C	2.227322	-0.067303	2.006695
H	-0.431898	1.016686	0.063918
H	-0.684833	-0.561947	-0.703014
H	3.105175	0.332714	2.521689
O	-0.330020	-0.644257	1.286793
C	2.445980	-0.012230	0.508843
C	1.382408	-0.055821	-0.409595
C	1.664846	-0.074496	-1.780389
C	2.976814	-0.042483	-2.250632
C	4.032284	0.005347	-1.340711
C	3.759742	0.021751	0.026442
H	5.060497	0.032781	-1.690743
H	3.171438	-0.058198	-3.319499
H	0.841137	-0.115760	-2.490362
H	4.582443	0.061793	0.737359
O	1.122005	0.728507	2.482054
H	2.090524	-1.106866	2.332640
C	-0.801865	-0.296283	3.630504
H	-1.877557	-0.401318	3.451170
H	-0.666062	0.483312	4.391669
C	-0.278543	-1.639803	4.185492
H	-0.425806	-2.427635	3.441660
O	-0.992768	-2.060298	5.340683
H	-0.833121	-1.404850	6.037674
H	0.801589	-1.567128	4.390047

Sum of electronic and thermal Enthalpies = -652.352542 Hartree
 $\langle S^2 \rangle = 0.7528$

AT_VOH

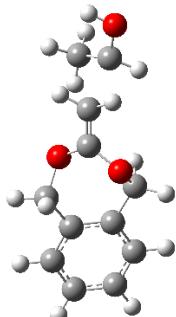


C	-0.078085	-0.135426	-0.134973
H	0.116744	-0.042695	0.935033
O	1.027089	-0.251925	-0.950498

H	1.731353	-0.698788	-0.457546
C	-1.217723	0.590397	-0.756409
H	-2.101058	0.533844	-0.111523
H	-0.998635	1.658568	-0.932179
H	-1.473210	0.152723	-1.729786

Sum of electronic and thermal Enthalpies = -154.306298 Hartree
 $\langle S^2 \rangle = 0.753007$

AT_A0-VOHts

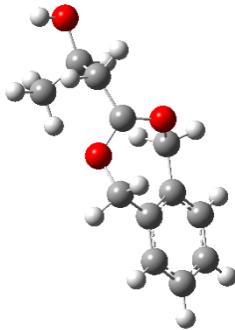


C	-0.005084	0.002043	0.005524
C	-0.006593	-0.003636	2.368910
C	2.322938	0.000504	1.936852
H	-0.642160	0.489178	-0.738382
H	-0.359049	-1.030972	0.126383
H	2.275334	1.036345	2.300151
O	-0.232344	0.722070	1.228196
C	2.516883	-0.030446	0.434225
C	1.435862	0.023234	-0.463204
C	1.692537	0.048625	-1.838654
C	2.995662	0.014610	-2.333535
C	4.067636	-0.040862	-1.443660
C	3.821256	-0.065388	-0.071478
H	5.089041	-0.069298	-1.813127
H	3.170692	0.035405	-3.405696
H	0.855711	0.097669	-2.532510
H	4.657089	-0.114881	0.623493
O	1.161129	-0.714252	2.393752
H	3.169976	-0.486826	2.428109
C	-0.818343	0.108432	3.456462
H	-0.611553	-0.509604	4.320961
H	-1.843400	0.423261	3.296182
C	-0.431683	1.976601	4.735873
O	-1.154646	1.807612	5.905545
C	-0.800089	3.134644	3.858378
H	-2.083262	2.022150	5.720963
H	-0.605252	4.108570	4.337908
H	-0.238877	3.093534	2.919470
H	-1.868525	3.108274	3.595848
H	0.624334	1.819231	4.944541

Sum of electronic and thermal Enthalpies = -691.603551 Hartree
 $\langle S^2 \rangle = 0.775569$

Imaginary frequency = i394 cm⁻¹

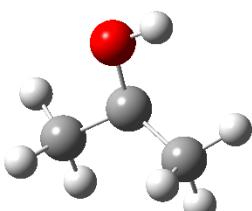
AT_A0-VOHpro



C	-0.097033	-0.020877	0.034643
C	-0.161011	-0.127440	2.390314
C	2.196512	0.141341	2.018703
H	-0.736237	0.462054	-0.710480
H	-0.410721	-1.070602	0.120298
H	2.049432	1.182063	2.336634
O	-0.386038	0.641571	1.274444
C	2.415797	0.076704	0.520940
C	1.352003	0.066690	-0.398374
C	1.634449	0.079612	-1.769277
C	2.946926	0.094163	-2.238899
C	4.002677	0.099811	-1.328053
C	3.730198	0.089186	0.039186
H	5.031447	0.109131	-1.677427
H	3.141658	0.104351	-3.307806
H	0.810115	0.078951	-2.479686
H	4.553464	0.090270	0.750583
O	1.101431	-0.663372	2.501426
H	3.079308	-0.243381	2.536752
C	-0.836812	0.330965	3.646809
H	-0.776119	-0.483614	4.377127
H	-1.899610	0.501227	3.426593
C	-0.259549	1.594897	4.341519
O	-0.801980	1.716247	5.658527
C	-0.466922	2.881327	3.542714
H	-1.747838	1.914505	5.561285
H	-0.037982	3.732554	4.081446
H	-0.014155	2.818497	2.548742
H	-1.539419	3.073144	3.398053
H	0.811215	1.432781	4.510402

Sum of electronic and thermal Enthalpies = -691.642927 Hartree
 $\langle S^2 \rangle = 0.752872$

AT__POH

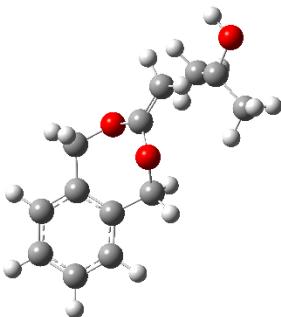


C	0.165265	0.089991	-0.094586
O	0.264614	0.233143	1.279584
H	0.507841	-0.624623	1.661560
C	-0.280454	1.350052	-0.758575
H	-0.123489	1.294414	-1.841216
H	-1.353232	1.559225	-0.590646

H	0.278544	2.208948	-0.370234
C	-0.245261	-1.253975	-0.610210
H	-1.301857	-1.492996	-0.383260
H	-0.127089	-1.307254	-1.697690
H	0.365009	-2.059095	-0.174563

Sum of electronic and thermal Enthalpies = -193.60038 Hartree
 $\langle S^2 \rangle = 0.753183$

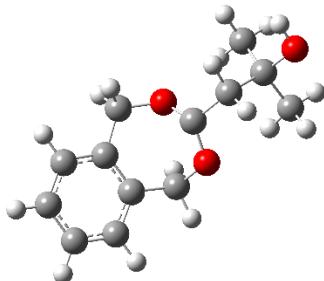
AT_A0-POHts



C	0.001685	-0.003571	-0.003111
C	0.001873	-0.000138	2.359160
C	2.334627	-0.003262	1.924071
H	-0.622845	0.496593	-0.749166
H	-0.380977	-1.025746	0.124304
H	2.291237	1.043737	2.254717
O	-0.204335	0.728498	1.216681
C	2.523414	-0.079810	0.422371
C	1.441740	-0.026095	-0.474080
C	1.695057	-0.042818	-1.850268
C	2.995775	-0.118021	-2.346829
C	4.068689	-0.173216	-1.458063
C	3.825436	-0.156184	-0.085208
H	5.088240	-0.233340	-1.828818
H	3.168270	-0.129391	-3.419544
H	0.857589	0.005853	-2.543397
H	4.661891	-0.205032	0.609024
O	1.174961	-0.701280	2.408637
H	3.182735	-0.477162	2.426386
C	-0.850431	0.081263	3.422434
H	-0.669251	-0.565099	4.272659
H	-1.879784	0.355924	3.218235
C	-0.628320	1.897553	4.761475
O	-1.609835	1.688655	5.726258
C	0.734133	1.752697	5.369312
C	-0.872866	3.055579	3.833641
H	-2.473890	1.868307	5.322804
H	1.501506	1.723884	4.588757
H	0.969649	2.592585	6.044313
H	0.800335	0.830136	5.956009
H	-0.783869	4.024660	4.353894
H	-0.158389	3.045046	3.004753
H	-1.878535	3.009110	3.392453

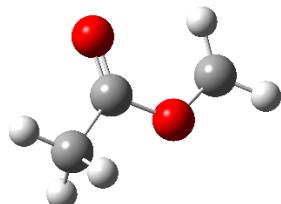
Sum of electronic and thermal Enthalpies = -730.897032 Hartree
 $\langle S^2 \rangle = 0.775544$

Imaginary frequency = i407 cm⁻¹

AT_A0-POHpro

C	0.270617	1.093646	0.056957
C	0.491259	0.446309	2.331937
C	2.764079	0.855495	1.781152
H	0.181247	2.040368	-0.489813
H	-0.619576	0.492780	-0.178112
H	2.649932	1.944988	1.725812
O	0.238019	1.470081	1.436979
C	2.674696	0.235295	0.401357
C	1.513520	0.340862	-0.386841
C	1.491948	-0.254649	-1.653264
C	2.603315	-0.930196	-2.154555
C	3.756043	-1.034038	-1.376610
C	3.778560	-0.460604	-0.106244
H	4.626551	-1.566213	-1.749885
H	2.564259	-1.380225	-3.142859
H	0.588793	-0.186051	-2.257007
H	4.670269	-0.553046	0.509593
O	1.809711	0.334923	2.716630
H	3.735804	0.635680	2.228620
C	-0.499333	0.221504	3.430970
H	-0.213900	-0.692433	3.963666
H	-1.475547	0.030346	2.962731
C	-0.708208	1.332880	4.513240
O	-1.646212	0.819183	5.476508
C	0.566674	1.594108	5.315090
C	-1.260415	2.628158	3.905647
H	-2.497933	0.713088	5.022474
H	1.364130	1.979533	4.675280
H	0.359925	2.320961	6.107767
H	0.918453	0.668712	5.782175
H	-1.463816	3.352189	4.702051
H	-0.563235	3.070002	3.188518
H	-2.199988	2.435967	3.369831

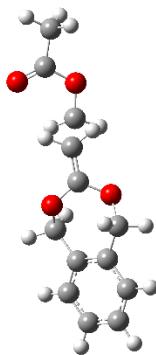
Sum of electronic and thermal Enthalpies = -730.931151 Hartree
 $\langle S^2 \rangle = 0.75286$

AT_MAC

C	-0.019646	-0.018626	0.010763
H	-0.053071	-0.013611	1.100584
H	1.021985	-0.020349	-0.328016
H	-0.488868	0.889506	-0.381765
C	-0.733764	-1.241420	-0.503804
O	-1.240319	-2.113799	0.159376
O	-0.737069	-1.244894	-1.879402
C	-1.319507	-2.303806	-2.521542
H	-1.886628	-3.011471	-1.934244
H	-1.412135	-2.160126	-3.587701

Sum of electronic and thermal Enthalpies = -267.640552 Hartree
 $\langle S^2 \rangle = 0.753531$

AT_A0-MACts



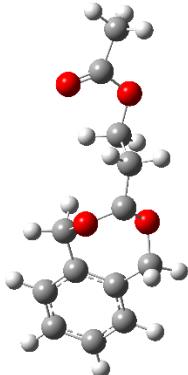
C	-0.000196	-0.000111	0.000163
C	-0.000104	-0.000440	2.367650
C	2.323066	-0.000182	1.934026
H	-0.341933	1.037513	0.113261
H	-0.643815	-0.485750	-0.738215
H	3.168016	0.491205	2.424283
O	-0.242193	-0.710470	1.229804
C	2.520000	0.017231	0.432202
C	1.440320	-0.040496	-0.465832
C	1.698188	-0.083197	-1.840574
C	3.002343	-0.062206	-2.333360
C	4.073341	-0.002426	-1.442517
C	3.825545	0.039024	-0.071042
H	5.095319	0.015763	-1.810881
H	3.178955	-0.096514	-3.404846
H	0.862091	-0.135222	-2.534906
H	4.660665	0.090724	0.624555
O	1.160323	0.718400	2.384064
H	2.271780	-1.032023	2.307216
C	-0.904748	0.086305	3.376599
H	-0.569786	0.426619	4.348228
H	-1.807159	-0.508248	3.320399
C	-2.213737	2.004112	3.220806
O	-2.877681	2.115539	4.436709
C	-3.996457	1.358280	4.622504
C	-4.585929	1.611931	5.988595
O	-4.440425	0.605270	3.784168
H	-3.822569	1.494580	6.764067
H	-5.407533	0.916072	6.162063
H	-4.959776	2.640173	6.051288

H	-1.473630	2.789190	3.124013
H	-2.841864	1.750747	2.374084

Sum of electronic and thermal Enthalpies = -804.940075 Hartree
 $\langle S^2 \rangle = 0.772557$

Imaginary frequency = i368 cm⁻¹

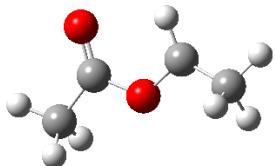
AT_A0-MACpro



C	-0.120812	-0.117673	0.330097
C	0.164321	-0.375630	2.697677
C	2.402703	-0.055076	2.019050
H	-0.508171	0.881772	0.569460
H	-0.805850	-0.576356	-0.388030
H	3.244575	0.491305	2.454142
O	-0.198443	-0.951606	1.505643
C	2.426341	0.081897	0.510351
C	1.263755	-0.012313	-0.275132
C	1.377566	0.053446	-1.668778
C	2.615116	0.218731	-2.289170
C	3.766897	0.317108	-1.509498
C	3.664291	0.250193	-0.120776
H	4.738897	0.448315	-1.977007
H	2.677891	0.266746	-3.372805
H	0.478764	-0.026977	-2.276644
H	4.562393	0.330473	0.488409
O	1.230454	0.488256	2.644207
H	2.496241	-1.109886	2.311980
C	-0.916395	0.042794	3.651380
H	-0.494964	0.106207	4.661211
H	-1.693665	-0.726968	3.650492
C	-1.556762	1.401449	3.312272
O	-2.478297	1.810687	4.347739
C	-3.752242	1.359721	4.241983
C	-4.589237	1.858440	5.397217
O	-4.150155	0.657357	3.338452
H	-4.173803	1.498188	6.344211
H	-5.613880	1.503144	5.283340
H	-4.573895	2.952673	5.430251
H	-0.800096	2.187572	3.282747
H	-2.090519	1.356711	2.360248

Sum of electronic and thermal Enthalpies = -804.984764 Hartree
 $\langle S^2 \rangle = 0.752814$

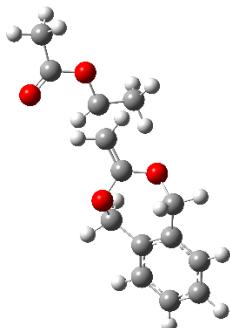
AT_VAC1



C	-0.004823	0.044546	-0.060822
H	0.559021	-0.283040	0.830132
H	0.726619	0.461084	-0.765107
H	-0.678064	0.848631	0.252572
C	0.350236	-4.087526	-2.392701
H	-0.129557	-5.039138	-2.623468
H	0.692161	-3.614531	-3.320007
H	1.232815	-4.253662	-1.766802
C	-0.635642	-3.189332	-1.689185
O	-1.804004	-3.426072	-1.489537
O	-0.022909	-2.026685	-1.297981
C	-0.783302	-1.055984	-0.678644
H	-1.779390	-1.356551	-0.379388

Sum of electronic and thermal Enthalpies = -306.935349 Hartree
 $\langle S^2 \rangle = 0.773878$

AT_A0-VACts2



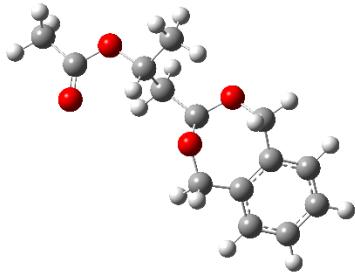
C	0.011287	0.047068	-0.037583
C	-0.108479	-0.202369	2.315910
C	2.230804	-0.285859	1.989848
H	-0.613152	-0.327569	-0.853126
H	-0.290456	1.083542	0.166066
H	3.074617	0.098999	2.569283
O	-0.326772	-0.772721	1.096755
C	2.504959	-0.116739	0.509734
C	1.471155	-0.016663	-0.437172
C	1.796983	0.078577	-1.794847
C	3.124056	0.081835	-2.222550
C	4.149643	-0.016190	-1.282990
C	3.834095	-0.111949	0.071726
H	5.188810	-0.014022	-1.600186
H	3.353361	0.156013	-3.281980
H	0.995957	0.149082	-2.527838
H	4.633916	-0.182869	0.806050
O	1.085883	0.446223	2.463056
H	2.104863	-1.347159	2.243455

C	-1.062489	-0.170344	3.285719
H	-0.755050	0.025772	4.305830
H	-1.978547	-0.723445	3.122448
C	-2.273799	1.777690	3.299322
O	-3.097083	1.653968	4.424333
C	-4.214350	0.881550	4.328612
C	-4.961071	0.866774	5.641085
O	-4.547974	0.302536	3.317586
H	-5.306453	1.876014	5.891020
H	-4.301997	0.538374	6.451270
H	-5.817291	0.195990	5.561953
H	-2.807171	1.638118	2.363827
C	-1.298767	2.897839	3.443926
H	-1.788125	3.885088	3.415240
H	-0.756177	2.827102	4.393752
H	-0.564130	2.858482	2.633593

Sum of electronic and thermal Enthalpies = -844.234031 Hartree
 $\langle S^2 \rangle = 0.752814$

Imaginary frequency = i392 cm⁻¹

AT_A0-VACpro

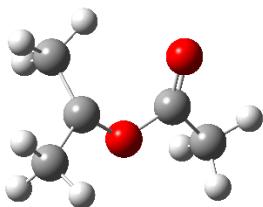


C	-0.011083	0.743660	-0.458893
C	-0.250422	0.351257	1.868171
C	1.999687	1.114104	1.791652
H	-0.565715	0.488151	-1.364358
H	0.018307	1.836602	-0.370191
H	2.498662	2.090669	1.780453
O	-0.805330	0.213714	0.613279
C	2.313884	0.341165	0.521867
C	1.391097	0.173396	-0.527953
C	1.782560	-0.536626	-1.669338
C	3.066904	-1.064334	-1.792981
C	3.978375	-0.899209	-0.750539
C	3.594642	-0.209308	0.398279
H	4.980183	-1.313452	-0.825131
H	3.348440	-1.608744	-2.690029
H	1.063949	-0.676781	-2.473665
H	4.302968	-0.093871	1.216589
O	0.616567	1.418503	1.997128
H	2.382890	0.559119	2.659229
C	-1.215530	0.150823	2.996791
H	-0.650283	-0.146868	3.886617
H	-1.895763	-0.667405	2.735500
C	-2.039904	1.403412	3.371088
C	-2.997031	1.873694	2.287195

O	-2.869586	1.083407	4.527064
H	-3.555313	2.752608	2.625699
H	-2.443335	2.135753	1.381809
H	-3.713494	1.085424	2.031573
C	-2.306562	1.192878	5.751766
C	-3.308339	0.841861	6.829334
O	-1.158463	1.528957	5.950033
H	-3.676251	-0.179086	6.683375
H	-4.173454	1.510689	6.771941
H	-2.835418	0.929840	7.808082
H	-1.351957	2.199779	3.664484

Sum of electronic and thermal Enthalpies = -844.274549 Hartree
 $\langle S^2 \rangle = 0.75275$

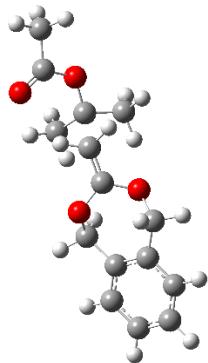
AT_MVAC



C	-0.024239	-0.011352	0.002150
C	0.074947	0.134379	1.485857
O	1.166087	-0.062701	-0.735278
C	-1.118451	0.619771	-0.791280
H	0.543605	1.094524	1.767421
H	-0.926383	0.117891	1.928184
H	0.668496	-0.668503	1.929672
C	2.125701	-0.996999	-0.465297
C	3.329451	-0.766775	-1.348764
O	2.016329	-1.871752	0.361434
H	3.026753	-0.691671	-2.397706
H	3.814740	0.178333	-1.080326
H	4.035219	-1.587764	-1.217893
H	-2.082179	0.479196	-0.291088
H	-0.968898	1.707105	-0.918006
H	-1.179039	0.184202	-1.794955

Sum of electronic and thermal Enthalpies = -346.224526 Hartree
 $\langle S^2 \rangle = 0.753561$

AT_A0-MVACts1

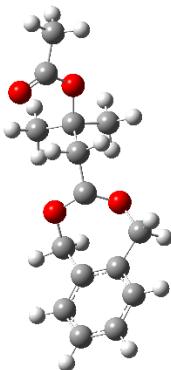


C	0.002150	-0.004825	0.001033
C	0.004166	0.000019	2.374897
C	2.326943	-0.001670	1.936993
H	-0.307910	1.044139	0.101570
H	-0.652474	-0.477611	-0.736097
H	3.172213	0.505894	2.410378
O	-0.266796	-0.696415	1.233691
C	2.522786	-0.033053	0.435240
C	1.441958	-0.092238	-0.461343
C	1.699572	-0.181809	-1.834039
C	3.003869	-0.206535	-2.326171
C	4.075827	-0.145534	-1.436528
C	3.828643	-0.057265	-0.067201
H	5.098043	-0.162770	-1.804315
H	3.179798	-0.277364	-3.395987
H	0.862665	-0.235073	-2.527291
H	4.664512	-0.004844	0.627488
O	1.162450	0.727088	2.365756
H	2.277016	-1.021193	2.343357
C	-0.871970	0.058892	3.418660
H	-0.482063	0.341169	4.389790
H	-1.749283	-0.573626	3.388950
C	-2.171722	1.922139	3.424246
C	-3.007511	1.861015	2.175751
O	-2.888584	1.857860	4.648883
H	-3.710075	2.710413	2.129163
H	-3.585101	0.937412	2.113634
H	-2.353776	1.929351	1.299631
C	-3.767950	0.865660	4.934216
C	-4.418174	1.123015	6.275821
O	-4.006002	-0.086129	4.221455
H	-3.658649	1.314088	7.040141
H	-5.024679	0.260460	6.554537
H	-5.054623	2.013233	6.218508
C	-1.172511	3.037466	3.535032
H	-0.599836	2.962325	4.465236
H	-0.468999	2.998777	2.698240
H	-1.664512	4.024265	3.524599

Sum of electronic and thermal Enthalpies = -883.522616 Hartree
 $\langle S^2 \rangle = 0.774867$

Imaginary frequency = i402 cm⁻¹

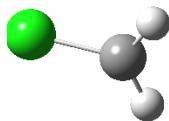
AT_A0-MVACpro



C	0.132241	1.035896	-0.404706
C	-0.104450	0.624567	1.920325
C	2.236962	0.993079	1.790933
H	0.338569	2.107051	-0.290424
H	-0.484201	0.898963	-1.295696
H	2.901948	1.865280	1.804526
O	-0.702448	0.605525	0.680627
C	2.387685	0.230165	0.485501
C	1.422021	0.252292	-0.538141
C	1.662969	-0.467653	-1.714599
C	2.841564	-1.188939	-1.897866
C	3.795892	-1.211165	-0.881253
C	3.559595	-0.512627	0.301529
H	4.715568	-1.777098	-1.002360
H	3.006951	-1.737322	-2.821010
H	0.909389	-0.460880	-2.498798
H	4.299761	-0.542846	1.099085
O	0.933922	1.529354	2.043169
H	2.530682	0.342036	2.626577
C	-1.042973	0.468106	3.075433
H	-0.439123	0.283347	3.971936
H	-1.656699	-0.418732	2.899833
C	-1.998477	1.658506	3.398076
C	-3.063201	1.885769	2.322287
O	-2.650392	1.380403	4.696582
H	-3.749744	2.678488	2.640714
H	-3.634736	0.976303	2.131713
H	-2.583664	2.194018	1.389596
C	-3.468323	0.324195	4.883758
C	-4.005960	0.332019	6.300530
O	-3.743841	-0.517037	4.053549
H	-3.180084	0.323391	7.019199
H	-4.641008	-0.541700	6.451743
H	-4.582636	1.245785	6.478847
C	-1.229041	2.947331	3.690182
H	-0.500100	2.791837	4.491738
H	-0.689326	3.281294	2.800920
H	-1.923380	3.734703	4.001814

Sum of electronic and thermal Enthalpies = -883.558164 Hartree
 $\langle S^2 \rangle = 0.752857$

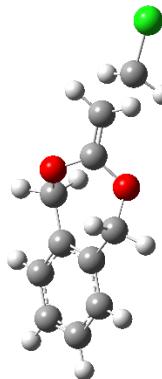
AT_MC



C	-0.002806	0.000000	0.001620
H	0.037407	0.000000	1.081346
Cl	1.480727	0.000000	-0.854898
H	-0.917770	0.000000	-0.573068

Sum of electronic and thermal Enthalpies = -499.412881 Hartree
 $\langle S^2 \rangle = 0.754113$

AT_A0-MCts

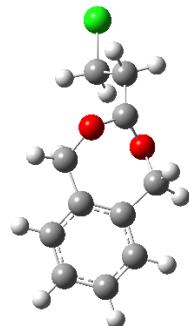


C	0.000791	-0.001174	-0.000338
C	0.000424	-0.000763	2.368474
C	2.323320	-0.001014	1.933772
H	-0.333871	1.038925	0.110249
H	-0.645612	-0.484737	-0.737408
H	3.165891	0.495453	2.422415
O	-0.250850	-0.706713	1.231604
C	2.520401	0.007100	0.432481
C	1.440835	-0.053193	-0.465159
C	1.698232	-0.106277	-1.839603
C	3.002516	-0.093635	-2.332209
C	4.073597	-0.031639	-1.441573
C	3.826157	0.020161	-0.070402
H	5.095604	-0.019638	-1.809921
H	3.179149	-0.135763	-3.403342
H	0.862124	-0.159409	-2.533793
H	4.661469	0.073248	0.624770
O	1.157909	0.718350	2.380509
H	2.272885	-1.030105	2.314140
C	-0.890720	0.068525	3.389045
H	-0.555190	0.410297	4.359101
H	-1.791812	-0.527988	3.337478
C	-2.164846	2.030206	3.194162
Cl	-3.235284	2.186000	4.576451
H	-2.699683	1.854847	2.266499
H	-1.372464	2.770804	3.187040

Sum of electronic and thermal Enthalpies = -1036.711832 Hartree
 $\langle S^2 \rangle = 0.771065$

Imaginary frequency = i346 cm⁻¹

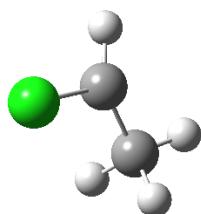
AT-A0-MCpro



C	-0.053754	0.090981	0.092529
C	0.020565	-0.157835	2.478230
C	2.321188	0.050636	1.990164
H	-0.333107	1.135313	0.285901
H	-0.726177	-0.300308	-0.675349
H	3.137878	0.613225	2.451750
O	-0.336994	-0.697978	1.267380
C	2.476207	0.061096	0.482999
C	1.378301	0.012593	-0.393601
C	1.611507	-0.047024	-1.772782
C	2.905715	-0.051143	-2.290806
C	3.993834	0.001616	-1.420447
C	3.772356	0.058838	-0.045375
H	5.009039	0.001391	-1.807494
H	3.061373	-0.098464	-3.364973
H	0.761755	-0.090817	-2.450729
H	4.621609	0.103181	0.633584
O	1.116083	0.666096	2.471714
H	2.361052	-0.978634	2.373228
C	-1.080270	0.268368	3.406322
H	-0.675425	0.368354	4.418343
H	-1.844165	-0.515222	3.423662
C	-1.724578	1.597583	2.990327
Cl	-3.048386	2.090283	4.144412
H	-2.192345	1.525955	2.006797
H	-0.996671	2.409919	2.991001

Sum of electronic and thermal Enthalpies = -1036.757651 Hartree
 $\langle S^2 \rangle = 0.752965$

AT_VC

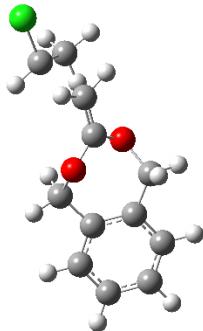


C	-0.027737	-0.026174	0.006834
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H	-0.054517	0.086469	1.097467
H	1.033174	-0.105378	-0.283793
H	-0.429068	0.887153	-0.446249
C	-0.825519	-1.197242	-0.439542
H	-1.309215	-1.255386	-1.407251
Cl	-0.555140	-2.742127	0.305438

Sum of electronic and thermal Enthalpies = -538.705542 Hartree
 $\langle S^2 \rangle = 0.753952$

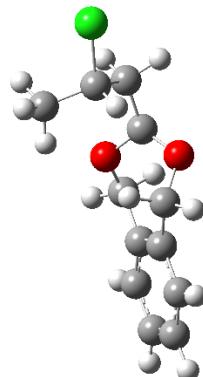
AT_A0-VCts



C	-0.002803	0.003147	0.002413
C	-0.001615	0.001944	2.373096
C	2.322600	0.001369	1.936365
H	-0.331388	1.045493	0.111300
H	-0.651662	-0.476807	-0.734981
H	3.166390	0.499916	2.420996
O	-0.258169	-0.700011	1.234089
C	2.517642	0.001198	0.434592
C	1.437118	-0.058084	-0.462278
C	1.693884	-0.120398	-1.836483
C	2.997923	-0.117347	-2.329874
C	4.069718	-0.055688	-1.440138
C	3.823144	0.005250	-0.069210
H	5.091611	-0.051258	-1.809012
H	3.173725	-0.166911	-3.400839
H	0.857113	-0.173387	-2.529880
H	4.659161	0.057907	0.625179
O	1.157562	0.722699	2.380593
H	2.271843	-1.025559	2.322554
C	-0.895204	0.078162	3.394886
H	-0.547813	0.395867	4.369817
H	-1.788938	-0.530203	3.346491
C	-2.162557	2.001805	3.241224
C	-1.211828	3.133525	3.470547
Cl	-3.463428	1.844823	4.438507
H	-1.691722	4.115713	3.339227
H	-0.794715	3.102200	4.483354
H	-0.381725	3.058898	2.758900
H	-2.561507	1.860445	2.240194

Sum of electronic and thermal Enthalpies = -1076.004272 Hartree
 $\langle S^2 \rangle = 0.773111$

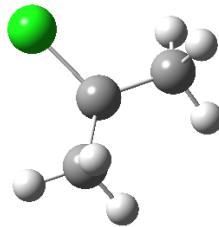
Imaginary frequency = i382 cm⁻¹

AT-A0-VCpro

C	-0.055782	0.170197	0.137455
C	0.022743	-0.103301	2.522192
C	2.326308	0.008244	2.021362
H	-0.308523	1.219978	0.338005
H	-0.741032	-0.197766	-0.630670
H	3.171385	0.517225	2.493891
O	-0.354951	-0.619615	1.306903
C	2.475174	0.051972	0.514540
C	1.371768	0.059069	-0.356556
C	1.596321	0.026578	-1.738107
C	2.887229	-0.004217	-2.263444
C	3.980866	-0.006395	-1.398478
C	3.768020	0.023425	-0.021196
H	4.993601	-0.028060	-1.791325
H	3.035900	-0.029684	-3.339349
H	0.742367	0.025491	-2.412204
H	4.621443	0.024961	0.653918
O	1.154067	0.670400	2.524129
H	2.314796	-1.031171	2.377479
C	-1.065628	0.302984	3.471613
H	-0.637114	0.446436	4.469302
H	-1.778523	-0.525624	3.529638
C	-1.835968	1.576505	3.063344
C	-1.035694	2.866343	3.173255
Cl	-3.340860	1.716372	4.126749
H	-1.633355	3.726456	2.858347
H	-0.709307	3.030406	4.205366
H	-0.142470	2.802055	2.542971
H	-2.241515	1.450240	2.056512

Sum of electronic and thermal Enthalpies = -1076.045836 Hartree
 $\langle S^2 \rangle = 0.753036$

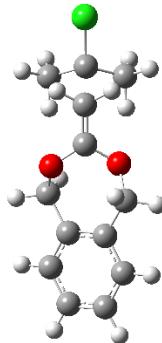
AT__PC



C	0.004710	-0.010059	-0.015026
H	0.082170	-0.030972	1.077290
H	1.032762	-0.042897	-0.415418
H	-0.433242	0.949313	-0.314713
C	-0.834738	-1.132330	-0.526784
Cl	-0.481558	-2.718507	0.145862
C	-1.464940	-1.127836	-1.879145
H	-1.848631	-0.126577	-2.107873
H	-0.747259	-1.395670	-2.673830
H	-2.294625	-1.840332	-1.938884

Sum of electronic and thermal Enthalpies = -577.99836 Hartree
 $\langle S^2 \rangle = 0.753925$

AT_A0-PCts



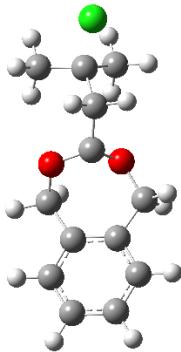
C	0.001617	-0.004967	0.000965
C	0.002005	-0.003556	2.376097
C	2.324589	-0.004468	1.939605
H	-0.292208	1.048586	0.100758
H	-0.659127	-0.468451	-0.736329
H	3.166944	0.511994	2.408008
O	-0.282557	-0.691799	1.234359
C	2.520614	-0.053758	0.438714
C	1.440396	-0.114690	-0.458227
C	1.698088	-0.223150	-1.829533
C	3.002529	-0.265037	-2.319978
C	4.073996	-0.202018	-1.429912
C	3.826688	-0.095128	-0.061943
H	5.096364	-0.232175	-1.796287
H	3.178885	-0.350173	-3.388604
H	0.861419	-0.276791	-2.522979
H	4.662654	-0.041426	0.632487
O	1.156477	0.725548	2.361037
H	2.277430	-1.018827	2.358809
C	-0.858945	0.040688	3.432127
H	-0.467597	0.319569	4.402428

H	-1.731173	-0.600520	3.407240
C	-2.176881	1.897189	3.445866
C	-1.207798	3.033249	3.599692
Cl	-3.185892	1.648057	4.910225
H	-1.720786	4.008214	3.605063
H	-0.635821	2.951226	4.528927
H	-0.499919	3.025154	2.762932
C	-2.980932	1.815443	2.180965
H	-2.305624	1.837658	1.317077
H	-3.570765	0.894794	2.133698
H	-3.674948	2.665333	2.084016

Sum of electronic and thermal Enthalpies = -1115.295584 Hartree
 $\langle S^2 \rangle = 0.774291$

Imaginary frequency = i407 cm⁻¹

AT-A0-PCpro

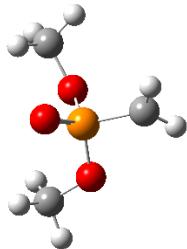


C	0.096074	0.903990	-0.398619
C	-0.016156	0.422652	1.922073
C	2.280845	0.993792	1.716054
H	0.210241	1.985682	-0.259394
H	-0.540853	0.735158	-1.269279
H	2.864546	1.922064	1.727041
O	-0.654750	0.372250	0.705012
C	2.445067	0.276780	0.387053
C	1.442653	0.239973	-0.600245
C	1.698914	-0.428183	-1.803731
C	2.926772	-1.041002	-2.048117
C	3.917174	-1.005924	-1.066992
C	3.667842	-0.358407	0.141838
H	4.876137	-1.488029	-1.236083
H	3.103289	-1.550671	-2.991120
H	0.918526	-0.467081	-2.560261
H	4.437638	-0.343814	0.911175
O	0.944981	1.406495	2.030786
H	2.662578	0.354384	2.524256
C	-0.889156	0.157890	3.111218
H	-0.238229	-0.038893	3.969529
H	-1.459182	-0.756655	2.916004
C	-1.891235	1.277186	3.512897
C	-1.200889	2.577484	3.917355
Cl	-2.756360	0.629762	5.047004
H	-1.933703	3.306642	4.275527
H	-0.465478	2.405570	4.708602

H	-0.675839	2.998239	3.053527
C	-2.977737	1.504999	2.464796
H	-2.524076	1.878333	1.540965
H	-3.502088	0.574045	2.230945
H	-3.708421	2.237439	2.820613

Sum of electronic and thermal Enthalpies = -1115.332624 Hartree
 $\langle S^2 \rangle = 0.752994$

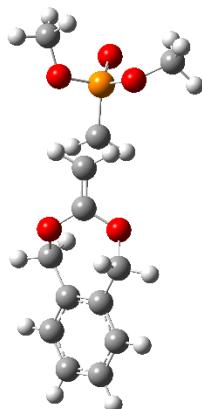
AT_MP



C	0.064541	-0.183177	0.066894
H	-0.140925	-0.153037	1.131642
P	1.720804	-0.069666	-0.560773
O	2.162816	1.497528	-0.471488
O	2.548488	-0.668403	0.686939
O	1.935489	-0.672424	-1.902167
C	2.021377	2.342914	-1.624962
H	2.324509	1.814883	-2.532515
H	2.667548	3.207329	-1.458522
H	0.983899	2.682238	-1.723975
C	3.980511	-0.768701	0.589001
H	4.311202	-1.315271	1.473603
H	4.266003	-1.315785	-0.314356
H	4.429772	0.229038	0.578952
H	-0.766501	-0.258797	-0.625710

Sum of electronic and thermal Enthalpies = -686.024307 Hartree
 $\langle S^2 \rangle = 0.753663$

AT_A0-MPtS



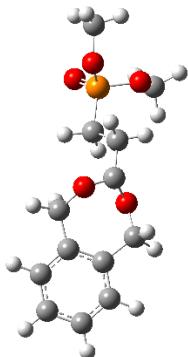
C	0.001099	0.000447	-0.000170
C	0.002551	-0.000032	2.364216
C	2.329949	0.000712	1.925014

H	-0.362634	1.029873	0.117954
H	-0.635450	-0.497247	-0.736382
H	3.171962	0.485009	2.426028
O	-0.226425	-0.715782	1.229940
C	2.521290	0.053274	0.424472
C	1.439976	-0.009586	-0.470643
C	1.692956	-0.024772	-1.846765
C	2.994906	0.027986	-2.342885
C	4.067890	0.092951	-1.454764
C	3.824629	0.107250	-0.081954
H	5.087905	0.135938	-1.826186
H	3.168318	0.014448	-3.415283
H	0.855799	-0.079995	-2.539540
H	4.660954	0.161829	0.611770
O	1.163839	0.705152	2.400812
H	2.282574	-1.038958	2.274577
C	-0.834824	-0.068706	3.429418
H	-1.845150	-0.427557	3.288100
H	-0.612801	0.511121	4.314596
C	-0.310692	-2.067628	4.604369
P	-1.480219	-2.187116	5.925622
O	-1.294452	-0.738319	6.632955
O	-2.943312	-2.036266	5.212802
O	-1.408926	-3.354615	6.851557
C	-1.990224	-0.483826	7.862899
C	-3.844383	-3.151642	5.153665
H	-1.790676	-1.274963	8.591493
H	-3.068476	-0.411517	7.682633
H	-1.618271	0.471722	8.237902
H	-3.710672	-3.690676	4.208479
H	-3.677367	-3.834333	5.990267
H	-4.859059	-2.747142	5.195026
H	-0.441455	-2.760486	3.778389
H	0.717755	-1.851876	4.878430

Sum of electronic and thermal Enthalpies = -1223.328488 Hartree
 $\langle S^2 \rangle = 0.76802$

Imaginary frequency = i276 cm⁻¹

AT_A0-MPpro

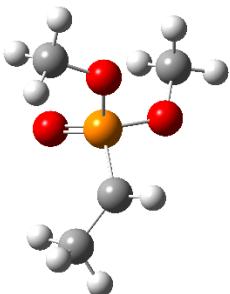


C	-0.101296	0.012121	0.017262
C	-0.184004	0.314777	2.356664
C	2.162557	-0.082513	2.039461

H	-0.423849	1.062818	0.005063
H	-0.726454	-0.539117	-0.691633
H	3.054768	0.277071	2.559019
O	-0.406172	-0.540519	1.305804
C	2.405515	-0.077682	0.544479
C	1.354624	-0.098123	-0.388878
C	1.655225	-0.163467	-1.754383
C	2.973914	-0.201574	-2.204815
C	4.017330	-0.178352	-1.280111
C	3.726355	-0.114994	0.081809
H	5.050601	-0.205574	-1.614843
H	3.183026	-0.252403	-3.269844
H	0.840806	-0.185529	-2.475890
H	4.539479	-0.093512	0.804340
O	1.100730	0.790220	2.478654
H	1.957898	-1.103126	2.387590
C	-0.910843	-0.051884	3.615951
H	-1.978117	-0.140119	3.390202
H	-0.789606	0.761864	4.336639
C	-0.412662	-1.375307	4.253730
P	-1.327546	-1.925441	5.724239
O	-1.263960	-0.594650	6.638887
O	-2.903223	-1.934751	5.300958
O	-0.864129	-3.195859	6.342693
C	-1.863213	-0.617870	7.945991
C	-3.535018	-3.173694	4.939628
H	-1.477185	-1.458104	8.530579
H	-2.951990	-0.692036	7.861682
H	-1.593447	0.324253	8.426185
H	-3.310763	-3.427483	3.896941
H	-3.202872	-3.984332	5.592920
H	-4.610740	-3.018950	5.047718
H	-0.475000	-2.194529	3.527625
H	0.637647	-1.289905	4.554617

Sum of electronic and thermal Enthalpies = -1223.369451 Hartree
 $\langle S^2 \rangle = 0.752734$

AT_VP

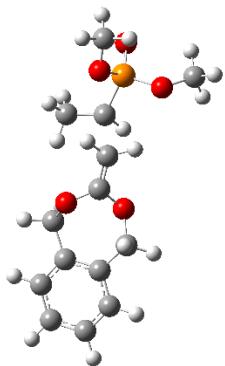


C	0.111244	-0.323669	0.078531
H	0.517351	-0.736723	1.014580
H	0.940448	0.048206	-0.528655
C	-0.688777	-1.341616	-0.660340
H	-1.549412	-1.800104	-0.177710
P	-0.310326	-1.832973	-2.327789
O	-0.212943	-3.462347	-2.333700
O	-1.739793	-1.646923	-3.054806

O	0.867896	-1.151832	-2.928442
C	1.061653	-4.083866	-2.108899
H	1.833593	-3.623551	-2.731332
H	0.944509	-5.136990	-2.372608
H	1.347663	-4.005838	-1.053258
C	-1.863376	-1.969013	-4.452200
H	-2.849352	-1.618802	-4.762415
H	-1.089155	-1.460008	-5.034111
H	-1.789780	-3.050827	-4.599295
H	-0.516113	0.532713	0.370344

Sum of electronic and thermal Enthalpies = -725.31745 Hartree
 $\langle S^2 \rangle = 0.753712$

AT_A0-VPts



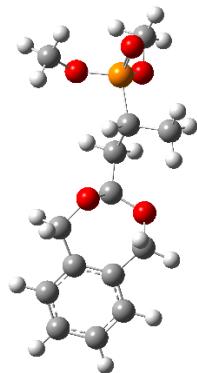
C	-0.000320	0.009749	-0.002855
C	-0.001467	0.006235	2.360292
C	2.332455	0.006757	1.922714
H	-0.428383	1.014522	0.116949
H	-0.601829	-0.522680	-0.744635
H	3.179060	0.454960	2.448804
O	-0.189930	-0.721980	1.224007
C	2.517791	0.153292	0.427835
C	1.438218	0.093098	-0.469414
C	1.687796	0.168626	-1.844277
C	2.984556	0.308720	-2.336840
C	4.056124	0.370805	-1.446749
C	3.815976	0.294931	-0.075529
H	5.072083	0.481470	-1.815301
H	3.155236	0.365027	-3.408314
H	0.852031	0.115263	-2.539019
H	4.650827	0.347544	0.620073
O	1.173898	0.686164	2.446381
H	2.282314	-1.053126	2.203864
C	-0.895830	-0.030697	3.388052
H	-1.915826	-0.322004	3.175301
H	-0.715957	0.593701	4.253256
C	-0.582640	-1.946038	4.625511
C	0.792865	-1.836773	5.229746
P	-1.985873	-2.007126	5.716836
H	0.845598	-1.018945	5.956317
H	1.079285	-2.760731	5.754276
H	1.545752	-1.652077	4.455254
O	-1.914026	-0.542017	6.412890

O	-3.292559	-1.857522	4.745591
O	-2.100712	-3.149285	6.670768
C	-2.805378	-0.253369	7.500991
C	-4.152784	-2.982856	4.513122
H	-2.770314	-1.048702	8.251088
H	-3.830339	-0.139119	7.131485
H	-2.467974	0.688370	7.938585
H	-3.820225	-3.532756	3.624909
H	-4.160230	-3.652430	5.376560
H	-5.155956	-2.587168	4.335183
H	-0.683154	-2.627062	3.781207

Sum of electronic and thermal Enthalpies = -1262.616118 Hartree
 $\langle S^2 \rangle = 0.7716$

Imaginary frequency = i359 cm⁻¹

AT_A0-VPpro

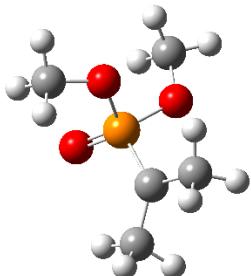


C	0.273747	-1.194034	0.228436
C	0.487469	-0.448775	2.474864
C	2.774582	-0.646035	1.869240
H	-0.680320	-0.698822	-0.001833
H	0.273012	-2.163427	-0.284889
H	3.730554	-0.315240	2.280762
O	0.314153	-1.522718	1.620110
C	2.582756	-0.079222	0.477315
C	1.418440	-0.329562	-0.272687
C	1.299877	0.222739	-1.553210
C	2.319896	0.995627	-2.105502
C	3.475915	1.242459	-1.365596
C	3.593170	0.712614	-0.081622
H	4.275005	1.851541	-1.778844
H	2.206740	1.409849	-3.103682
H	0.392822	0.042560	-2.127354
H	4.486594	0.915896	0.504346
O	1.797673	-0.199980	2.821740
H	2.770853	-1.742603	1.846137
C	-0.487847	-0.358426	3.609501
H	-1.480283	-0.167923	3.186688
H	-0.225737	0.503609	4.230851
C	-0.556574	-1.638894	4.493818
C	0.710777	-1.879712	5.331939
P	-2.032731	-1.656870	5.569968
H	0.879743	-1.050138	6.026945

H	0.622729	-2.801825	5.914093
H	1.585531	-1.954001	4.680767
O	-1.899337	-0.228874	6.319256
O	-3.312423	-1.376932	4.593170
O	-2.198513	-2.855991	6.435966
C	-2.857515	0.121275	7.331885
C	-4.131691	-2.474438	4.159905
H	-2.946054	-0.679975	8.071419
H	-3.833907	0.317009	6.877058
H	-2.485408	1.029137	7.810084
H	-3.700077	-2.941552	3.266927
H	-4.231749	-3.220927	4.951736
H	-5.110039	-2.057664	3.909788
H	-0.707746	-2.497201	3.824187

Sum of electronic and thermal Enthalpies = -1262.653216 Hartree
 $\langle S^2 \rangle = 0.752731$

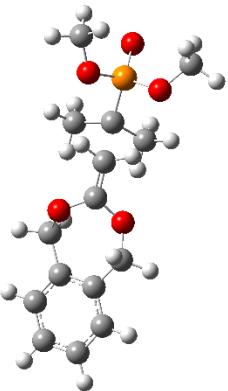
AT_PP1



C	-0.036650	0.053709	-0.136108
H	-0.036705	0.206366	0.953694
H	0.997058	0.026524	-0.488515
C	-0.780091	-1.192485	-0.501805
P	-0.019687	-2.372813	-1.602366
O	-0.330412	-3.857206	-0.993284
O	-1.046269	-2.382732	-2.853198
O	1.417344	-2.126475	-1.899862
C	0.617463	-4.449746	-0.092309
H	1.635268	-4.348768	-0.478497
H	0.350168	-5.505355	-0.009306
H	0.553859	-3.982501	0.897669
C	-0.785078	-3.257489	-3.965765
H	-1.514064	-3.001702	-4.736796
H	0.228540	-3.101526	-4.346965
H	-0.913263	-4.301879	-3.665221
H	-0.523370	0.942642	-0.570175
C	-2.199440	-1.368639	-0.055697
H	-2.324609	-1.052163	0.989028
H	-2.877996	-0.743184	-0.658486
H	-2.539599	-2.403786	-0.148909

Sum of electronic and thermal Enthalpies = -764.609614 Hartree
 $\langle S^2 \rangle = 0.753777$

AT_A0-PPts



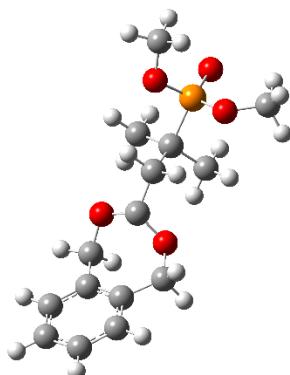
C	-0.000536	0.003836	-0.001461
C	-0.001938	0.001671	2.375823
C	2.321290	0.000845	1.940660
H	-0.266540	1.064488	0.095427
H	-0.671676	-0.444494	-0.738459
H	3.160910	0.534335	2.394643
O	-0.307291	-0.672490	1.232919
C	2.515865	-0.086146	0.441205
C	1.435769	-0.145553	-0.455682
C	1.693243	-0.289340	-1.823906
C	2.997149	-0.368300	-2.311004
C	4.068493	-0.307225	-1.420579
C	3.821668	-0.164844	-0.055841
H	5.090557	-0.366020	-1.784342
H	3.173237	-0.480588	-3.377151
H	0.856535	-0.341250	-2.517346
H	4.657705	-0.111936	0.638635
O	1.149302	0.732925	2.349334
H	2.281254	-1.002806	2.386043
C	-0.843500	0.022217	3.454319
H	-0.425215	0.278911	4.419065
H	-1.697767	-0.642438	3.439751
C	-2.154908	1.861811	3.450655
C	-2.949746	1.731877	2.170970
P	-3.105759	1.655942	4.953033
H	-3.571232	0.831882	2.160987
H	-3.612903	2.598637	2.024608
H	-2.274115	1.693302	1.307777
O	-3.754305	0.176233	4.731628
O	-1.948799	1.450808	6.087269
O	-4.110817	2.692507	5.336607
C	-4.874924	-0.226313	5.531944
C	-2.112526	1.981344	7.411004
H	-5.610637	0.579322	5.603332
H	-4.544300	-0.511631	6.537655
H	-5.315332	-1.095660	5.038824
H	-1.122508	2.287586	7.758820
H	-2.792277	2.836976	7.407304
H	-2.503555	1.204630	8.077973
C	-1.158473	2.999322	3.486058
H	-0.570597	2.999361	4.408693
H	-0.462326	2.922025	2.643009
H	-1.665118	3.974081	3.410600

Sum of electronic and thermal Enthalpies = -1301.904384 Hartree

$\langle S^2 \rangle = 0.773151$

Imaginary frequency = i401 cm⁻¹

AT_A0-PPpro

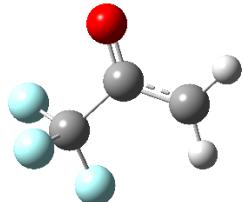


C	0.159384	1.005018	-0.372821
C	-0.150661	0.585795	1.940666
C	2.200688	0.895645	1.877835
H	0.395955	2.068271	-0.245231
H	-0.435230	0.892505	-1.281914
H	2.886534	1.751340	1.903619
O	-0.718544	0.594667	0.686403
C	2.361039	0.124964	0.578336
C	1.426272	0.179971	-0.472760
C	1.675310	-0.549218	-1.641755
C	2.832560	-1.311920	-1.791081
C	3.755712	-1.367193	-0.747305
C	3.510400	-0.659488	0.428200
H	4.657685	-1.965786	-0.841790
H	3.005037	-1.866676	-2.709129
H	0.945197	-0.516685	-2.447244
H	4.225529	-0.715748	1.246893
O	0.905377	1.463732	2.098891
H	2.459896	0.240307	2.721496
C	-1.111258	0.426452	3.078056
H	-0.519538	0.197670	3.971169
H	-1.733056	-0.450153	2.869204
C	-2.059860	1.633858	3.406053
C	-3.077715	1.887041	2.274081
P	-3.019545	1.247186	4.933276
H	-3.664239	0.988590	2.057943
H	-3.768423	2.690585	2.549687
H	-2.551736	2.172563	1.359026
O	-3.647736	-0.200793	4.563509
O	-1.916457	0.849852	6.071724
O	-3.987438	2.284529	5.387556
C	-4.544511	-0.827487	5.494657
C	-1.706225	1.685714	7.221311
H	-5.354060	-0.144739	5.769006
H	-4.001335	-1.139779	6.392936
H	-4.952814	-1.704918	4.989822
H	-0.816420	2.305408	7.066754
H	-2.573075	2.325785	7.402028
H	-1.542345	1.025015	8.076666

C	-1.264761	2.923797	3.700840
H	-0.509619	2.764484	4.478225
H	-0.738846	3.252674	2.799909
H	-1.936123	3.725936	4.024280

Sum of electronic and thermal Enthalpies = -1301.935639 Hartree
 $\langle S^2 \rangle = 0.7529$

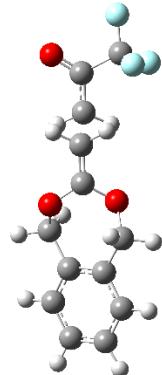
AT_F



C	0.193019	0.004576	0.052351
C	-0.007325	-0.008228	1.459655
H	0.228762	-0.917841	2.000675
H	-0.380810	0.853394	1.999622
C	-0.100847	1.307651	-0.724477
O	0.618465	-0.965901	-0.587184
F	-0.748041	1.042345	-1.865883
F	1.052836	1.932419	-1.027470
F	-0.856059	2.165631	-0.001490

Sum of electronic and thermal Enthalpies = -490.15019 Hartree
 $\langle S^2 \rangle = 0.770336$

AT_A0-Fts1



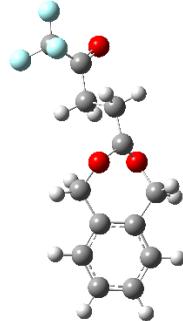
C	0.000066	0.002075	0.001477
C	0.001314	0.004673	2.367557
C	2.333949	0.004068	1.928282
H	-0.410660	1.014235	0.113451
H	-0.612980	-0.529129	-0.730450
H	3.173607	0.467234	2.450993
O	-0.210534	-0.714113	1.239932
C	2.517972	0.127375	0.432695
C	1.438980	0.054372	-0.463425
C	1.688880	0.097555	-1.839525
C	2.987049	0.218412	-2.333254

C	4.058290	0.294372	-1.443826
C	3.817661	0.250443	-0.071389
H	5.074927	0.390794	-1.814024
H	3.158971	0.249458	-3.405382
H	0.853341	0.035380	-2.533474
H	4.652441	0.312313	0.623284
O	1.166399	0.684217	2.448005
H	2.285543	-1.049928	2.229235
C	-0.869751	-0.053807	3.419674
H	-1.889400	-0.360038	3.230475
H	-0.672986	0.565688	4.285447
C	-0.365425	-1.933080	4.575750
C	-1.319904	-1.876230	5.641267
H	-0.500634	-2.634446	3.760996
C	-2.698608	-2.521411	5.364588
O	-1.161364	-1.283293	6.711246
F	-3.363339	-2.772096	6.495577
F	-2.586899	-3.681692	4.675060
F	-3.465618	-1.688994	4.609071
H	0.647529	-1.633959	4.819909

Sum of electronic and thermal Enthalpies = -1027.457871 Hartree
 $\langle S^2 \rangle = 0.769591$

Imaginary frequency = i307 cm⁻¹

AT_A0-Fpro2

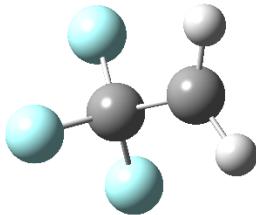


C	-0.061388	-0.064841	-0.034862
C	-0.159787	0.184497	2.311693
C	2.205929	-0.062115	1.992273
H	-0.487891	0.948009	-0.035484
H	-0.627271	-0.668050	-0.750700
H	3.073488	0.322637	2.534080
O	-0.317147	-0.661061	1.247107
C	2.444656	0.044093	0.501093
C	1.399426	-0.023218	-0.436189
C	1.703591	0.009075	-1.802108
C	3.020077	0.112947	-2.248197
C	4.057925	0.182638	-1.319459
C	3.763363	0.149640	0.042544
H	5.089136	0.265761	-1.651031
H	3.232213	0.135770	-3.313505
H	0.894216	-0.048757	-2.527227
H	4.571800	0.206844	0.768252
O	1.093193	0.716160	2.483745

H	2.063295	-1.111227	2.281185
C	-0.911163	-0.211492	3.541238
H	-1.972545	-0.318071	3.296020
H	-0.805545	0.583590	4.284386
C	-0.410103	-1.564737	4.157147
C	-1.255846	-1.952625	5.342870
H	-0.508084	-2.350846	3.403136
C	-0.722263	-1.513531	6.729986
O	-2.319972	-2.525851	5.272093
F	-1.539515	-1.871382	7.719487
F	-0.571536	-0.167653	6.761104
F	0.492607	-2.062779	6.955907
H	0.640468	-1.466795	4.446892

Sum of electronic and thermal Enthalpies = -1027.482638 Hartree
 $\langle S^2 \rangle = 0.753348$

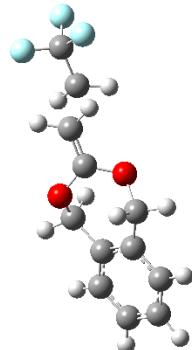
AT_MF



C	0.116665	-0.179086	0.082502
H	-0.085883	0.154370	1.091813
H	1.000596	0.154542	-0.445026
C	-0.689281	-1.282376	-0.487392
F	-0.706489	-1.238445	-1.837684
F	-0.199054	-2.502237	-0.140971
F	-1.967997	-1.238657	-0.053242

Sum of electronic and thermal Enthalpies = -376.833557 Hartree
 $\langle S^2 \rangle = 0.75351$

AT_A0-MFts



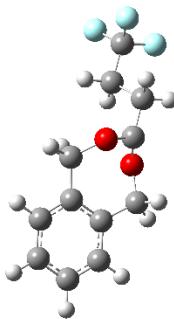
C	-0.003594	0.004131	0.002199
C	-0.002307	0.002419	2.371306
C	2.320797	0.001942	1.933203
H	-0.329257	1.046647	0.113549
H	-0.656130	-0.475083	-0.731892

H	3.161340	0.504281	2.418832
O	-0.261691	-0.697951	1.236496
C	2.515313	0.002426	0.432027
C	1.434825	-0.061153	-0.463841
C	1.690215	-0.127177	-1.838062
C	2.994107	-0.123693	-2.331783
C	4.066274	-0.057288	-1.442767
C	3.820722	0.007031	-0.071811
H	5.087882	-0.051936	-1.812242
H	3.169585	-0.176177	-3.402596
H	0.853226	-0.182919	-2.530886
H	4.656992	0.062683	0.621950
O	1.153050	0.719124	2.382244
H	2.274151	-1.025041	2.319328
C	-0.881692	0.055563	3.401452
H	-0.545583	0.405657	4.367567
H	-1.791204	-0.527032	3.348722
C	-2.187791	2.056232	3.220734
H	-2.686817	1.907909	2.269943
C	-3.039810	1.944063	4.421405
H	-1.400328	2.799658	3.259309
F	-3.814908	0.829655	4.388913
F	-2.304142	1.889585	5.561272
F	-3.896679	2.995683	4.575523

Sum of electronic and thermal Enthalpies = -914.140034 Hartree
 $\langle S^2 \rangle = 0.768418$

Imaginary frequency = i260 cm⁻¹

AT_A0-MFpro

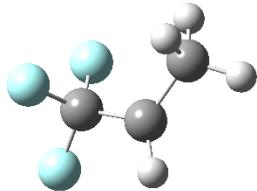


C	-0.081091	0.104283	0.153961
C	0.031252	-0.234256	2.529435
C	2.320314	0.038229	2.017596
H	-0.346784	1.143924	0.385635
H	-0.766339	-0.254179	-0.618592
H	3.129427	0.617255	2.472631
O	-0.358148	-0.722100	1.303334
C	2.453777	0.065894	0.508236
C	1.343843	0.029651	-0.353556
C	1.558350	-0.012703	-1.736527
C	2.845234	-0.011662	-2.272347
C	3.945229	0.028866	-1.416263
C	3.742658	0.068773	-0.037719
H	4.955071	0.032384	-1.817157
H	2.986204	-0.045502	-3.349066

H	0.699244	-0.046755	-2.403147
H	4.601258	0.103543	0.630046
O	1.107620	0.616136	2.523144
H	2.393249	-0.993483	2.389433
C	-1.056495	0.154631	3.485430
H	-0.628570	0.239299	4.489375
H	-1.800563	-0.647892	3.505653
C	-1.755026	1.485792	3.122541
H	-2.232516	1.414781	2.139907
C	-2.826846	1.871352	4.115010
H	-1.026873	2.301920	3.088333
F	-3.800102	0.933742	4.192949
F	-2.323984	2.027077	5.361923
F	-3.420438	3.037736	3.773515

Sum of electronic and thermal Enthalpies = -914.184704 Hartree
 $\langle S^2 \rangle = 0.752679$

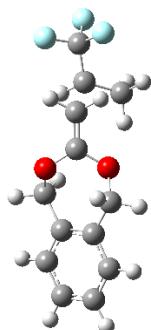
AT_VF



C	-0.012459	-0.040731	-0.015880
H	0.044987	-0.172626	1.059242
C	1.283478	0.086187	-0.725389
F	2.243165	0.588803	0.080508
F	1.739270	-1.114465	-1.182525
F	1.191665	0.892692	-1.811199
C	-1.273033	-0.300430	-0.761023
H	-2.146695	0.009788	-0.178491
H	-1.283241	0.227389	-1.720327
H	-1.396928	-1.374372	-0.981231

Sum of electronic and thermal Enthalpies = -416.127867 Hartree
 $\langle S^2 \rangle = 0.753616$

AT_A0-VFts



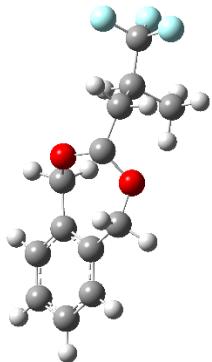
C	-0.002172	0.003531	0.003267
C	0.000293	0.002097	2.374283
C	2.324859	0.000484	1.935210

H	-0.330207	1.045839	0.111615
H	-0.652449	-0.477569	-0.731810
H	3.167253	0.499941	2.420829
O	-0.259644	-0.697428	1.237436
C	2.518081	0.003565	0.433674
C	1.437032	-0.058711	-0.462009
C	1.692328	-0.120906	-1.836480
C	2.995950	-0.114507	-2.330865
C	4.068428	-0.049396	-1.442173
C	3.823203	0.011123	-0.071017
H	5.089889	-0.042020	-1.812075
H	3.170926	-0.163881	-3.401934
H	0.855091	-0.175825	-2.529098
H	4.659702	0.066015	0.622541
O	1.158512	0.718945	2.384854
H	2.275683	-1.026998	2.319744
C	-0.891721	0.074787	3.398624
H	-0.545067	0.394415	4.372380
H	-1.785990	-0.531994	3.348146
C	-2.154680	2.021524	3.218484
H	-2.577124	1.839660	2.233420
C	-3.139966	1.814934	4.307434
F	-3.897995	0.708942	4.103965
F	-2.543809	1.676325	5.521415
F	-4.013349	2.858766	4.439111
C	-1.187199	3.158614	3.358847
H	-0.751473	3.183891	4.363328
H	-0.368688	3.063436	2.638592
H	-1.674556	4.131640	3.188493

Sum of electronic and thermal Enthalpies = -953.430967 Hartree
 $\langle S^2 \rangle = 0.772038$

Imaginary frequency = i336 cm⁻¹

AT_A0-VFpro

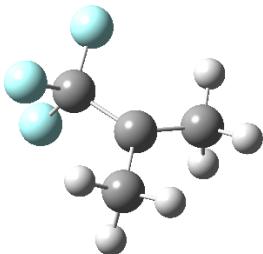


C	-0.061376	0.237253	0.188062
C	0.061957	-0.098010	2.564442
C	2.355354	0.008609	2.019977
H	-0.276662	1.289294	0.416469
H	-0.771707	-0.092127	-0.574774
H	3.212803	0.512562	2.475753
O	-0.362568	-0.570270	1.344287
C	2.473362	0.055136	0.510164

C	1.352320	0.094574	-0.337212
C	1.547387	0.065636	-1.723398
C	2.825803	0.006342	-2.276075
C	3.936902	-0.028879	-1.434318
C	3.753632	-0.002533	-0.052739
H	4.940372	-0.073224	-1.848534
H	2.951314	-0.015562	-3.355030
H	0.679798	0.090180	-2.379409
H	4.620716	-0.026325	0.604393
O	1.197069	0.672807	2.548962
H	2.347674	-1.032079	2.373062
C	-0.997342	0.308463	3.543654
H	-0.527986	0.482210	4.517566
H	-1.681208	-0.540106	3.653127
C	-1.832584	1.558373	3.142950
H	-2.215972	1.399916	2.127139
C	-3.070381	1.656847	4.021093
F	-3.849765	0.554372	3.920019
F	-2.750498	1.798445	5.329872
F	-3.842615	2.716277	3.683056
C	-1.032316	2.866774	3.198535
H	-0.707192	3.074774	4.223639
H	-0.138515	2.792805	2.575272
H	-1.636069	3.711417	2.853907

Sum of electronic and thermal Enthalpies = -953.470444 Hartree
 $\langle S^2 \rangle = 0.752791$

AT_PF



C	-0.076151	-0.132731	0.004400
C	0.053678	0.093891	1.470828
F	1.346107	0.156692	1.868987
F	-0.546768	1.240207	1.868906
F	-0.522115	-0.911600	2.195078
C	0.885941	-1.066697	-0.655314
H	0.975979	-0.840404	-1.724148
H	1.879138	-1.014668	-0.201099
H	0.546318	-2.114295	-0.579980
C	-1.371901	0.216470	-0.653065
H	-1.835826	1.094698	-0.195967
H	-1.224831	0.412757	-1.721520
H	-2.097174	-0.612397	-0.579370

Sum of electronic and thermal Enthalpies = -455.420934 Hartree
 $\langle S^2 \rangle = 0.753688$

AT_A0-PFts

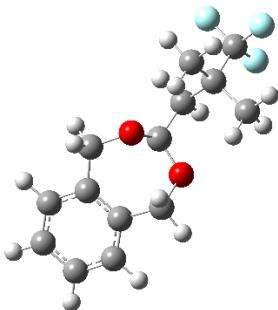


C	-0.002987	0.015428	-0.003443
C	-0.005877	0.011128	2.372897
C	2.317840	0.008114	1.938547
H	-0.293584	1.069598	0.095989
H	-0.664522	-0.446401	-0.740765
H	3.158617	0.524372	2.409564
O	-0.294846	-0.669631	1.230558
C	2.515048	-0.038108	0.438152
C	1.435891	-0.098780	-0.459770
C	1.694877	-0.206707	-1.830898
C	2.999871	-0.248077	-2.319790
C	4.070408	-0.184973	-1.428589
C	3.821772	-0.078890	-0.060834
H	5.093133	-0.214379	-1.793928
H	3.177412	-0.332572	-3.388236
H	0.859030	-0.259629	-2.525324
H	4.656967	-0.025368	0.634489
O	1.148338	0.736612	2.362845
H	2.270117	-1.006850	2.355927
C	-0.863356	0.045088	3.434409
H	-0.464731	0.312271	4.404364
H	-1.731458	-0.600988	3.406520
C	-2.167876	1.923617	3.420371
C	-2.987968	1.659792	4.639476
F	-3.733284	0.530340	4.532068
F	-2.232069	1.528910	5.759403
F	-3.872135	2.672137	4.897626
C	-2.931816	1.848840	2.125040
H	-2.242135	1.866159	1.274016
H	-3.538364	0.941017	2.057446
H	-3.609786	2.710321	2.011687
C	-1.178700	3.051530	3.555931
H	-0.643360	3.010866	4.508938
H	-0.438761	3.009769	2.749894
H	-1.680737	4.030940	3.498436

Sum of electronic and thermal Enthalpies = -992.721196 Hartree
 $\langle S^2 \rangle = 0.773711$

Imaginary frequency = i374 cm⁻¹

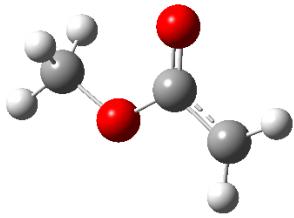
AT_A0-PFadd



C	0.151992	0.722549	-0.482798
C	0.095902	0.331088	1.856145
C	2.358235	1.009107	1.588037
H	0.224605	1.813122	-0.391698
H	-0.487985	0.491526	-1.336916
H	2.890334	1.966769	1.536838
O	-0.561583	0.209596	0.652512
C	2.534700	0.232036	0.294768
C	1.522034	0.105214	-0.674519
C	1.789525	-0.612188	-1.846634
C	3.038344	-1.186448	-2.078779
C	4.039334	-1.061466	-1.115960
C	3.779305	-0.364543	0.062866
H	5.015094	-1.512227	-1.275296
H	3.223224	-1.735933	-2.997535
H	1.001245	-0.721200	-2.588004
H	4.557821	-0.280295	0.818850
O	1.009175	1.365155	1.913724
H	2.792768	0.434826	2.418267
C	-0.749570	0.068855	3.062185
H	-0.076837	-0.124405	3.905134
H	-1.303573	-0.856885	2.873198
C	-1.774745	1.172912	3.502471
C	-2.532974	0.614726	4.714043
F	-3.211557	-0.519500	4.414612
F	-1.701310	0.312062	5.741299
F	-3.441487	1.496717	5.195686
C	-2.798855	1.472704	2.391940
H	-2.294326	1.898736	1.522282
H	-3.315069	0.564257	2.067726
H	-3.547990	2.189058	2.744063
C	-1.060881	2.467246	3.937427
H	-0.349133	2.275732	4.746620
H	-0.507497	2.889866	3.096645
H	-1.787397	3.207019	4.288030

Sum of electronic and thermal Enthalpies = -992.754991 Hartree
 $\langle S^2 \rangle = 0.752855$

AT_MEST



C	0.004549	0.000075	0.006207
H	-0.020602	0.000766	1.089167
C	1.258550	0.000572	-0.716555
C	3.606799	-0.000005	-0.523862
H	4.343838	0.001242	0.279963
H	3.722757	0.887963	-1.152192
H	3.723081	-0.889759	-1.149627
O	1.360473	-0.001230	-1.935331
O	2.328581	0.000687	0.124636
H	-0.915687	-0.001173	-0.563685

Sum of electronic and thermal Enthalpies = -267.643234 Hartree
 $\langle S^2 \rangle = 0.75759$

AT_A0-MESTts



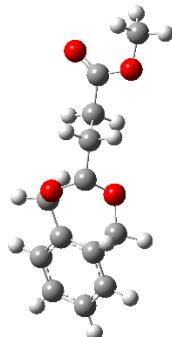
C	-0.001358	0.003054	-0.000159
C	-0.003080	0.003972	2.364980
C	2.326425	-0.000356	1.930334
H	-0.356303	1.035838	0.114299
H	-0.640556	-0.491871	-0.735607
H	3.166581	0.488372	2.429734
O	-0.241178	-0.707132	1.232328
C	2.518320	0.043288	0.430052
C	1.438430	-0.021110	-0.466405
C	1.693549	-0.048116	-1.842019
C	2.996551	-0.005197	-2.336179
C	4.068183	0.061933	-1.446580
C	3.822808	0.087771	-0.074420
H	5.089002	0.097784	-1.816476
H	3.171821	-0.027926	-3.408078
H	0.857229	-0.104557	-2.535642
H	4.658283	0.144026	0.620146
O	1.158001	0.705094	2.403912
H	2.279528	-1.037777	2.286304
C	-0.829687	-0.084684	3.445002
H	-1.849856	-0.413185	3.294513
H	-0.604810	0.515876	4.316880

C	-0.345105	-2.019916	4.580397
C	-1.262938	-1.886316	5.692839
O	-1.016136	-1.351602	6.765467
O	-2.503827	-2.382078	5.387120
C	-3.475836	-2.250625	6.428132
H	-3.165475	-2.796788	7.324256
H	-3.623683	-1.200196	6.697036
H	-4.398152	-2.674430	6.026945
H	-0.583713	-2.703543	3.774755
H	0.697982	-1.823423	4.794443

Sum of electronic and thermal Enthalpies = -804.946222 Hartree
 $\langle S^2 \rangle = 0.769635$

Imaginary frequency = i355 cm⁻¹

AT_A0-MESTpro

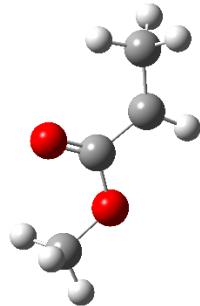


C	-0.067189	0.003853	-0.001374
C	-0.153282	0.293459	2.339209
C	2.206285	-0.008764	2.013037
H	-0.413884	1.046763	-0.007638
H	-0.681781	-0.558854	-0.710257
H	3.084517	0.393382	2.525090
O	-0.354756	-0.561734	1.285729
C	2.442612	-0.009613	0.517072
C	1.389426	-0.071018	-0.412155
C	1.687357	-0.143350	-1.777886
C	3.005100	-0.147337	-2.232736
C	4.050442	-0.081877	-1.312238
C	3.762337	-0.012098	0.049968
H	5.082945	-0.081693	-1.650440
H	3.212049	-0.204372	-3.297859
H	0.871503	-0.197862	-2.495992
H	4.577052	0.041864	0.769022
O	1.110108	0.823006	2.448694
H	2.046521	-1.033385	2.372762
C	-0.855950	-0.104075	3.600848
H	-1.928346	-0.186203	3.398377
H	-0.709987	0.694182	4.336451
C	-0.357779	-1.452936	4.202226
C	-1.101086	-1.808624	5.470391
O	-0.642952	-1.775260	6.592348
O	-2.386155	-2.146771	5.201497
C	-3.190359	-2.464142	6.348054
H	-2.774800	-3.321880	6.883972

H	-3.241120	-1.612225	7.031618
H	-4.180119	-2.700789	5.955996
H	-0.503929	-2.244710	3.460180
H	0.703112	-1.387962	4.455315

Sum of electronic and thermal Enthalpies = -804.979798 Hartree
 $\langle S^2 \rangle = 0.752844$

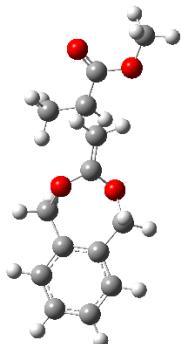
AT_MA2



C	0.005401	0.008091	0.001847
H	0.000771	-0.000163	1.094267
H	1.047449	0.025874	-0.350514
H	-0.450249	0.946447	-0.348406
C	-0.720546	-1.171409	-0.532355
H	-0.808366	-1.328895	-1.603146
C	-1.333813	-2.144956	0.349724
C	-2.577442	-4.144974	0.452629
H	-3.014702	-4.853718	-0.251929
H	-3.354407	-3.704822	1.084767
H	-1.846446	-4.645415	1.094742
O	-1.317682	-2.100165	1.573253
O	-1.945962	-3.141236	-0.350463

Sum of electronic and thermal Enthalpies = -306.938829 Hartree
 $\langle S^2 \rangle = 0.756682$

AT_A0-MAts



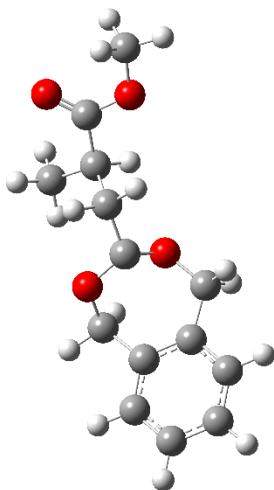
C	-0.001467	0.002262	-0.000109
C	-0.000609	0.000207	2.376425
C	2.322515	0.001503	1.941145
H	-0.274363	1.060824	0.097708
H	-0.671644	-0.451717	-0.734069
H	3.160182	0.534444	2.398781

O	-0.305144	-0.674379	1.237804
C	2.515232	-0.073898	0.441129
C	1.434835	-0.138818	-0.454691
C	1.691290	-0.277024	-1.823655
C	2.995198	-0.344337	-2.312253
C	4.067122	-0.276827	-1.422960
C	3.821061	-0.140576	-0.057487
H	5.089086	-0.326207	-1.788240
H	3.170902	-0.452297	-3.378867
H	0.854194	-0.333046	-2.516222
H	4.657394	-0.083781	0.636215
O	1.148852	0.727532	2.359174
H	2.285928	-1.005533	2.378779
C	-0.854506	0.045856	3.445954
H	-0.439870	0.301548	4.413015
H	-1.726953	-0.596164	3.422186
C	-2.068737	1.917491	3.424229
C	-2.898743	1.859429	2.177247
C	-2.743960	1.731039	4.701332
H	-3.430496	2.808616	2.009917
H	-2.280778	1.674057	1.292160
H	-3.657182	1.074911	2.253724
O	-3.862449	1.259814	4.858561
O	-1.944811	2.089839	5.754744
C	-2.524755	1.888866	7.047260
H	-1.765420	2.205559	7.764421
H	-3.432383	2.488545	7.165681
H	-2.781825	0.836719	7.203074
H	-1.209129	2.580680	3.437653

Sum of electronic and thermal Enthalpies = -844.236411 Hartree
 $\langle S^2 \rangle = 0.771258$

Imaginary frequency = i416 cm⁻¹

AT_A0-MApro

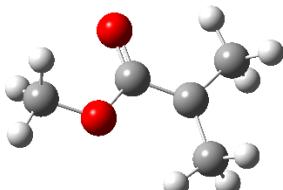


C	-0.022792	0.582211	-0.425412
C	-0.131204	0.380658	1.937002
C	2.100145	1.157087	1.674456
H	-0.017192	1.679008	-0.422827

H	-0.621766	0.244615	-1.273830
H	2.586408	2.134645	1.570183
O	-0.739812	0.120498	0.728986
C	2.361944	0.300459	0.447172
C	1.387041	0.037693	-0.533365
C	1.732114	-0.745912	-1.641172
C	3.020034	-1.255164	-1.799264
C	3.983463	-0.995715	-0.824923
C	3.647129	-0.231202	0.290977
H	4.989419	-1.393857	-0.926373
H	3.264707	-1.858112	-2.669254
H	0.973684	-0.959269	-2.390941
H	4.396946	-0.041240	1.056813
O	0.725960	1.463892	1.929178
H	2.533636	0.666521	2.557451
C	-1.033391	0.272516	3.126605
H	-0.417947	0.052473	4.005978
H	-1.710392	-0.575100	2.971058
C	-1.869406	1.561347	3.431335
C	-2.899898	1.882294	2.346759
C	-2.546068	1.392553	4.782085
H	-3.442620	2.802885	2.585327
H	-2.410587	2.006431	1.377703
H	-3.636105	1.077369	2.261552
O	-3.724540	1.172426	4.965162
O	-1.647475	1.489395	5.794498
C	-2.183986	1.297594	7.112179
H	-1.338530	1.406870	7.792566
H	-2.949978	2.047227	7.328814
H	-2.628048	0.302869	7.208292
H	-1.150118	2.383095	3.528403

Sum of electronic and thermal Enthalpies = -844.265462 Hartree
 $\langle S^2 \rangle = 0.752832$

AT_MMA2

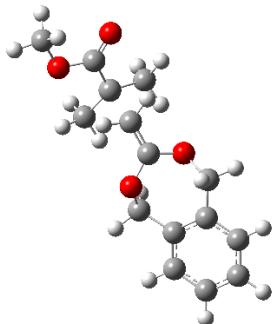


C	0.021263	0.037729	-0.010234
H	-0.572753	0.545195	0.765791
H	1.018017	-0.151952	0.388734
H	0.104263	0.753066	-0.842103
C	-0.659380	-1.214756	-0.459157
C	-0.067501	-2.534763	-0.294731
C	1.777115	-3.780554	0.481562
H	2.733850	-3.579590	0.965901
H	1.932058	-4.275743	-0.481553
H	1.157672	-4.426679	1.110481
O	-0.594726	-3.584227	-0.647286
O	1.159480	-2.501552	0.302414
C	-2.007317	-1.123729	-1.095134
H	-2.728377	-0.639456	-0.419241

H	-2.382863	-2.112851	-1.362208
H	-1.972366	-0.499641	-2.000940

Sum of electronic and thermal Enthalpies = -346.231305 Hartree
 $\langle S^2 \rangle = 0.756645$

AT_A0-MMAts

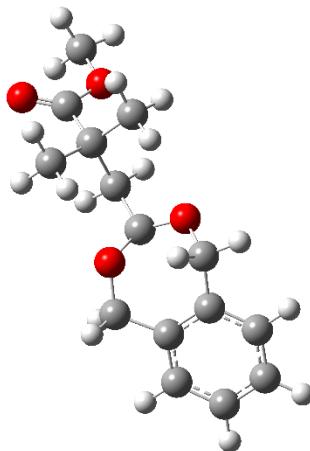


C	0.001294	-0.001613	-0.000479
C	-0.000640	-0.000847	2.377632
C	2.323671	-0.003744	1.946565
H	-0.252184	1.062204	0.092293
H	-0.673573	-0.445480	-0.736480
H	3.160949	0.539617	2.392707
O	-0.319085	-0.668568	1.237098
C	2.516227	-0.110244	0.448263
C	1.436754	-0.171838	-0.449173
C	1.694661	-0.337355	-1.814943
C	2.998360	-0.435471	-2.298935
C	4.069092	-0.371770	-1.407960
C	3.821928	-0.208043	-0.045761
H	5.090978	-0.445124	-1.769449
H	3.174690	-0.564648	-3.363100
H	0.858388	-0.391132	-2.508708
H	4.657484	-0.153644	0.649101
O	1.148718	0.728613	2.349657
H	2.287999	-1.001369	2.405518
C	-0.846669	0.028339	3.461040
H	-0.411863	0.252448	4.428370
H	-1.686621	-0.656696	3.440696
C	-2.114430	1.812041	3.509302
C	-1.119657	2.937041	3.642505
C	-2.801757	1.440237	4.753431
C	-2.877431	1.741871	2.209680
H	-0.612894	2.901546	4.609449
H	-0.370674	2.898055	2.844513
H	-1.627631	3.911753	3.571886
O	-2.412210	1.702394	5.883454
O	-3.916770	0.677626	4.533021
H	-3.598052	2.570959	2.134415
H	-2.194334	1.834340	1.357204
H	-3.439627	0.810795	2.108285
C	-4.588138	0.233952	5.716578
H	-4.931060	1.085081	6.312220
H	-5.438996	-0.355024	5.369747
H	-3.926134	-0.378723	6.335794

Sum of electronic and thermal Enthalpies = -883.524801 Hartree
 $\langle S^2 \rangle = 0.752974$

Imaginary frequency = i454 cm⁻¹

AT_A0-MMApro

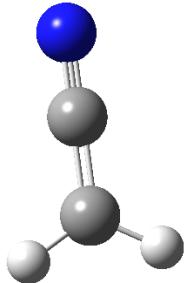


C	0.160705	0.951008	-0.359350
C	-0.064567	0.495633	1.958967
C	2.283653	0.807174	1.815273
H	0.385866	2.014953	-0.218205
H	-0.466597	0.848182	-1.247393
H	2.971177	1.660846	1.851692
O	-0.670455	0.504707	0.722462
C	2.409311	0.080497	0.486630
C	1.435323	0.149183	-0.526951
C	1.653070	-0.541013	-1.725670
C	2.816691	-1.277746	-1.940280
C	3.779380	-1.345969	-0.933567
C	3.566164	-0.677228	0.270579
H	4.687818	-1.924100	-1.079400
H	2.964282	-1.802101	-2.880265
H	0.893158	-0.497949	-2.502617
H	4.312936	-0.742655	1.059811
O	0.996085	1.369774	2.089021
H	2.563024	0.124033	2.629882
C	-0.992551	0.332731	3.120295
H	-0.375828	0.090888	3.995066
H	-1.629304	-0.535263	2.920875
C	-1.927539	1.544432	3.506609
C	-1.109261	2.800799	3.839149
C	-2.685998	1.112153	4.767701
C	-2.943677	1.844656	2.383968
H	-0.388626	2.606433	4.638578
H	-0.558879	3.139115	2.957698
H	-1.767290	3.607934	4.176476
O	-2.579207	1.614168	5.866746
O	-3.504481	0.057213	4.525956
H	-3.632426	2.639913	2.693828
H	-2.422919	2.175842	1.482246
H	-3.533758	0.960143	2.130110
C	-4.236644	-0.426221	5.661939

H	-4.884062	0.357258	6.065117
H	-4.831490	-1.262803	5.293278
H	-3.553554	-0.757595	6.448933

Sum of electronic and thermal Enthalpies = -883.548148 Hartree
 $\langle S^2 \rangle = 0.771851$

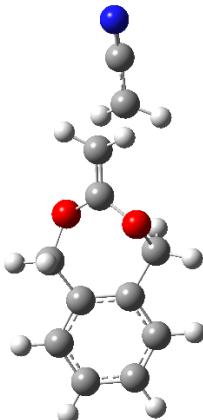
AT_MCN



C	0.002084	0.000001	0.001801
N	-0.002026	0.000003	1.178526
C	0.007298	-0.000002	-1.381047
H	-0.927079	0.005346	-1.930837
H	0.945802	-0.005348	-1.923765

Sum of electronic and thermal Enthalpies = -132.060076 Hartree
 $\langle S^2 \rangle = 0.768735$

AT_A0-MCNts



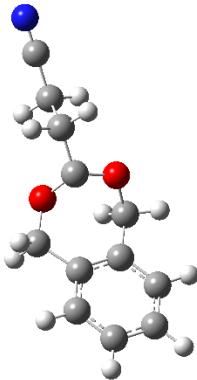
C	0.001001	0.000731	0.000644
C	0.002043	0.000583	2.365890
C	2.334058	-0.000284	1.928240
H	-0.628816	0.508603	-0.733927
H	-0.376130	-1.023935	0.117076
H	2.290711	1.044719	2.261863
O	-0.223554	0.716104	1.234416
C	2.520847	-0.075850	0.428759
C	1.440378	-0.006693	-0.466599
C	1.692867	-0.007392	-1.842960
C	2.993825	-0.082189	-2.338600
C	4.066067	-0.154224	-1.450130
C	3.823286	-0.152573	-0.077295

H	5.085179	-0.214836	-1.821312
H	3.167030	-0.080569	-3.411020
H	0.856362	0.052161	-2.536034
H	4.659244	-0.211966	0.616374
O	1.165969	-0.693104	2.423185
H	3.174499	-0.480602	2.434944
C	-0.839461	0.090636	3.439208
H	-0.632894	-0.527760	4.303042
H	-1.865006	0.389711	3.266175
C	-0.390614	2.008929	4.554103
C	-1.346466	2.048739	5.584624
N	-2.166814	2.023096	6.420491
H	0.635629	1.801216	4.840126
H	-0.524681	2.692825	3.722364

Sum of electronic and thermal Enthalpies = -669.360524 Hartree
 $\langle S^2 \rangle = 0.774622$

Imaginary frequency = i399 cm⁻¹

AT_A0-MCNpro

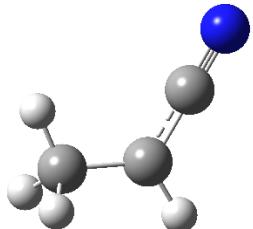


C	0.139385	0.898832	0.026018
C	0.383058	0.253583	2.306268
C	2.609702	0.908453	1.796720
H	-0.026448	1.843552	-0.505302
H	-0.682962	0.221045	-0.241999
H	2.376160	1.978745	1.744460
O	0.031693	1.244971	1.412280
C	2.611244	0.287459	0.415472
C	1.459937	0.276551	-0.393765
C	1.521401	-0.316579	-1.659819
C	2.704753	-0.875226	-2.139881
C	3.847763	-0.862779	-1.341101
C	3.789339	-0.292052	-0.070738
H	4.774096	-1.303816	-1.698164
H	2.729439	-1.326053	-3.128155
H	0.627248	-0.339472	-2.279945
H	4.674338	-0.294620	0.561350
O	1.697536	0.282653	2.713604
H	3.590035	0.793001	2.263346
C	-0.572857	0.049653	3.440536
H	-0.239120	-0.803161	4.039485
H	-1.562693	-0.187991	3.039112
C	-0.674746	1.309544	4.351310

C	-1.612543	1.125212	5.459074
N	-2.363786	0.950942	6.327519
H	0.316331	1.544230	4.755729
H	-0.995627	2.168661	3.751362

Sum of electronic and thermal Enthalpies = -669.393175 Hartree
 $\langle S^2 \rangle = 0.752688$

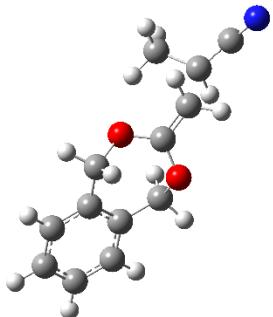
AT_AN



C	0.004981	-0.043635	-0.015781
H	-0.246804	0.218448	1.021432
H	1.091796	-0.115535	-0.100575
H	-0.338664	0.791409	-0.642297
C	0.020837	-2.442840	-0.842730
N	0.611828	-3.394482	-1.202911
C	-0.669980	-1.317467	-0.417198
H	-1.754415	-1.381041	-0.379373

Sum of electronic and thermal Enthalpies = -171.35237 Hartree
 $\langle S^2 \rangle = 0.766961$

AT_A0-ANts7



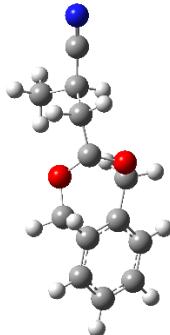
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.365328
C	2.333669	0.000000	1.927804
H	-0.625527	0.510642	-0.736551
H	-0.385987	-1.020988	0.120259
H	2.290035	1.047935	2.252447
O	-0.217267	0.720566	1.232055
C	2.519884	-0.087821	0.428579
C	1.439418	-0.020619	-0.467251
C	1.691332	-0.034197	-1.843650
C	2.991555	-0.120534	-2.339304
C	4.063706	-0.190919	-1.450632
C	3.821505	-0.176241	-0.077719
H	5.082328	-0.260660	-1.821640

H	3.164329	-0.129202	-3.411784
H	0.854758	0.024094	-2.536790
H	4.657411	-0.234866	0.616088
O	1.167480	-0.690410	2.427340
H	3.175697	-0.474902	2.437249
C	-0.847660	0.083509	3.439683
H	-0.655900	-0.572185	4.279863
H	-1.877130	0.364216	3.253257
C	-0.438461	1.920374	4.621282
C	-0.795171	3.067276	3.705091
C	-1.232611	1.696362	5.770648
H	-1.873370	3.104929	3.518529
H	-0.501778	4.033531	4.140259
H	-0.285911	2.960946	2.742467
N	-1.920273	1.456539	6.687076
H	0.622849	1.732587	4.770961

Sum of electronic and thermal Enthalpies = -708.64861 Hartree
 $\langle S^2 \rangle = 0.775476$

Imaginary frequency = i447 cm⁻¹

AT_A0-ANpro

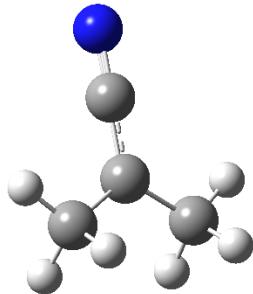


C	-0.069044	0.027150	-0.019701
C	-0.118991	-0.106555	2.336917
C	2.234392	0.214439	1.964524
H	-0.669180	0.569820	-0.755979
H	-0.457044	-0.999084	0.043165
H	2.066920	1.273880	2.199453
O	-0.323617	0.681721	1.234346
C	2.447502	0.035299	0.475724
C	1.385235	0.017419	-0.444651
C	1.667894	-0.073328	-1.812624
C	2.979545	-0.153901	-2.277184
C	4.034334	-0.141163	-1.365209
C	3.761301	-0.048812	-0.001497
H	5.062201	-0.206107	-1.710884
H	3.174631	-0.223377	-3.343723
H	0.845030	-0.080468	-2.524700
H	4.583303	-0.041080	0.711070
O	1.161647	-0.569027	2.525519
H	3.126388	-0.112210	2.504934
C	-0.888583	0.257332	3.568542
H	-0.850940	-0.599946	4.249421
H	-1.937257	0.421898	3.300385

C	-0.352992	1.512422	4.339087
C	-0.567724	2.834416	3.576023
C	-0.983932	1.579934	5.665294
H	-1.636074	3.024504	3.430038
H	-0.142974	3.677959	4.128817
H	-0.096704	2.779770	2.591588
N	-1.503406	1.624388	6.703387
H	0.721584	1.359215	4.506217

Sum of electronic and thermal Enthalpies = -708.677155 Hartree
 $\langle S^2 \rangle = 0.752903$

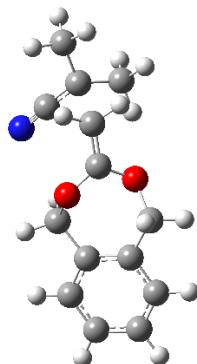
AT_AZO



C	-0.132298	0.264985	0.056916
C	-0.034684	0.069480	1.542490
H	0.923811	0.410300	1.940651
H	-0.837903	0.615305	2.058621
H	-0.160115	-0.991694	1.802602
C	0.929324	0.824952	-0.647601
C	-1.383578	-0.148088	-0.663050
H	-1.325032	0.047831	-1.736174
H	-1.578444	-1.220543	-0.516938
H	-2.256427	0.386319	-0.260541
N	1.826899	1.298354	-1.243243

Sum of electronic and thermal Enthalpies = -210.644595 Hartree
 $\langle S^2 \rangle = 0.765669$

AT_A0-AZOts1



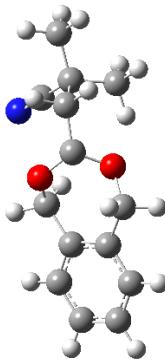
C	0.002191	0.000152	-0.000441
C	0.002090	0.003332	2.381715
C	2.329791	0.003554	1.951608
H	-0.410754	1.011353	0.082892

H	-0.606463	-0.541905	-0.727896
H	3.173259	0.471089	2.465713
O	-0.228877	-0.698367	1.249306
C	2.523096	0.092311	0.453865
C	1.447472	0.024572	-0.447700
C	1.710970	0.045260	-1.822501
C	3.014070	0.136756	-2.308914
C	4.080920	0.205082	-1.413452
C	3.828479	0.185075	-0.042818
H	5.101937	0.278631	-1.777348
H	3.193479	0.151588	-3.380357
H	0.878906	-0.009934	-2.521057
H	4.659075	0.243784	0.657574
O	1.166662	0.700881	2.446522
H	2.273122	-1.043256	2.277789
C	-2.067875	2.005061	3.301493
C	-0.944539	0.122465	3.374452
H	-1.816700	-0.514646	3.287008
H	-0.593386	0.347349	4.375558
C	-1.040648	3.014791	3.775732
H	-0.167552	3.039343	3.117733
H	-1.467998	4.027651	3.815747
H	-0.700529	2.761133	4.786507
C	-2.418975	2.097279	1.925447
C	-3.206691	1.703239	4.254631
H	-3.879714	0.937340	3.856952
H	-2.815045	1.353904	5.217662
H	-3.807159	2.603495	4.453481
N	-2.656041	2.129918	0.780586

Sum of electronic and thermal Enthalpies = -747.938803 Hartree
 $\langle S^2 \rangle = 0.772576$

Imaginary frequency = i455 cm⁻¹

AT_A0-AZOprom

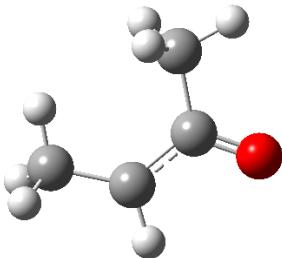


C	-0.010358	0.293113	0.020361
C	-0.030053	-0.041851	2.399983
C	2.291860	0.105762	2.008816
H	-0.267508	1.337551	0.227546
H	-0.669213	-0.052625	-0.779229
H	3.109447	0.626928	2.515654
O	-0.368164	-0.516763	1.162197
C	2.501692	0.155001	0.508972
C	1.436468	0.171225	-0.408606

C	1.722534	0.143775	-1.779150
C	3.034951	0.107890	-2.247672
C	4.090015	0.095630	-1.336060
C	3.816847	0.121062	0.030538
H	5.118942	0.070067	-1.684264
H	3.230260	0.086919	-3.316267
H	0.898585	0.152253	-2.489305
H	4.640032	0.115262	0.742455
O	1.090079	0.745980	2.470544
H	2.283402	-0.935056	2.361940
C	-1.906373	1.625000	3.262762
C	-1.128327	0.257921	3.368937
H	-1.861973	-0.551379	3.284409
H	-0.715194	0.224785	4.384513
C	-0.971251	2.827836	3.521213
H	-0.146948	2.855466	2.806169
H	-1.527327	3.769014	3.459951
H	-0.544996	2.743449	4.527113
C	-2.504496	1.763152	1.921528
C	-3.052060	1.615321	4.302270
H	-3.745287	0.787266	4.123388
H	-2.631178	1.503517	5.307793
H	-3.619037	2.551101	4.269046
N	-2.983827	1.896608	0.871520

Sum of electronic and thermal Enthalpies = -747.962768 Hartree
 $\langle S^2 \rangle = 0.753036$

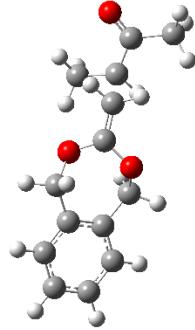
AT_MVC



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.440947
C	1.319280	0.000000	2.203852
H	1.923185	-0.883161	1.961615
H	1.923071	0.883292	1.961889
H	1.102518	-0.000197	3.273645
O	-1.080594	0.000036	2.052833
H	-0.989060	-0.000056	-0.453350
C	1.188959	0.000049	-0.897232
H	2.135860	0.000421	-0.351214
H	1.178385	-0.877797	-1.560662
H	1.177948	0.877572	-1.561087

Sum of electronic and thermal Enthalpies = -231.713993 Hartree
 $\langle S^2 \rangle = 0.765243$

AT_A0-MVCts

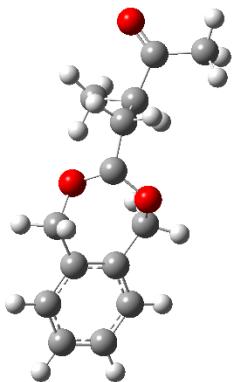


C	-0.003222	-0.004345	-0.000352
C	-0.005308	-0.002317	2.364283
C	2.328357	0.005833	1.929861
H	-0.628258	0.505170	-0.738133
H	-0.387776	-1.026121	0.118961
H	2.278395	1.053375	2.254383
O	-0.223288	0.715572	1.230297
C	2.517092	-0.083065	0.430924
C	1.437040	-0.023337	-0.465911
C	1.690284	-0.042209	-1.842049
C	2.991138	-0.126009	-2.336418
C	4.062985	-0.187885	-1.446712
C	3.819482	-0.168042	-0.074078
H	5.082213	-0.254879	-1.816665
H	3.164723	-0.138852	-3.408754
H	0.854032	0.010255	-2.536046
H	4.654938	-0.220058	0.620843
O	1.164491	-0.690675	2.426598
H	3.172144	-0.464722	2.440662
C	-0.849182	0.086535	3.443980
H	-0.647192	-0.585108	4.269722
H	-1.882960	0.357099	3.265272
C	-0.474300	1.941044	4.568215
C	-1.334677	1.664909	5.714849
H	0.592255	1.778888	4.719582
C	-0.731267	0.898676	6.888479
O	-2.518641	2.015014	5.742222
H	0.056322	0.202983	6.577669
H	-0.280356	1.608096	7.595150
H	-1.519340	0.355517	7.416518
C	-0.869753	3.029176	3.611562
H	-0.412547	2.896048	2.626309
H	-1.957777	3.055764	3.503881
H	-0.557327	4.012622	3.994252

Sum of electronic and thermal Enthalpies = -769.012482 Hartree
 $\langle S^2 \rangle = 0.773633$

Imaginary frequency = i444 cm⁻¹

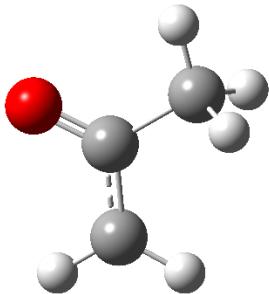
AT_A0-MVCpro



C	-0.083578	-0.050819	-0.040273
C	-0.205501	-0.129886	2.314404
C	2.155510	0.177933	2.002258
H	-0.684437	0.448274	-0.806217
H	-0.434257	-1.089241	0.041222
H	1.976202	1.231859	2.251191
O	-0.391145	0.628015	1.186976
C	2.416710	0.025076	0.518247
C	1.380152	-0.015359	-0.430587
C	1.702112	-0.084692	-1.791035
C	3.027695	-0.121652	-2.220744
C	4.056808	-0.085268	-1.280450
C	3.744598	-0.014296	0.076233
H	5.095108	-0.115380	-1.598931
H	3.253320	-0.175176	-3.282233
H	0.899004	-0.108982	-2.524964
H	4.546624	0.011010	0.810977
O	1.065210	-0.619978	2.508061
H	3.031353	-0.155734	2.565231
C	-0.965970	0.294500	3.532486
H	-0.949616	-0.554030	4.228014
H	-2.011070	0.472989	3.258350
C	-0.418141	1.566568	4.272437
C	-1.111854	1.631116	5.636278
H	0.654969	1.403265	4.441354
C	-0.425054	0.922350	6.791964
O	-2.176150	2.204302	5.782128
H	-0.085835	-0.080153	6.504984
H	0.470647	1.487578	7.082880
H	-1.099958	0.859040	7.648110
C	-0.645920	2.853903	3.473438
H	-0.228289	2.772855	2.466648
H	-1.717532	3.056720	3.390007
H	-0.184511	3.711918	3.975703

Sum of electronic and thermal Enthalpies = -769.038605 Hartree
 $\langle S^2 \rangle = 0.753055$

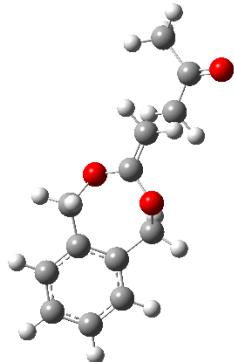
AT__ACE



C	0.018270	0.000012	0.014055
C	-0.011592	0.000232	1.453279
C	1.312186	0.000010	2.205337
H	1.909438	-0.882604	1.945289
H	1.909432	0.882754	1.945719
H	1.118443	-0.000244	3.279636
O	-1.094614	-0.000054	2.055789
H	-0.922207	-0.000120	-0.526703
H	0.948105	-0.000017	-0.547620

Sum of electronic and thermal Enthalpies = -192.420996 Hartree
 $\langle S^2 \rangle = 0.766434$

AT_A0-ACEts1



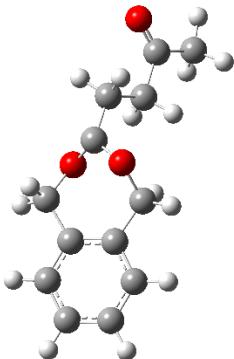
C	0.002249	0.001887	-0.000710
C	0.003711	0.003945	2.364355
C	2.333738	0.002291	1.926610
H	-0.629771	0.505396	-0.736605
H	-0.369266	-1.024869	0.116178
H	2.288371	1.045177	2.265796
O	-0.225971	0.717657	1.231294
C	2.522373	-0.065922	0.426942
C	1.441732	0.001674	-0.468482
C	1.694425	0.007133	-1.844787
C	2.995712	-0.060629	-2.340624
C	4.068036	-0.131352	-1.452162
C	3.825080	-0.135593	-0.079309
H	5.087496	-0.186648	-1.823357
H	3.169165	-0.054651	-3.413032
H	0.857691	0.065735	-2.537732
H	4.661018	-0.194296	0.614444
O	1.164862	-0.694243	2.413781
H	3.173689	-0.479770	2.432565

C	-0.828253	0.100755	3.443243
H	-0.626816	-0.514116	4.310737
H	-1.848631	0.418585	3.269710
C	-0.258202	1.952583	4.608930
C	-1.213974	1.899019	5.697546
H	0.751924	1.623304	4.828882
C	-2.511593	2.688163	5.538950
O	-1.007848	1.221207	6.710004
H	-2.324285	3.758351	5.697197
H	-2.935121	2.581721	4.532804
H	-3.237148	2.349124	6.281773
H	-0.378350	2.680083	3.811162

Sum of electronic and thermal Enthalpies = -729.722394 Hartree
 $\langle S^2 \rangle = 0.772783$

Imaginary frequency = i380 cm⁻¹

AT_A0-ACEpro

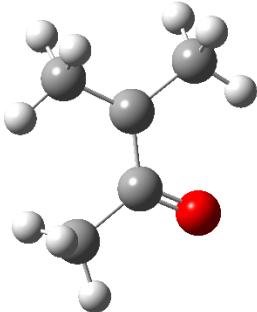


C	0.079545	-0.770229	0.187473
C	0.111193	-0.498352	2.532138
C	2.172248	0.576147	1.927333
H	-0.696101	-0.644868	-0.574200
H	0.129217	-1.837506	0.445629
H	1.622583	1.520933	2.030720
O	-0.388603	-0.047389	1.334191
C	2.406752	0.267944	0.462824
C	1.413174	-0.296891	-0.355742
C	1.676786	-0.486698	-1.717259
C	2.905571	-0.134187	-2.273309
C	3.893515	0.422266	-1.461649
C	3.638026	0.616619	-0.105056
H	4.857420	0.700029	-1.879071
H	3.087390	-0.290787	-3.333052
H	0.904468	-0.917600	-2.351463
H	4.409134	1.047562	0.530146
O	1.483050	-0.456656	2.658098
H	3.133341	0.688505	2.436732
C	-0.703934	-0.115254	3.730229
H	-0.298345	-0.632656	4.605398
H	-1.728003	-0.476274	3.595731
C	-0.741503	1.400806	4.009509
C	-1.613602	1.774217	5.203808
H	0.271185	1.790945	4.185950

C	-1.629161	3.243287	5.597121
O	-2.261812	0.944304	5.812642
H	-0.632355	3.553703	5.935883
H	-1.885520	3.875956	4.738601
H	-2.349294	3.403285	6.402205
H	-1.118413	1.941403	3.129383

Sum of electronic and thermal Enthalpies = -729.755037 Hartree
 $\langle S^2 \rangle = 0.752686$

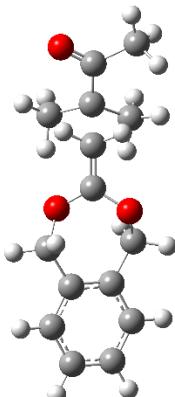
AT_PK



C	0.016790	0.349686	0.071337
C	0.017852	0.034237	1.487751
C	1.339631	-0.141489	2.228684
O	-1.051163	-0.094876	2.106345
H	1.938052	-0.956893	1.804277
H	1.952193	0.767477	2.188111
H	1.118067	-0.371991	3.272312
C	-1.292265	0.516710	-0.630844
H	-1.385780	-0.198243	-1.461987
H	-2.121973	0.369091	0.061909
H	-1.371905	1.518200	-1.079600
C	1.265519	0.519548	-0.736620
H	1.298755	1.520406	-1.193282
H	2.181963	0.383103	-0.159040
H	1.284511	-0.192737	-1.575446

Sum of electronic and thermal Enthalpies = -271.008062 Hartree
 $\langle S^2 \rangle = 0.762843$

AT_A0-PKts

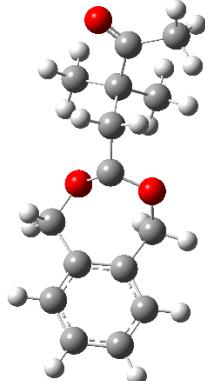


C	0.000131	-0.002123	-0.000132
C	0.000268	-0.001584	2.363667
C	2.339376	-0.001639	1.927605
H	-0.585254	0.548751	-0.741081
H	-0.455389	-0.994965	0.117425
H	2.293669	1.064893	2.182107
O	-0.175426	0.730342	1.230107
C	2.516353	-0.187265	0.436120
C	1.437334	-0.123470	-0.461666
C	1.683601	-0.233117	-1.834907
C	2.976389	-0.410827	-2.325419
C	4.047446	-0.477160	-1.435052
C	3.810607	-0.367326	-0.065649
H	5.060345	-0.617334	-1.801875
H	3.144476	-0.493087	-3.395581
H	0.848318	-0.177080	-2.529944
H	4.645094	-0.422563	0.630122
O	1.182340	-0.663413	2.478463
H	3.187223	-0.439468	2.460110
C	-0.916938	0.022888	3.392002
H	-0.740612	-0.684999	4.194623
H	-1.950947	0.226401	3.137961
C	-0.776063	1.807195	4.608880
C	-1.838945	1.420747	5.554123
C	-1.461245	0.682151	6.835096
O	-3.028070	1.639715	5.305348
H	-0.897783	-0.236554	6.627037
H	-0.828752	1.302607	7.482199
H	-2.377229	0.424958	7.370652
C	-1.142139	2.893348	3.625975
H	-0.510875	2.856845	2.732306
H	-2.190647	2.810702	3.332377
H	-1.007041	3.884096	4.087179
C	0.661455	1.813487	5.076256
H	0.853207	2.662862	5.750734
H	0.943183	0.900600	5.610192
H	1.343777	1.927720	4.226179

Sum of electronic and thermal Enthalpies = -808.299195 Hartree
 $\langle S^2 \rangle = 0.773277$

Imaginary frequency = i499 cm⁻¹

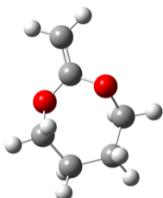
AT_A0-PKpro



C	0.331771	1.032242	0.039579
C	0.370097	0.383904	2.323896
C	2.700008	0.576696	1.897279
H	0.335443	1.979918	-0.511994
H	-0.588882	0.496316	-0.230345
H	2.685748	1.672591	1.854282
O	0.267157	1.418401	1.417311
C	2.638024	-0.017942	0.504808
C	1.536080	0.189905	-0.345405
C	1.539518	-0.387638	-1.620417
C	2.620260	-1.144638	-2.069235
C	3.715123	-1.349216	-1.229974
C	3.710654	-0.793935	0.048418
H	4.560566	-1.944962	-1.562509
H	2.601803	-1.578936	-3.065099
H	0.680794	-0.239860	-2.272783
H	4.555990	-0.964018	0.711333
O	1.650554	0.131726	2.768072
H	3.620443	0.266077	2.396290
C	-0.679914	0.257959	3.382379
H	-0.407455	-0.625119	3.972609
H	-1.642880	0.040734	2.905468
C	-0.905223	1.488437	4.353436
C	-1.805085	0.926443	5.476579
C	-1.150423	0.226772	6.660873
O	-3.018868	1.003969	5.406301
H	-0.381769	-0.487851	6.346408
H	-0.654418	0.962995	7.305300
H	-1.920926	-0.287631	7.238658
C	-1.656365	2.615190	3.624274
H	-1.081169	2.961776	2.762734
H	-2.635825	2.271245	3.283299
H	-1.822743	3.463466	4.298778
C	0.432325	2.016132	4.905194
H	0.260550	2.793235	5.660025
H	1.045592	1.228746	5.352931
H	1.018080	2.465362	4.097678

Sum of electronic and thermal Enthalpies = -808.320134 Hartree
 $\langle S^2 \rangle = 0.753089$

AT_AC77_1

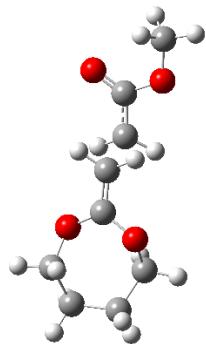


C	-0.000269	0.000011	0.006461
C	-0.000131	-0.000153	1.341513
H	0.935148	-0.011626	-0.537421
H	-0.935791	0.011804	-0.537239
O	1.152673	0.143135	2.057038
O	-1.152812	-0.143591	2.057218
C	1.322325	-0.710633	3.206096
C	-1.321928	0.709269	3.207008

C	0.764377	-0.063608	4.472079
H	0.863624	-1.688971	3.016322
H	2.403894	-0.848763	3.293828
C	-0.763621	0.061216	4.472315
H	-0.863204	1.687717	3.017858
H	-2.403452	0.847429	3.295245
H	1.223308	0.928928	4.571499
H	1.089531	-0.652476	5.340189
H	-1.222527	-0.931400	4.571060
H	-1.088560	0.649388	5.340977

Sum of electronic and thermal Enthalpies = -384.911174 Hartree

AT_A7-MEST_ts

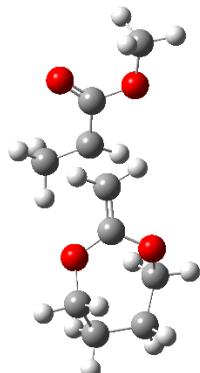


C	-0.000389	0.002929	0.003675
O	0.003039	-0.000175	1.360112
O	1.194983	0.002395	-0.637729
C	0.996649	0.802963	2.037997
C	2.221220	-0.884469	-0.139080
C	2.303017	0.040730	2.243786
H	1.157439	1.734746	1.482347
H	0.537984	1.046556	2.999808
C	3.068926	-0.221394	0.942510
H	1.760234	-1.812472	0.220795
H	2.830895	-1.117996	-1.015857
H	2.066744	-0.908354	2.742544
H	2.933095	0.614812	2.935763
H	3.459340	0.721466	0.537519
H	3.936592	-0.863144	1.144512
C	-1.163879	0.117791	-0.698828
H	-2.098438	0.102615	-0.153505
H	-1.171817	-0.157924	-1.745238
C	-1.450670	2.330729	-1.274773
C	-2.642616	2.210489	-2.085744
H	-1.532437	2.742708	-0.276016
O	-2.673515	1.966327	-3.284903
O	-3.783157	2.336454	-1.333412
C	-5.002485	2.180961	-2.063498
H	-5.803353	2.297746	-1.331062
H	-5.056151	1.193644	-2.532737
H	-5.090377	2.940622	-2.846445
H	-0.512352	2.443135	-1.802405

Sum of electronic and thermal Enthalpies = -652.550428 Hartree
 $\langle S^2 \rangle = 0.768485$

Imaginary frequency = i336 cm⁻¹

AT_A7-MA_1ts

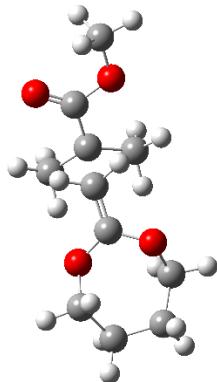


C	0.000198	-0.000281	-0.000186
O	0.000109	0.000677	1.357528
O	1.200688	-0.000391	-0.637934
C	0.969994	0.831086	2.036052
C	2.234704	-0.863469	-0.115768
C	2.290528	0.098177	2.255762
H	1.114155	1.762874	1.475342
H	0.500658	1.072104	2.993525
C	3.065087	-0.168943	0.960145
H	1.783859	-1.791382	0.257249
H	2.855033	-1.103981	-0.983233
H	2.071329	-0.848394	2.767002
H	2.908196	0.693562	2.940977
H	3.439062	0.774996	0.542248
H	3.944088	-0.790986	1.174621
C	-1.166817	0.130249	-0.707164
H	-2.095288	0.060717	-0.154554
H	-1.171356	-0.174565	-1.746734
C	-1.534869	2.274731	-1.215808
C	-0.391291	2.673605	-2.100197
C	-2.849797	2.113408	-1.818672
H	-1.534261	2.625169	-0.187641
H	-0.492680	2.211268	-3.086325
H	-0.368811	3.763805	-2.252577
H	0.570953	2.379900	-1.668593
O	-3.082024	1.978676	-3.013012
O	-3.838722	2.057482	-0.870049
C	-5.156291	1.848718	-1.385633
H	-5.813508	1.818012	-0.514651
H	-5.216488	0.908213	-1.941891
H	-5.449145	2.664931	-2.053260

Sum of electronic and thermal Enthalpies = -691.841004 Hartree
 $\langle S^2 \rangle = 0.770661$

Imaginary frequency = i417.6355 cm⁻¹

AT_A7-MMA_ts

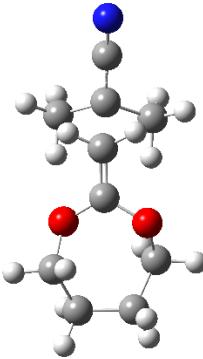


C	-0.001073	-0.000938	0.001344
O	0.001469	-0.004152	1.360553
O	1.197529	-0.002374	-0.640928
C	1.046629	0.712925	2.051330
C	2.188279	-0.955106	-0.193709
C	2.306312	-0.132298	2.225468
H	1.262515	1.651434	1.525958
H	0.610552	0.953815	3.024440
C	3.063699	-0.382087	0.916560
H	1.688917	-1.880147	0.120881
H	2.786978	-1.170265	-1.082977
H	2.013639	-1.086364	2.683207
H	2.965727	0.374611	2.942274
H	3.503173	0.555759	0.552214
H	3.896860	-1.074791	1.094593
C	-1.176721	0.119796	-0.703994
H	-2.095300	0.020421	-0.137331
H	-1.183741	-0.234727	-1.728226
C	-1.599176	2.185866	-1.302686
C	-0.465600	2.508208	-2.243016
C	-2.875063	1.867601	-1.954122
H	-0.533228	1.914407	-3.157352
H	-0.494734	3.569681	-2.536228
H	0.504044	2.324621	-1.768307
O	-3.009993	1.522754	-3.120904
O	-3.936315	1.912660	-1.088810
C	-5.194799	1.541660	-1.659210
H	-5.921498	1.622526	-0.848799
H	-5.163963	0.517803	-2.043834
H	-5.464098	2.212384	-2.480572
C	-1.617337	2.935610	0.006370
H	-2.349454	2.528586	0.707503
H	-0.627832	2.908098	0.477730
H	-1.868084	3.995911	-0.152872

Sum of electronic and thermal Enthalpies = -731.128976 Hartree
 $\langle S^2 \rangle = 0.771127$

Imaginary frequency = 1446 cm⁻¹

AT_A7-PCN_ts

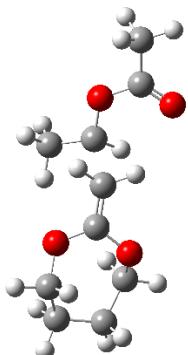


C	0.000032	0.004814	-0.003275
O	-0.004885	0.007855	1.355219
O	1.201307	0.004523	-0.640396
C	1.052221	0.701624	2.051801
C	2.181878	-0.965014	-0.201941
C	2.297486	-0.164752	2.224274
H	1.285406	1.639768	1.532589
H	0.618009	0.943597	3.025327
C	3.059177	-0.414401	0.917763
H	1.670363	-1.887488	0.099929
H	2.780377	-1.176197	-1.092198
H	1.987710	-1.117890	2.672451
H	2.960093	0.326101	2.949127
H	3.515078	0.519898	0.564351
H	3.880761	-1.120913	1.094651
C	-1.172599	0.118490	-0.714656
H	-2.097332	0.016436	-0.159338
H	-1.172008	-0.244064	-1.735652
C	-0.460905	2.513850	-2.273403
H	-0.495008	1.887134	-3.169780
H	-0.505481	3.564119	-2.599025
H	0.504349	2.354713	-1.781540
C	-1.607084	2.951941	-0.012035
H	-2.384836	2.586007	0.665241
H	-0.637860	2.855142	0.490016
H	-1.785930	4.024752	-0.178543
C	-1.594644	2.191289	-1.321213
C	-2.866631	1.978713	-1.922019
N	-3.905808	1.734319	-2.400436

Sum of electronic and thermal Enthalpies = -595.541043 Hartree
 $\langle S^2 \rangle = 0.774378$

Imaginary frequency = i451 cm⁻¹

AT_A7-VAC_1ts

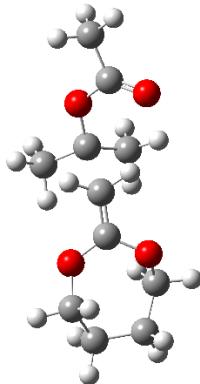


C	-0.000811	0.000043	-0.006368
O	-0.005771	0.002637	1.355980
O	1.214318	0.003064	-0.630953
C	0.946484	0.852412	2.028001
C	2.233050	-0.862117	-0.091080
C	2.270609	0.131102	2.270459
H	1.090412	1.777911	1.455952
H	0.470135	1.106004	2.979264
C	3.056534	-0.159022	0.986116
H	1.774837	-1.784152	0.288341
H	2.865132	-1.117795	-0.946539
H	2.050204	-0.807011	2.796699
H	2.881908	0.740206	2.949702
H	3.438310	0.777699	0.558698
H	3.931236	-0.780949	1.218934
C	-1.153946	0.111296	-0.722287
H	-2.093606	0.088289	-0.185560
H	-1.147886	-0.186843	-1.763635
C	-1.596399	2.279384	-1.358740
C	-0.434135	2.735767	-2.175803
O	-2.766146	2.187179	-2.123073
H	-1.764653	2.698800	-0.371517
H	-0.337168	2.137386	-3.089294
H	-0.522312	3.791670	-2.480385
H	0.490079	2.622400	-1.600741
C	-3.958012	2.080447	-1.475583
C	-5.091771	1.979595	-2.468559
O	-4.072291	2.077108	-0.268765
H	-6.031372	1.844296	-1.931671
H	-5.143497	2.888664	-3.077814
H	-4.927081	1.139480	-3.151111

Sum of electronic and thermal Enthalpies = -691.837445 Hartree
 $\langle S^2 \rangle = 0.773457$

Imaginary frequency = 1385 cm⁻¹

AT_A7-MVAC_ts

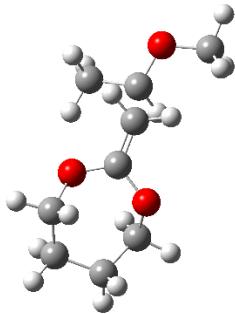


C	0.003929	-0.005007	0.000406
O	0.005102	-0.009862	1.363897
O	1.216839	-0.005043	-0.629280
C	1.004760	0.774439	2.043218
C	2.210878	-0.925566	-0.135002
C	2.295688	-0.013794	2.256823
H	1.190070	1.705280	1.491883
H	0.550672	1.028202	3.005336
C	3.066242	-0.294736	0.961425
H	1.722885	-1.845205	0.211817
H	2.826746	-1.168966	-1.005815
H	2.034424	-0.957606	2.753285
H	2.934794	0.545134	2.953394
H	3.486464	0.638969	0.564536
H	3.914293	-0.960563	1.170235
C	-1.156204	0.107635	-0.709457
H	-2.094050	0.065264	-0.171945
H	-1.148811	-0.207737	-1.746317
C	-1.603182	2.247363	-1.365260
C	-0.449230	2.575516	-2.268302
O	-2.771579	2.155900	-2.169444
H	-0.430433	1.912055	-3.139284
H	-0.505480	3.612563	-2.639644
H	0.495901	2.456562	-1.730282
C	-3.962419	1.723585	-1.688104
C	-5.017005	1.806930	-2.770170
O	-4.162666	1.332872	-0.557338
H	-5.934655	1.334720	-2.417197
H	-5.218547	2.855607	-3.016400
H	-4.668146	1.318538	-3.685204
C	-1.743595	3.047931	-0.100647
H	-2.522303	2.649201	0.551511
H	-0.791200	3.036839	0.440284
H	-1.985112	4.101523	-0.322763

Sum of electronic and thermal Enthalpies = -731.126045 Hartree
 $\langle S^2 \rangle = 0.774395$

Imaginary frequency = i391 cm⁻¹

AT_A7-VE_1ts



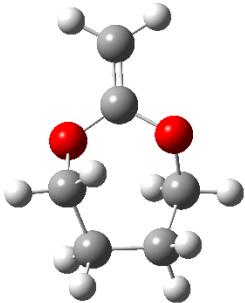
C	-0.006109	-0.002237	-0.008507
O	-0.010670	0.002380	1.359090
O	1.212924	0.001025	-0.631236
C	0.965125	0.826740	2.025632
C	2.214056	-0.894608	-0.112895
C	2.273633	0.072925	2.259718
H	1.129399	1.750496	1.455898
H	0.503748	1.089203	2.982521
C	3.053623	-0.224994	0.973467
H	1.738536	-1.813815	0.252544
H	2.840343	-1.149132	-0.973350
H	2.031319	-0.863877	2.778792
H	2.899859	0.661814	2.943441
H	3.458961	0.706678	0.556784
H	3.912589	-0.870329	1.201697
C	-1.157633	0.141450	-0.727348
H	-2.093590	0.094403	-0.184696
H	-1.163867	-0.174412	-1.763419
C	-1.514445	2.301373	-1.420839
C	-0.441881	2.522607	-2.440766
O	-2.779116	2.392168	-1.967202
H	-1.407732	2.820029	-0.461952
H	-0.428500	3.559576	-2.813982
H	0.538161	2.294334	-2.011386
H	-0.594676	1.867038	-3.306663
C	-3.833864	2.466927	-1.026992
H	-3.894902	1.559509	-0.410870
H	-4.761252	2.577514	-1.594454
H	-3.712722	3.334433	-0.360236

Sum of electronic and thermal Enthalpies = -578.486358 Hartree
 $\langle S^2 \rangle = 0.775871$

Imaginary frequency = i396 cm⁻¹

UBMK/6-31G(d)

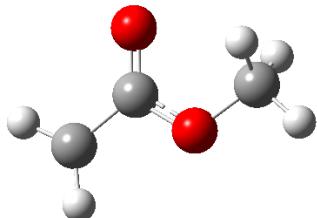
AT_AC77_1_K



C	-0.000013	0.000063	0.009583
C	0.000016	-0.000021	1.347309
H	0.939507	0.014700	-0.530702
H	-0.939552	-0.014498	-0.530670
O	1.136556	0.162740	2.061033
O	-1.136501	-0.162883	2.061048
C	1.324561	-0.688754	3.189003
C	-1.324282	0.688097	3.189435
C	0.768405	-0.049684	4.470039
H	0.863412	-1.669132	3.001032
H	2.409058	-0.823438	3.270638
C	-0.768021	0.048400	4.470117
H	-0.863081	1.668528	3.001869
H	-2.408758	0.822822	3.271270
H	1.210569	0.953100	4.561582
H	1.106518	-0.637258	5.335780
H	-1.210183	-0.954426	4.561207
H	-1.106068	0.635556	5.336166

Sum of electronic and thermal Enthalpies = -384.681769 Hartree

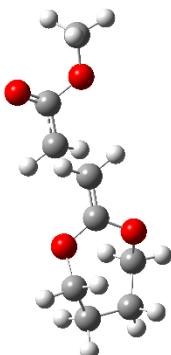
AT_MEST_K



C	-0.000426	-0.000022	0.002961
H	0.002740	0.000212	1.088501
C	1.250286	-0.000726	-0.752838
C	3.581505	-0.002433	-0.612590
H	4.338122	-0.002480	0.175713
H	3.684100	0.887470	-1.244466
H	3.683089	-0.893099	-1.243562
O	1.320824	-0.001357	-1.965015
O	2.326657	-0.001389	0.052111
H	-0.932152	0.000221	-0.552580

Sum of electronic and thermal Enthalpies = -267.4953 Hartree
 $\langle S^2 \rangle = 0.758157$

AT_A7-MEST_ts_K

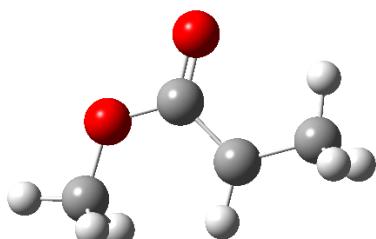


C	0.894455	0.104396	-0.566014
O	1.535911	-1.086531	-0.666853
O	1.570725	1.150211	-0.028200
C	2.400541	-1.485850	0.421622
C	2.938814	1.349495	-0.448864
C	3.818688	-0.947681	0.250807
H	1.961518	-1.168215	1.375135
H	2.396690	-2.578260	0.383965
C	3.920388	0.571769	0.422781
H	3.039047	1.082179	-1.507969
H	3.102794	2.425391	-0.346230
H	4.174980	-1.241301	-0.745280
H	4.468679	-1.447848	0.980701
H	3.736300	0.846579	1.469689
H	4.937980	0.906053	0.181423
C	-0.425427	0.224555	-0.888327
H	-0.928349	-0.627713	-1.326183
H	-0.832278	1.211553	-1.065427
C	-1.665335	0.055437	1.046894
C	-2.981430	0.319054	0.507202
H	-1.399484	-0.960274	1.314441
O	-3.489336	1.423170	0.360534
O	-3.602354	-0.833996	0.097770
C	-4.891118	-0.643630	-0.491138
H	-5.240555	-1.640031	-0.767853
H	-4.827823	-0.002585	-1.375963
H	-5.583223	-0.182671	0.220425
H	-1.183302	0.869046	1.573349

Sum of electronic and thermal Enthalpies = -652.170619 Hartree
 $\langle S^2 \rangle = 0.773905$

Imaginary frequency = i437 cm⁻¹

AT_MA_K

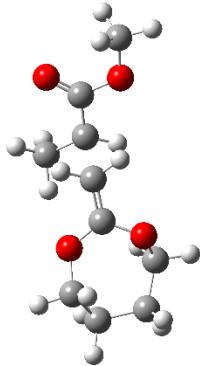


C	0.000659	0.000996	0.000355
H	-0.009457	-0.014826	1.093918
H	1.043536	-0.000911	-0.353997

H	-0.448713	0.942050	-0.354122
C	-0.743805	-1.177182	-0.539518
H	-0.822288	-1.301938	-1.616163
C	-1.354310	-2.142590	0.382725
C	-2.155142	-3.410887	-1.502397
H	-2.736104	-4.330338	-1.615241
H	-2.695178	-2.585148	-1.986567
H	-1.177319	-3.544276	-1.986107
O	-1.277934	-2.021362	1.588174
O	-2.025596	-3.205207	-0.111894

Sum of electronic and thermal Enthalpies = -306.747702 Hartree
 $\langle S^2 \rangle = 0.760814$

AT_A7-MA_1ts_K

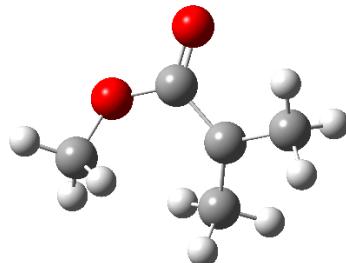


C	0.954886	-0.164758	-0.645888
O	1.541076	-1.326415	-0.258176
O	1.690939	0.975884	-0.574746
C	2.384478	-1.302574	0.916028
C	3.065279	0.912899	-1.015170
C	3.827721	-0.945360	0.571523
H	1.964138	-0.612470	1.657970
H	2.325180	-2.318534	1.315314
C	4.006504	0.507318	0.115798
H	3.144869	0.231986	-1.871585
H	3.290527	1.926749	-1.356523
H	4.168213	-1.632525	-0.214149
H	4.452792	-1.136828	1.453646
H	3.837601	1.190926	0.958216
H	5.039804	0.666714	-0.219561
C	-0.375851	-0.118728	-0.971155
H	-0.897092	-1.062088	-1.074361
H	-0.730804	0.723122	-1.553335
C	-1.595170	0.453718	0.811695
C	-1.141900	1.836663	1.173666
C	-2.911731	0.293857	0.212012
H	-1.263125	-0.373524	1.432461
H	-1.504728	2.561309	0.439004
H	-1.539288	2.140677	2.154441
H	-0.050214	1.900459	1.224742
O	-3.580082	1.180648	-0.303195
O	-3.317194	-1.016293	0.221621
C	-4.583020	-1.259216	-0.398113
H	-4.750636	-2.334780	-0.317148
H	-4.571693	-0.953251	-1.448757
H	-5.380626	-0.711434	0.113210

Sum of electronic and thermal Enthalpies = -691.433669 Hartree
 $\langle S^2 \rangle = 0.776225$

Imaginary frequency = i477 cm⁻¹

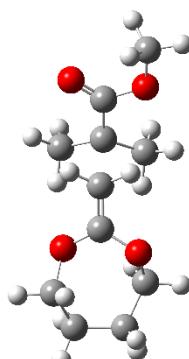
AT_MMA_K



C	-0.005418	0.010100	0.003386
H	0.006858	-0.001744	1.096757
H	1.025491	0.034517	-0.381511
H	-0.486609	0.948157	-0.321242
C	-0.746850	-1.176169	-0.543605
C	-1.605308	-1.935162	0.382006
C	-1.199028	-4.065306	-0.665901
H	-1.307935	-5.038651	-0.174633
H	-1.487712	-4.163734	-1.719914
H	-0.148339	-3.753065	-0.606645
O	-1.978627	-1.468837	1.437115
O	-2.052100	-3.162107	0.012056
C	-0.754165	-1.398022	-2.034085
H	-0.786772	-0.429220	-2.553183
H	0.160883	-1.909282	-2.378110
H	-1.615724	-1.991726	-2.358341

Sum of electronic and thermal Enthalpies = -349.003218 Hartree
 $\langle S^2 \rangle = 0.760748$

AT_A7-MMA_ts_K



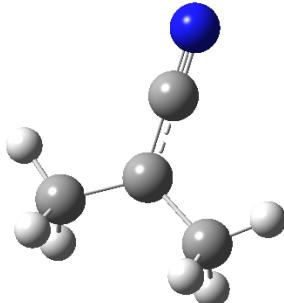
C	1.041147	0.024797	-0.640100
O	1.642855	-1.192841	-0.587442
O	1.764678	1.113039	-0.264073
C	2.595427	-1.447910	0.466730
C	3.097018	1.244060	-0.809043
C	3.998913	-0.969367	0.102378
H	2.245856	-0.991760	1.401155
H	2.581134	-2.534523	0.585896
C	4.137823	0.556702	0.069404

H	3.111568	0.854330	-1.834679
H	3.276500	2.322002	-0.845902
H	4.259220	-1.395879	-0.875247
H	4.706263	-1.388538	0.830077
H	4.047018	0.964013	1.084929
H	5.136419	0.832116	-0.294805
C	-0.294617	0.141411	-0.950523
H	-0.784278	-0.747873	-1.330229
H	-0.638448	1.097585	-1.327746
C	-1.571893	0.261740	0.827011
C	-1.137477	1.552524	1.473758
C	-2.827999	0.337373	0.072012
H	-1.407447	2.411594	0.855455
H	-1.629668	1.681722	2.450796
H	-0.056109	1.561949	1.646431
O	-3.345038	1.365655	-0.344896
O	-3.351958	-0.897230	-0.207764
C	-4.540951	-0.880817	-1.003255
H	-4.819741	-1.927358	-1.138991
H	-4.357827	-0.405629	-1.971671
H	-5.342621	-0.335839	-0.495956
C	-1.249847	-1.005832	1.579089
H	-1.425664	-1.900902	0.978099
H	-0.203075	-1.002761	1.905150
H	-1.868653	-1.091326	2.485864

Sum of electronic and thermal Enthalpies = -730.694056 Hartree
 $\langle S^2 \rangle = 0.776914$

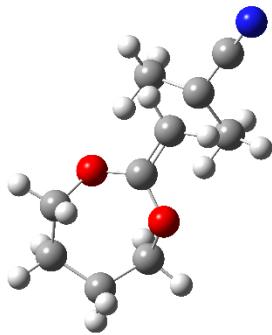
Imaginary frequency = 1540 cm⁻¹

AT_AZO_K



C	-0.001051	0.000002	0.000613
C	0.000243	-0.000009	1.508778
H	1.015772	-0.000005	1.916968
H	-0.532628	0.884783	1.891346
H	-0.532615	-0.884814	1.891336
C	1.210724	-0.000021	-0.705786
C	-1.312791	-0.000037	-0.743634
H	-1.167606	0.000169	-1.828457
H	-1.908136	-0.884963	-0.468606
H	-1.908362	0.884634	-0.468288
N	2.222009	-0.000040	-1.295307

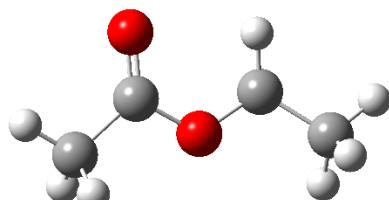
Sum of electronic and thermal Enthalpies = -210.495169 Hartree
 $\langle S^2 \rangle = 0.767514$

AT_A7-PCN_ts_K

C	-0.431392	-0.198672	-0.678890
O	-1.100019	0.960869	-0.911142
O	-1.034619	-1.144004	0.090167
C	-1.969133	1.479351	0.118340
C	-2.400569	-1.490466	-0.238328
C	-3.363310	0.859285	0.065155
H	-1.504623	1.337458	1.102295
H	-2.020265	2.551410	-0.088829
C	-3.400753	-0.609177	0.502973
H	-2.537930	-1.433990	-1.325376
H	-2.503766	-2.534289	0.070119
H	-3.740161	0.960328	-0.961036
H	-4.028001	1.452263	0.706997
H	-3.190427	-0.686122	1.577917
H	-4.407299	-1.018963	0.346803
C	0.865191	-0.365373	-1.109161
H	1.255363	0.376317	-1.795881
H	1.222063	-1.381101	-1.230885
C	2.077805	-0.965081	1.506917
H	2.290891	-1.969611	1.128843
H	2.704890	-0.803799	2.396769
H	1.030052	-0.934092	1.823495
C	2.013339	1.521286	0.848689
H	2.122169	2.211112	0.006191
H	0.983108	1.584758	1.216679
H	2.673508	1.872151	1.655972
C	2.340484	0.095660	0.457201
C	3.524203	-0.075163	-0.313341
N	4.456049	-0.232665	-1.002801

Sum of electronic and thermal Enthalpies = -595.164428 Hartree
 $\langle S^2 \rangle = 0.780112$

Imaginary frequency = i550 cm⁻¹

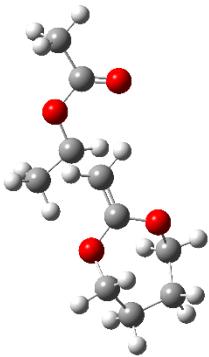
AT_VAC1_K

C	0.005437	-0.005826	-0.005703
H	0.005297	-0.025082	1.098905
H	1.054414	-0.014682	-0.332496

H	-0.452864	0.936909	-0.326020
C	0.032982	-4.728176	-0.470982
H	-0.566384	-5.623897	-0.648990
H	0.883453	-4.701662	-1.163644
H	0.434728	-4.736294	0.549398
C	-0.834225	-3.502296	-0.678950
O	-1.983395	-3.500727	-1.032367
O	-0.133872	-2.373794	-0.413341
C	-0.743988	-1.159307	-0.588363
H	-1.822066	-1.189549	-0.715546

Sum of electronic and thermal Enthalpies = -306.758086 Hartree
 $\langle S^2 \rangle = 0.753828$

AT_A7-VAc_1ts_K

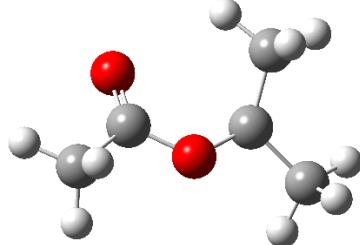


C	1.005810	-0.102716	-0.674422
O	1.578580	-1.286474	-0.318510
O	1.766782	1.025590	-0.554005
C	2.391661	-1.306178	0.872721
C	3.138315	0.943039	-0.989777
C	3.848291	-0.965855	0.564836
H	1.969363	-0.627479	1.624741
H	2.310013	-2.330097	1.248275
C	4.062176	0.491851	0.139707
H	3.212198	0.280234	-1.861155
H	3.392881	1.958731	-1.306441
H	4.190640	-1.643254	-0.228567
H	4.454660	-1.185707	1.453683
H	3.898561	1.161209	0.994736
H	5.102571	0.635876	-0.181128
C	-0.308518	-0.024419	-1.022343
H	-0.867458	-0.946074	-1.120855
H	-0.647997	0.845328	-1.571545
C	-1.658198	0.579097	0.742756
C	-1.171132	1.904247	1.225952
O	-2.940860	0.666514	0.187643
H	-1.518222	-0.307127	1.354182
H	-1.281814	2.670261	0.449486
H	-1.718589	2.254914	2.116345
H	-0.109309	1.837437	1.482443
C	-3.638695	-0.483109	-0.018688
C	-4.985103	-0.181065	-0.633128
O	-3.222338	-1.585423	0.265972
H	-5.507367	-1.116551	-0.836869
H	-5.583172	0.433515	0.048691
H	-4.861909	0.387770	-1.560513

Sum of electronic and thermal Enthalpies = -691.429235 Hartree
 $\langle S^2 \rangle = 0.777747$

Imaginary frequency = i401 cm⁻¹

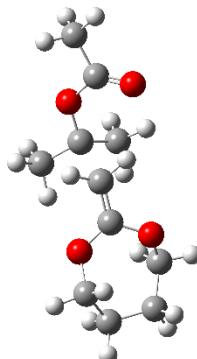
AT_MVAC_K



C	-0.002520	-0.031005	-0.013171
C	0.002678	-0.017036	1.492065
O	1.225811	-0.022318	-0.661307
C	-1.027204	0.736530	-0.798684
H	0.458338	0.913979	1.877276
H	-1.028343	-0.060845	1.862513
H	0.564859	-0.865233	1.895189
C	2.156696	-0.967806	-0.411658
C	3.425923	-0.673149	-1.191806
O	1.992548	-1.906373	0.321652
H	3.194910	-0.566739	-2.258277
H	3.860272	0.274354	-0.849019
H	4.137472	-1.487273	-1.036257
H	-2.026600	0.571919	-0.378694
H	-0.828145	1.823830	-0.777692
H	-1.028300	0.421970	-1.850022

Sum of electronic and thermal Enthalpies = -346.017249 Hartree
 $\langle S^2 \rangle = 0.753882$

AT_A7-MVAc_ts_K



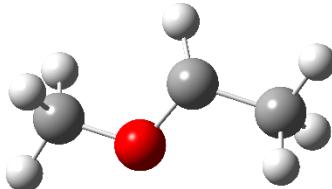
C	1.094525	-0.035616	-0.683698
O	1.698462	-1.232738	-0.436127
O	1.834261	1.095485	-0.481071
C	2.586475	-1.322361	0.694942
C	3.179786	1.099286	-1.000046
C	4.015050	-0.925407	0.327472
H	2.201804	-0.713569	1.523299
H	2.548975	-2.373881	0.993545
C	4.179689	0.568588	0.024795
H	3.216768	0.526287	-1.935172

H	3.389964	2.148124	-1.229423
H	4.315942	-1.522713	-0.543278
H	4.680113	-1.210800	1.153491
H	4.059285	1.153810	0.946169
H	5.195589	0.763445	-0.344119
C	-0.227702	0.039289	-1.013250
H	-0.763825	-0.881415	-1.200723
H	-0.578231	0.941154	-1.501473
C	-1.574493	0.485575	0.774287
C	-1.109480	1.841435	1.221697
O	-2.880146	0.631428	0.231861
H	-1.266235	2.589494	0.437489
H	-1.651276	2.181159	2.120345
H	-0.041391	1.814737	1.456986
C	-3.528879	-0.375711	-0.401781
C	-4.917392	0.075246	-0.800070
O	-3.073466	-1.479470	-0.615557
H	-5.380849	-0.690505	-1.423357
H	-5.529595	0.236294	0.094493
H	-4.872549	1.026120	-1.339832
C	-1.389873	-0.660813	1.729055
H	-1.628254	-1.620242	1.267153
H	-0.348815	-0.682405	2.068934
H	-2.026541	-0.539803	2.622214

Sum of electronic and thermal Enthalpies = -730.690985 Hartree
 $\langle S^2 \rangle = 0.779072$

Imaginary frequency = i437 cm⁻¹

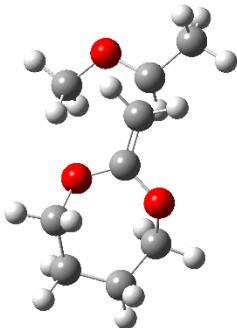
AT_VE1_K



C	-0.000779	-0.018439	-0.011687
C	0.002170	0.000545	1.488161
O	1.234731	-0.014507	-0.568598
H	0.389828	0.952296	1.893575
H	-1.015889	-0.141132	1.870301
H	0.637770	-0.805187	1.879655
C	1.254865	0.052928	-1.972524
H	2.304204	0.084702	-2.281191
H	0.767546	-0.827606	-2.417258
H	0.743111	0.961317	-2.330483
H	-0.772354	0.526648	-0.568586

Sum of electronic and thermal Enthalpies = -193.457532 Hartree
 $\langle S^2 \rangle = 0.75305$

AT_A7-VE_1ts_K



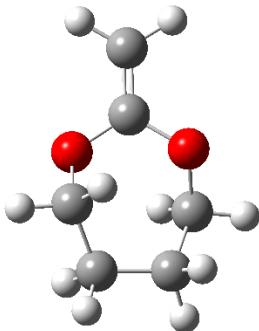
C	0.433541	-0.093737	-0.731391
O	1.063833	-1.278932	-0.469845
O	1.094079	1.055901	-0.391004
C	1.790646	-1.387493	0.769502
C	2.490808	1.132640	-0.732119
C	3.235836	-0.914475	0.618145
H	1.267818	-0.836250	1.561770
H	1.765688	-2.453159	1.016739
C	3.371163	0.596693	0.395345
H	2.673848	0.601930	-1.675225
H	2.685984	2.197374	-0.892275
H	3.679660	-1.460690	-0.224719
H	3.796251	-1.207064	1.516340
H	3.104317	1.136216	1.313846
H	4.417432	0.846602	0.173453
C	-0.859425	-0.053047	-1.167247
H	-1.317957	-0.990383	-1.456815
H	-1.213904	0.848050	-1.652655
C	-2.363249	0.312063	0.529431
C	-2.092800	1.726165	0.937795
O	-3.642226	0.148225	0.035950
H	-2.051009	-0.477143	1.221902
H	-2.689363	2.028874	1.813724
H	-1.032876	1.852035	1.177952
H	-2.340537	2.415381	0.121398
C	-4.059570	-1.195647	-0.112080
H	-3.441434	-1.735674	-0.842160
H	-5.093395	-1.172656	-0.465589
H	-4.017714	-1.733974	0.847221

Sum of electronic and thermal Enthalpies = -578.127563 Hartree
 $\langle S^2 \rangle = 0.780618$

Imaginary frequency = i468 cm⁻¹

UBMK/6-311++G(2dp3df)

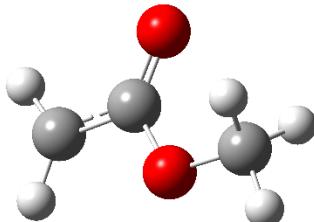
AT_AC77_1_K-GB



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.335051
H	0.935546	0.000000	-0.543785
H	-0.935540	0.000022	-0.543798
O	1.150847	0.157786	2.050677
O	-1.150871	-0.157758	2.050655
C	1.331045	-0.693654	3.199858
C	-1.330763	0.693059	3.200323
C	0.764917	-0.053506	4.465703
H	0.884639	-1.677676	3.010157
H	2.414250	-0.818232	3.287718
C	-0.764524	0.052195	4.465768
H	-0.884295	1.677145	3.011101
H	-2.413939	0.817690	3.288432
H	1.211385	0.944706	4.565049
H	1.097320	-0.638154	5.333920
H	-1.210988	-0.946072	4.564587
H	-1.096886	0.636361	5.334324

Sum of electronic and thermal Enthalpies = -384.9684 Hartree

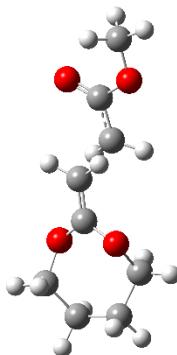
AT__MEST_K-GB



C	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.083253
C	1.236883	0.000000	-0.751682
C	3.588971	-0.002525	-0.613563
H	4.344475	-0.002377	0.172935
H	3.691011	0.885766	-1.243849
H	3.689990	-0.891957	-1.242427
O	1.310480	-0.001081	-1.972497
O	2.326155	-0.001268	0.064439
H	-0.933220	-0.000159	-0.548373

Sum of electronic and thermal Enthalpies = -267.6686 Hartree
 $\langle S^2 \rangle = 0.758507$

AT_A7-MEst_ts_K-GB

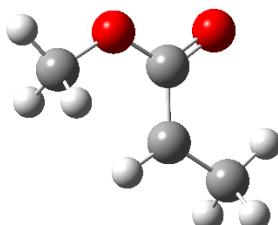


C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.356444
O	1.196991	0.000000	-0.638378
C	0.990551	0.806344	2.034999
C	2.223438	-0.884006	-0.135110
C	2.297662	0.046769	2.245832
H	1.151193	1.737123	1.477626
H	0.529048	1.051366	2.995088
C	3.067298	-0.217046	0.947099
H	1.763090	-1.811954	0.225722
H	2.835719	-1.118515	-1.009806
H	2.061710	-0.901568	2.746162
H	2.925030	0.623482	2.938084
H	3.457164	0.725538	0.540940
H	3.935518	-0.856882	1.152762
C	-1.161898	0.111312	-0.705702
H	-2.097808	0.095818	-0.162709
H	-1.166729	-0.166806	-1.751495
C	-1.450918	2.322445	-1.287432
C	-2.640605	2.198360	-2.101136
H	-1.535899	2.736568	-0.289831
O	-2.668063	1.951408	-3.299807
O	-3.783256	2.324136	-1.351979
C	-5.000471	2.164938	-2.084786
H	-5.803384	2.282056	-1.354645
H	-5.051304	1.176464	-2.551899
H	-5.087647	2.922660	-2.869689
H	-0.511457	2.435214	-1.812948

Sum of electronic and thermal Enthalpies = -652.6315 Hartree
 $\langle S^2 \rangle = 0.773293$

Imaginary frequency = i437 cm⁻¹

AT_MA_K-GB

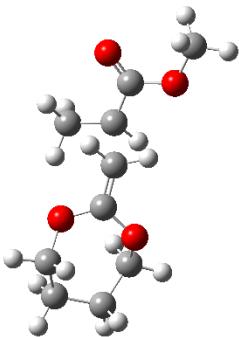


C	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.091494
H	1.039732	0.000000	-0.359623

H	-0.446470	0.939003	-0.359613
C	-0.743177	-1.176189	-0.522390
H	-0.823584	-1.303963	-1.596685
C	-1.348391	-2.133385	0.388380
C	-2.157352	-3.414422	-1.514203
H	-2.737527	-4.332231	-1.625269
H	-2.697010	-2.591505	-1.998828
H	-1.182260	-3.549116	-1.998295
O	-1.277183	-2.020126	1.604203
O	-2.028428	-3.209686	-0.110005

Sum of electronic and thermal Enthalpies = -306.9623 Hartree
 $\langle S^2 \rangle = 0.76098$

AT_A7-MA_1ts_K-GB

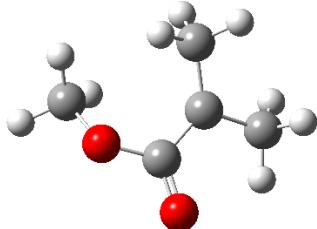


C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.357714
O	1.200449	0.000000	-0.637826
C	0.970164	0.829655	2.036761
C	2.234255	-0.863739	-0.116336
C	2.290504	0.096218	2.255869
H	1.114552	1.761798	1.476699
H	0.500957	1.070131	2.994433
C	3.064903	-0.170207	0.960012
H	1.783171	-1.791787	0.256054
H	2.854459	-1.103814	-0.984012
H	2.071070	-0.850652	2.766454
H	2.908385	0.690944	2.941463
H	3.439118	0.773921	0.542758
H	3.943742	-0.792650	1.173992
C	-1.167023	0.131359	-0.706810
H	-2.095479	0.061700	-0.154190
H	-1.171716	-0.172720	-1.746594
C	-1.534501	2.276304	-1.213917
C	-0.390867	2.675478	-2.098098
C	-2.849514	2.115779	-1.816810
H	-1.533728	2.626015	-0.185503
H	-0.492451	2.213865	-3.084546
H	-0.368089	3.765778	-2.249711
H	0.571321	2.381196	-1.666764
O	-3.081857	1.981956	-3.011229
O	-3.838393	2.059463	-0.868162
C	-5.156054	1.851436	-1.383808
H	-5.813224	1.820302	-0.512805
H	-5.216554	0.911341	-1.940725
H	-5.448720	2.668202	-2.050839

Sum of electronic and thermal Enthalpies = -691.93229 Hartree
 $\langle S^2 \rangle = 0.775547$

Imaginary frequency = i477 cm⁻¹

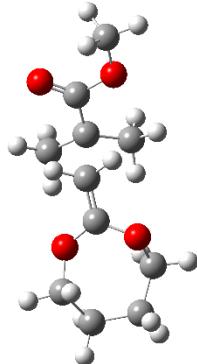
AT_MMA_K-GB



C	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.091183
H	1.036180	0.000000	-0.367619
H	-0.446109	0.948990	-0.336971
C	-0.758646	-1.166623	-0.546894
C	-1.606102	-1.922614	0.371521
C	-1.193300	-4.084206	-0.661328
H	-1.313398	-5.050905	-0.163972
H	-1.467913	-4.190908	-1.716191
H	-0.144260	-3.777171	-0.590913
O	-1.988186	-1.456717	1.433877
O	-2.061512	-3.165583	0.004609
C	-0.765686	-1.377801	-2.030519
H	-0.840507	-0.411050	-2.546246
H	0.167359	-1.843028	-2.386216
H	-1.599276	-2.002637	-2.360173

Sum of electronic and thermal Enthalpies = -346.2588 Hartree
 $\langle S^2 \rangle = 0.760828$

AT_A7-MMA_ts_K-GB



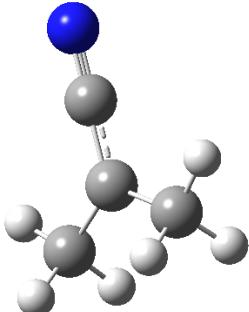
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.359216
O	1.199806	0.000000	-0.640023
C	1.042096	0.721279	2.050248
C	2.192055	-0.949230	-0.188699
C	2.303524	-0.120426	2.228741
H	1.256658	1.659074	1.523062
H	0.603602	0.963390	3.021968
C	3.063977	-0.371437	0.921846
H	1.694379	-1.874753	0.127142
H	2.792948	-1.165012	-1.076335

H	2.012339	-1.074126	2.688187
H	2.960344	0.389796	2.945578
H	3.501827	0.566625	0.556106
H	3.898504	-1.061665	1.103076
C	-1.174616	0.116173	-0.707820
H	-2.094009	0.015873	-0.142642
H	-1.178842	-0.240783	-1.731221
C	-1.601025	2.179776	-1.312185
C	-0.466482	2.502689	-2.251153
C	-2.874900	1.856833	-1.965252
H	-0.530934	1.906568	-3.164207
H	-0.497676	3.563393	-2.546928
H	0.502718	2.322612	-1.774198
O	-3.006793	1.508901	-3.131465
O	-3.937882	1.901320	-1.102036
C	-5.194378	1.525876	-1.673911
H	-5.922793	1.606865	-0.865054
H	-5.160302	0.501194	-2.056054
H	-5.463782	2.193994	-2.497359
C	-1.623485	2.932562	-0.004943
H	-2.355913	2.525392	0.695780
H	-0.634802	2.908600	0.468331
H	-1.876539	3.991864	-0.167162

Sum of electronic and thermal Enthalpies = -731.23196 Hartree
 $\langle S^2 \rangle = 0.776491$

Imaginary frequency = i540 cm⁻¹

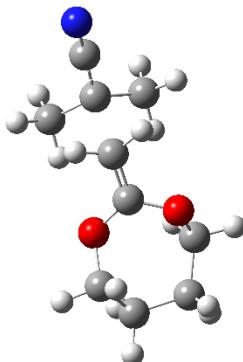
AT_AZO_K-GB



C	0.309013	0.000000	0.000023
C	1.065226	1.297237	-0.000004
H	0.398508	2.162621	-0.000008
H	1.719578	1.364169	0.881369
H	1.719541	1.364157	-0.881410
C	-1.082730	-0.000004	0.000019
C	1.065238	-1.297230	-0.000003
H	0.398525	-2.162621	0.000256
H	1.719349	-1.364266	-0.881550
H	1.719782	-1.364046	0.881234
N	-2.259395	-0.000004	-0.000014

Sum of electronic and thermal Enthalpies = -210.6561 Hartree
 $\langle S^2 \rangle = 0.76802$

AT_A7-PCN_ts_K-GB

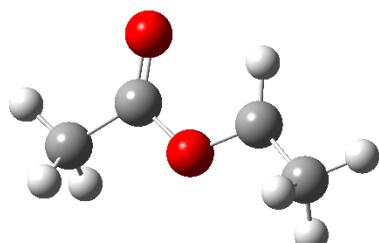


C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.358506
O	1.198961	0.000000	-0.641464
C	1.060281	0.691204	2.052809
C	2.180185	-0.971446	-0.208733
C	2.305333	-0.176736	2.218833
H	1.292483	1.630288	1.534858
H	0.629825	0.931404	3.028440
C	3.062055	-0.424177	0.909019
H	1.668884	-1.894109	0.092921
H	2.775258	-1.181200	-1.101620
H	1.996271	-1.130582	2.665994
H	2.971027	0.311863	2.942381
H	3.517567	0.510480	0.556051
H	3.883598	-1.131861	1.081349
C	-1.175088	0.116382	-0.706876
H	-2.097902	0.013959	-0.148445
H	-1.178537	-0.243882	-1.728677
C	-0.466748	2.514555	-2.262822
H	-0.504693	1.889884	-3.160470
H	-0.511499	3.565594	-2.585929
H	0.500126	2.353403	-1.774813
C	-1.604321	2.948661	0.003655
H	-2.379966	2.581947	0.682921
H	-0.633380	2.849818	0.501976
H	-1.782743	4.022012	-0.159802
C	-1.597344	2.190935	-1.307260
C	-2.871698	1.980911	-1.903932
N	-3.912831	1.738575	-2.379130

Sum of electronic and thermal Enthalpies = -595.61035 Hartree
 $\langle S^2 \rangle = 0.779831$

Imaginary frequency = i550 cm⁻¹

AT_VAC_K-GB

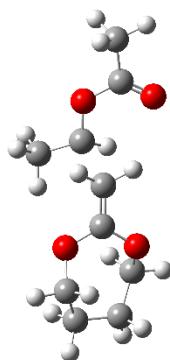


C	0.000000	0.000000	0.000000
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H	0.000000	0.000000	1.104097
H	1.050317	0.000000	-0.318378
H	-0.459981	0.936949	-0.329493
C	0.028381	-4.734119	-0.474407
H	-0.573535	-5.631084	-0.623303
H	0.859445	-4.727148	-1.188420
H	0.462093	-4.735141	0.530674
C	-0.835028	-3.514587	-0.676668
O	-1.987173	-3.505550	-1.041984
O	-0.123576	-2.377214	-0.393031
C	-0.736961	-1.153848	-0.569582
H	-1.804466	-1.182641	-0.747603

Sum of electronic and thermal Enthalpies = -306.9717 Hartree
 $\langle S^2 \rangle = 0.754145$

AT_A7-VAc_1ts_K-GB



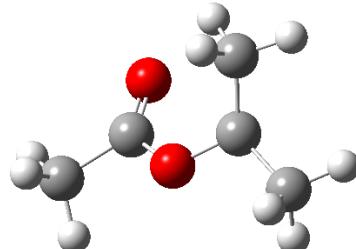
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.362359
O	1.212854	0.000000	-0.628998
C	0.957640	0.845176	2.032525
C	2.230526	-0.869744	-0.094487
C	2.280122	0.118812	2.268787
H	1.102706	1.771264	1.461719
H	0.485637	1.098597	2.985997
C	3.060361	-0.171575	0.981041
H	1.770492	-1.790909	0.284844
H	2.858604	-1.125974	-0.952726
H	2.058371	-0.819536	2.794039
H	2.896000	0.724489	2.946958
H	3.443836	0.764632	0.554019
H	3.933735	-0.796979	1.209488
C	-1.155336	0.116625	-0.711502
H	-2.093113	0.095851	-0.171402
H	-1.154097	-0.179537	-1.753431
C	-1.592557	2.287450	-1.342212
C	-0.431691	2.741363	-2.162631
O	-2.765388	2.200770	-2.102454
H	-1.755762	2.705555	-0.353587
H	-0.340125	2.144400	-3.077606
H	-0.517302	3.798147	-2.464879
H	0.494207	2.623687	-1.591155
C	-3.955257	2.096935	-1.450834
C	-5.092961	2.001920	-2.439865
O	-4.065160	2.091680	-0.243616
H	-6.031069	1.868855	-1.899818
H	-5.143740	2.912329	-3.047196

H -4.933675 1.162549 -3.124610

Sum of electronic and thermal Enthalpies = -691.022583 Hartree
 $\langle S^2 \rangle = 0.777167$

Imaginary frequency = i401 cm⁻¹

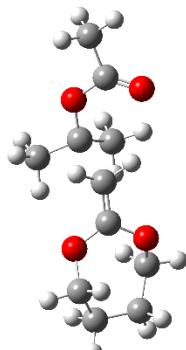
AT_MVAC_K-GB



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.494143
O	1.236930	0.000000	-0.658267
C	-1.031357	0.723256	-0.798969
H	0.458469	0.920380	1.898499
H	-1.029101	-0.042198	1.865301
H	0.553758	-0.851935	1.895951
C	2.166299	-0.972119	-0.417597
C	3.429436	-0.678021	-1.192529
O	1.992111	-1.920677	0.310781
H	3.199257	-0.496811	-2.246914
H	3.905230	0.228382	-0.801570
H	4.116152	-1.519638	-1.095796
H	-2.028151	0.551343	-0.379957
H	-0.862273	1.815059	-0.808829
H	-1.028366	0.387784	-1.842139

Sum of electronic and thermal Enthalpies = -346.2708 Hartree
 $\langle S^2 \rangle = 0.754148$

AT_A7-MVAc_ts_K-GB



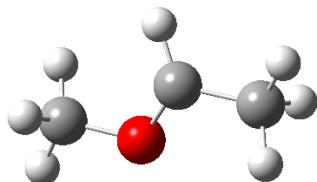
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.363500
O	1.213454	0.000000	-0.628638
C	0.997596	0.788587	2.040884
C	2.208788	-0.916890	-0.130230
C	2.289813	0.003545	2.258407
H	1.181639	1.717808	1.486401

H	0.542198	1.044919	3.001702
C	3.062016	-0.280557	0.964680
H	1.722219	-1.836204	0.219440
H	2.825867	-1.162229	-0.999639
H	2.029888	-0.938984	2.758000
H	2.927265	0.566146	2.953533
H	3.480832	0.652517	0.564832
H	3.911132	-0.944044	1.176590
C	-1.159725	0.107936	-0.711258
H	-2.097956	0.065718	-0.174406
H	-1.150842	-0.211108	-1.746982
C	-1.610144	2.244475	-1.375059
C	-0.456027	2.571580	-2.278268
O	-2.777669	2.147957	-2.179918
H	-0.435229	1.905059	-3.146867
H	-0.513898	3.607190	-2.653349
H	0.488859	2.456314	-1.739016
C	-3.968114	1.715122	-1.698067
C	-5.021915	1.792636	-2.781331
O	-4.168609	1.328061	-0.566091
H	-5.938984	1.319963	-2.427469
H	-5.225210	2.840050	-3.031465
H	-4.671348	1.301647	-3.694319
C	-1.753155	3.049272	-0.113425
H	-2.531681	2.651404	0.539478
H	-0.801211	3.041894	0.428361
H	-1.996454	4.101612	-0.339498

Sum of electronic and thermal Enthalpies = -731.22715 Hartree
 $\langle S^2 \rangle = 0.778541$

Imaginary frequency = i437 cm⁻¹

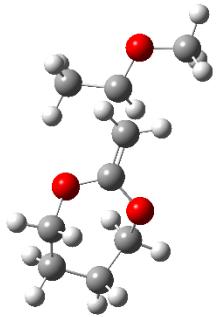
AT__VE1_K-GB



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.488810
O	1.245362	0.000000	-0.566449
H	0.386599	0.942083	1.916141
H	-1.017702	-0.142560	1.867399
H	0.629008	-0.809852	1.878751
C	1.256889	0.051186	-1.983942
H	2.303910	0.085224	-2.293113
H	0.775918	-0.836016	-2.416838
H	0.741139	0.950310	-2.352248
H	-0.775921	0.531189	-0.557145

Sum of electronic and thermal Enthalpies = -193.6254 Hartree
 $\langle S^2 \rangle = 0.753604$

AT_A7-VE_1ts_K-GB



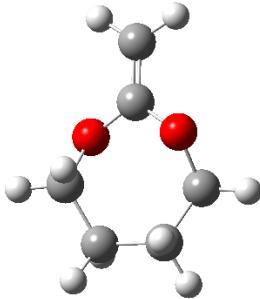
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.367612
O	1.216960	0.000000	-0.626776
C	0.981636	0.817785	2.033675
C	2.215839	-0.901791	-0.114804
C	2.287570	0.057419	2.260850
H	1.148100	1.742734	1.466519
H	0.524603	1.079033	2.992979
C	3.061961	-0.239572	0.971006
H	1.737479	-1.820127	0.249114
H	2.838135	-1.156153	-0.978198
H	2.042843	-0.880060	2.777563
H	2.918660	0.641220	2.944465
H	3.470027	0.691712	0.556121
H	3.918819	-0.889458	1.194190
C	-1.153259	0.151200	-0.714507
H	-2.087607	0.106439	-0.168898
H	-1.164328	-0.161117	-1.751612
C	-1.502821	2.315013	-1.399508
C	-0.432683	2.534975	-2.422254
O	-2.768885	2.413235	-1.941341
H	-1.390633	2.829939	-0.439237
H	-0.415958	3.573133	-2.792010
H	0.547761	2.300928	-1.996919
H	-0.591248	1.883024	-3.289845
C	-3.820166	2.489454	-0.997370
H	-3.883167	1.580231	-0.384116
H	-4.748935	2.606053	-1.561360
H	-3.692977	3.354153	-0.328098

Sum of electronic and thermal Enthalpies = -578.5778 Hartree
 $\langle S^2 \rangle = 0.779925$

Imaginary frequency = i468 cm⁻¹

G3(MP2)RAD

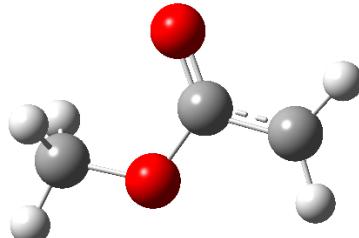
AT_AC77_1_G3



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.335051
H	0.935546	0.000000	-0.543785
H	-0.935540	0.000022	-0.543798
O	1.150847	0.157786	2.050677
O	-1.150871	-0.157758	2.050655
C	1.331045	-0.693654	3.199858
C	-1.330763	0.693059	3.200323
C	0.764917	-0.053506	4.465703
H	0.884639	-1.677676	3.010157
H	2.414250	-0.818232	3.287718
C	-0.764524	0.052195	4.465768
H	-0.884295	1.677145	3.011101
H	-2.413939	0.817690	3.288432
H	1.211385	0.944706	4.565049
H	1.097320	-0.638154	5.333920
H	-1.210988	-0.946072	4.564587
H	-1.096886	0.636361	5.334324

Sum of electronic and thermal Enthalpies = -384.454712 Hartree

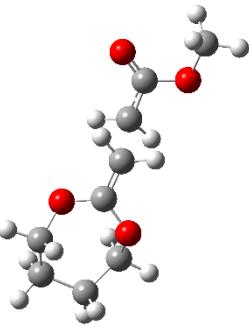
AT__MEST_G3MP2RAD



C	-0.000087	-0.000028	-0.000143
H	0.000371	0.000056	1.083166
C	1.236810	-0.000955	-0.751761
C	3.589019	-0.002464	-0.613493
H	4.344500	-0.002126	0.173036
H	3.690790	0.885878	-1.243729
H	3.690289	-0.891810	-1.242410
O	1.310579	-0.001110	-1.972639
O	2.326045	-0.001621	0.064298
H	-0.933571	0.000579	-0.548090

Sum of electronic and thermal Enthalpies = -267.338409 Hartree
 $\langle S^2 \rangle = 0.757593$

AT_A7-MEst_ts_G3

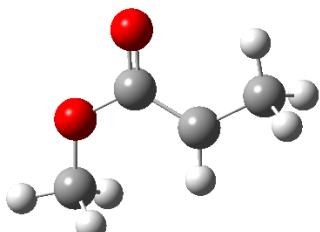


C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.356444
O	1.196991	0.000000	-0.638378
C	0.990551	0.806344	2.034999
C	2.223438	-0.884006	-0.135110
C	2.297662	0.046769	2.245832
H	1.151193	1.737123	1.477626
H	0.529048	1.051366	2.995088
C	3.067298	-0.217046	0.947099
H	1.763090	-1.811954	0.225722
H	2.835719	-1.118515	-1.009806
H	2.061710	-0.901568	2.746162
H	2.925030	0.623482	2.938084
H	3.457164	0.725538	0.540940
H	3.935518	-0.856882	1.152762
C	-1.161898	0.111312	-0.705702
H	-2.097808	0.095818	-0.162709
H	-1.166729	-0.166806	-1.751495
C	-1.450918	2.322445	-1.287432
C	-2.640605	2.198360	-2.101136
H	-1.535899	2.736568	-0.289831
O	-2.668063	1.951408	-3.299807
O	-3.783256	2.324136	-1.351979
C	-5.000471	2.164938	-2.084786
H	-5.803384	2.282056	-1.354645
H	-5.051304	1.176464	-2.551899
H	-5.087647	2.922660	-2.869689
H	-0.511457	2.435214	-1.812948

Sum of electronic and thermal Enthalpies = -651.787476 Hartree
 $\langle S^2 \rangle = 0.768485$

Imaginary frequency = i336 cm⁻¹

AT_MA_G3MP2RAD

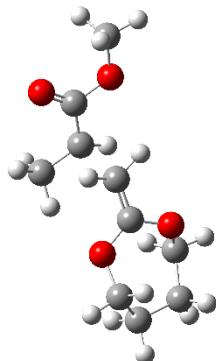


C	-0.000000	-0.000000	-0.000000
H	-0.000000	-0.000000	1.091494
H	1.039732	-0.000000	-0.359623
H	-0.446470	0.939003	-0.359613
C	-0.743177	-1.176189	-0.522390

H	-0.823584	-1.303963	-1.596685
C	-1.348391	-2.133385	0.388380
C	-2.157352	-3.414422	-1.514203
H	-2.737527	-4.332231	-1.625269
H	-2.697010	-2.591505	-1.998828
H	-1.182260	-3.549116	-1.998295
O	-1.277183	-2.020126	1.604203
O	-2.028428	-3.209686	-0.110005

Enthalpy = -306.566315 Hartree
 $\langle S^2 \rangle = 0.759559$

AT_A7-MA_1ts_G3b



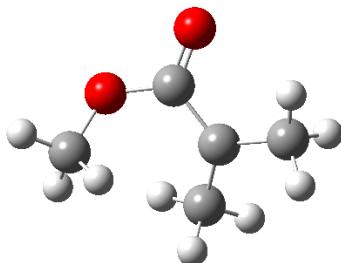
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.357714
O	1.200449	0.000000	-0.637826
C	0.970164	0.829655	2.036761
C	2.234255	-0.863739	-0.116336
C	2.290504	0.096218	2.255869
H	1.114552	1.761798	1.476699
H	0.500957	1.070131	2.994433
C	3.064903	-0.170207	0.960012
H	1.783171	-1.791787	0.256054
H	2.854459	-1.103814	-0.984012
H	2.071070	-0.850652	2.766454
H	2.908385	0.690944	2.941463
H	3.439118	0.773921	0.542758
H	3.943742	-0.792650	1.173992
C	-1.167023	0.131359	-0.706810
H	-2.095479	0.061700	-0.154190
H	-1.171716	-0.172720	-1.746594
C	-1.534501	2.276304	-1.213917
C	-0.390867	2.675478	-2.098098
C	-2.849514	2.115779	-1.816810
H	-1.533728	2.626015	-0.185503
H	-0.492451	2.213865	-3.084546
H	-0.368089	3.765778	-2.249711
H	0.571321	2.381196	-1.666764
O	-3.081857	1.981956	-3.011229
O	-3.838393	2.059463	-0.868162
C	-5.156054	1.851436	-1.383808
H	-5.813224	1.820302	-0.512805
H	-5.216554	0.911341	-1.940725
H	-5.448720	2.668202	-2.050839

Enthalpy = -690.026428 Hartree

$\langle S^2 \rangle = 0.770661$

Imaginary frequency = i418 cm⁻¹

AT_MMA_G3MP2RAD

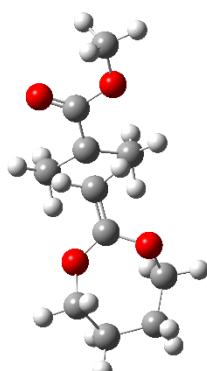


C	0.000709	-0.001109	0.000055
H	0.001451	-0.001385	1.091231
H	1.036635	-0.001579	-0.368234
H	-0.445250	0.948035	-0.336658
C	-0.758655	-1.167232	-0.546836
C	-1.606946	-1.922717	0.371168
C	-1.192394	-4.083849	-0.660577
H	-1.312948	-5.050810	-0.163905
H	-1.464926	-4.189992	-1.716016
H	-0.143762	-3.776091	-0.587836
O	-1.990663	-1.455861	1.432503
O	-2.062059	-3.165847	0.004407
C	-0.766528	-1.377340	-2.030806
H	-0.841622	-0.410202	-2.545806
H	0.166008	-1.842534	-2.387857
H	-1.600404	-2.001740	-2.360684

Enthalpy = -345.799866 Hartree

$\langle S^2 \rangle = 0.759147$

AT_A7-MMA_ts_G3b



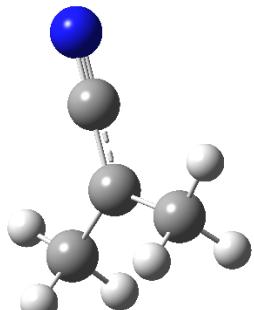
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.359216
O	1.199806	0.000000	-0.640023
C	1.042096	0.721279	2.050248
C	2.192055	-0.949230	-0.188699
C	2.303524	-0.120426	2.228741
H	1.256658	1.659074	1.523062
H	0.603602	0.963390	3.021968
C	3.063977	-0.371437	0.921846
H	1.694379	-1.874753	0.127142

H	2.792948	-1.165012	-1.076335
H	2.012339	-1.074126	2.688187
H	2.960344	0.389796	2.945578
H	3.501827	0.566625	0.556106
H	3.898504	-1.061665	1.103076
C	-1.174616	0.116173	-0.707820
H	-2.094009	0.015873	-0.142642
H	-1.178842	-0.240783	-1.731221
C	-1.601025	2.179776	-1.312185
C	-0.466482	2.502689	-2.251153
C	-2.874900	1.856833	-1.965252
H	-0.530934	1.906568	-3.164207
H	-0.497676	3.563393	-2.546928
H	0.502718	2.322612	-1.774198
O	-3.006793	1.508901	-3.131465
O	-3.937882	1.901320	-1.102036
C	-5.194378	1.525876	-1.673911
H	-5.922793	1.606865	-0.865054
H	-5.160302	0.501194	-2.056054
H	-5.463782	2.193994	-2.497359
C	-1.623485	2.932562	-0.004943
H	-2.355913	2.525392	0.695780
H	-0.634802	2.908600	0.468331
H	-1.876539	3.991864	-0.167162

Enthalpy = -730.266052 Hartree
 $\langle S^2 \rangle = 0.771127$

Imaginary frequency = i446 cm⁻¹

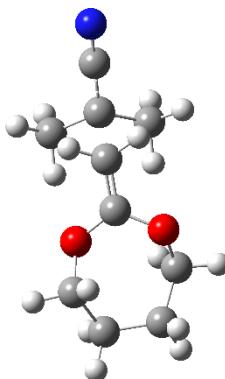
AT_AZO_G3MP2RAD



C	-0.000000	0.000000	-0.000000
C	0.000000	0.000000	1.501560
H	1.011818	0.000000	1.913416
H	-0.531601	0.881382	1.888912
H	-0.531581	-0.881397	1.888915
C	1.202361	-0.000021	-0.700911
C	-1.306631	-0.000035	-0.739862
H	-1.166467	0.000204	-1.823265
H	-1.905499	-0.881575	-0.468338
H	-1.905756	0.881209	-0.467962
N	2.218913	-0.000068	-1.293501

Enthalpy = -210.365585 Hartree
 $\langle S^2 \rangle = 0.765669$

AT_A7-PCN_ts_G3

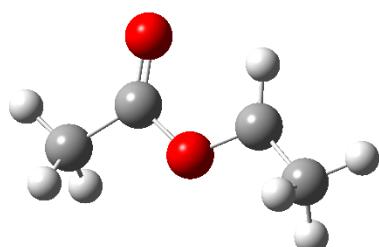


C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.358506
O	1.198961	0.000000	-0.641464
C	1.060281	0.691204	2.052809
C	2.180185	-0.971446	-0.208733
C	2.305333	-0.176736	2.218833
H	1.292483	1.630288	1.534858
H	0.629825	0.931404	3.028440
C	3.062055	-0.424177	0.909019
H	1.668884	-1.894109	0.092921
H	2.775258	-1.181200	-1.101620
H	1.996271	-1.130582	2.665994
H	2.971027	0.311863	2.942381
H	3.517567	0.510480	0.556051
H	3.883598	-1.131861	1.081349
C	-1.175088	0.116382	-0.706876
H	-2.097902	0.013959	-0.148445
H	-1.178537	-0.243882	-1.728677
C	-0.466748	2.514555	-2.262822
H	-0.504693	1.889884	-3.160470
H	-0.511499	3.565594	-2.585929
H	0.500126	2.353403	-1.774813
C	-1.604321	2.948661	0.003655
H	-2.379966	2.581947	0.682921
H	-0.633380	2.849818	0.501976
H	-1.782743	4.022012	-0.159802
C	-1.597344	2.190935	-1.307260
C	-2.871698	1.980911	-1.903932
N	-3.912831	1.738575	-2.379130

Enthalpy = -594.55986 Hartree
 $\langle S^2 \rangle = 0.774378$

Imaginary frequency = i451 cm⁻¹

AT_VAC1_G3MP2RAD



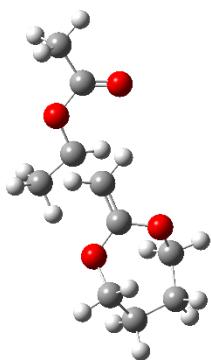
C	-0.000000	-0.000000	0.000000
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H	0.000000	0.000000	1.104097
H	1.050317	-0.000000	-0.318378
H	-0.459981	0.936949	-0.329493
C	0.028381	-4.734119	-0.474407
H	-0.573535	-5.631084	-0.623303
H	0.859445	-4.727148	-1.188420
H	0.462093	-4.735141	0.530674
C	-0.835028	-3.514587	-0.676668
O	-1.987173	-3.505550	-1.041984
O	-0.123576	-2.377214	-0.393031
C	-0.736961	-1.153848	-0.569582
H	-1.804466	-1.182641	-0.747603

Enthalpy = -306.575867 Hartree

$\langle S^2 \rangle = 0.75362$

AT_A7-VAc_1ts_G3



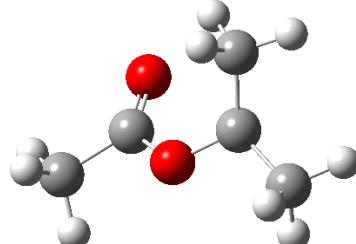
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.362359
O	1.212854	0.000000	-0.628998
C	0.957640	0.845176	2.032525
C	2.230526	-0.869744	-0.094487
C	2.280122	0.118812	2.268787
H	1.102706	1.771264	1.461719
H	0.485637	1.098597	2.985997
C	3.060361	-0.171575	0.981041
H	1.770492	-1.790909	0.284844
H	2.858604	-1.125974	-0.952726
H	2.058371	-0.819536	2.794039
H	2.896000	0.724489	2.946958
H	3.443836	0.764632	0.554019
H	3.933735	-0.796979	1.209488
C	-1.155336	0.116625	-0.711502
H	-2.093113	0.095851	-0.171402
H	-1.154097	-0.179537	-1.753431
C	-1.592557	2.287450	-1.342212
C	-0.431691	2.741363	-2.162631
O	-2.765388	2.200770	-2.102454
H	-1.755762	2.705555	-0.353587
H	-0.340125	2.144400	-3.077606
H	-0.517302	3.798147	-2.464879
H	0.494207	2.623687	-1.591155
C	-3.955257	2.096935	-1.450834
C	-5.092961	2.001920	-2.439865
O	-4.065160	2.091680	-0.243616
H	-6.031069	1.868855	-1.899818

H	-5.143740	2.912329	-3.047196
H	-4.933675	1.162549	-3.124610

Enthalpy = -690.03037 Hartree
 $\langle S^2 \rangle = 0.773456$

Imaginary frequency = i385 cm⁻¹

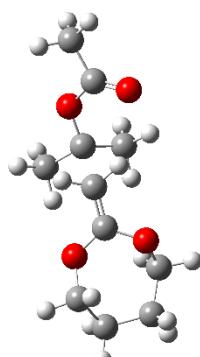
AT__MVAC_G3MP2RAD



C	0.000509	-0.000437	-0.000156
C	-0.000938	-0.000689	1.494102
O	1.237415	-0.000461	-0.658195
C	-1.030820	0.723460	-0.798553
H	0.458500	0.918892	1.899243
H	-1.030926	-0.040581	1.862839
H	0.550186	-0.853685	1.897304
C	2.167218	-0.972043	-0.417338
C	3.429668	-0.677954	-1.193418
O	1.994487	-1.919260	0.313097
H	3.198671	-0.498489	-2.247925
H	3.904943	0.229411	-0.804071
H	4.117112	-1.518872	-1.095923
H	-2.027353	0.552176	-0.378514
H	-0.861233	1.815188	-0.808590
H	-1.029044	0.388148	-1.841796

Enthalpy = -345.812012 Hartree
 $\langle S^2 \rangle = 0.753562$

AT_A7-MVAc_ts_G3b



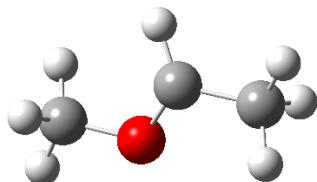
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.363500
O	1.213454	0.000000	-0.628638
C	0.997596	0.788587	2.040884
C	2.208788	-0.916890	-0.130230
C	2.289813	0.003545	2.258407
H	1.181639	1.717808	1.486401

H	0.542198	1.044919	3.001702
C	3.062016	-0.280557	0.964680
H	1.722219	-1.836204	0.219440
H	2.825867	-1.162229	-0.999639
H	2.029888	-0.938984	2.758000
H	2.927265	0.566146	2.953533
H	3.480832	0.652517	0.564832
H	3.911132	-0.944044	1.176590
C	-1.159725	0.107936	-0.711258
H	-2.097956	0.065718	-0.174406
H	-1.150842	-0.211108	-1.746982
C	-1.610144	2.244475	-1.375059
C	-0.456027	2.571580	-2.278268
O	-2.777669	2.147957	-2.179918
H	-0.435229	1.905059	-3.146867
H	-0.513898	3.607190	-2.653349
H	0.488859	2.456314	-1.739016
C	-3.968114	1.715122	-1.698067
C	-5.021915	1.792636	-2.781331
O	-4.168609	1.328061	-0.566091
H	-5.938984	1.319963	-2.427469
H	-5.225210	2.840050	-3.031465
H	-4.671348	1.301647	-3.694319
C	-1.753155	3.049272	-0.113425
H	-2.531681	2.651404	0.539478
H	-0.801211	3.041894	0.428361
H	-1.996454	4.101612	-0.339498

Enthalpy = -730.261536 Hartree
 $\langle S^2 \rangle = 0.774395$

Imaginary frequency = i391 cm⁻¹

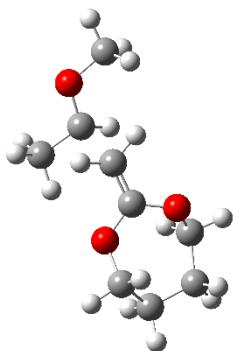
AT__VE1_G3MP2RAD



C	-0.000000	-0.000000	0.000000
C	-0.000000	-0.000000	1.488810
O	1.245362	-0.000000	-0.566449
H	0.386599	0.942083	1.916141
H	-1.017702	-0.142560	1.867399
H	0.629008	-0.809852	1.878751
C	1.256889	0.051186	-1.983942
H	2.303910	0.085224	-2.293113
H	0.775918	-0.836016	-2.416838
H	0.741139	0.950310	-2.352248
H	-0.775921	0.531189	-0.557145

Enthalpy = -730.261536 Hartree
 $\langle S^2 \rangle = 0.752941$

AT_A7-VE_1ts_G3



C	-0.000110	0.000046	-0.000298
O	-0.000318	0.000003	1.367314
O	1.216944	0.000186	-0.626904
C	0.981187	0.817794	2.033568
C	2.215829	-0.901554	-0.114866
C	2.287132	0.057480	2.260870
H	1.147684	1.742785	1.466489
H	0.524010	1.078956	2.992827
C	3.061737	-0.239347	0.971118
H	1.737502	-1.819965	0.248909
H	2.838274	-1.155791	-0.978191
H	2.042381	-0.880061	2.777460
H	2.918085	0.641254	2.944635
H	3.469786	0.692005	0.556367
H	3.918618	-0.889177	1.194377
C	-1.153272	0.151536	-0.715006
H	-2.087681	0.106400	-0.169520
H	-1.164201	-0.161077	-1.752029
C	-1.502409	2.314672	-1.399469
C	-0.432625	2.534668	-2.422588
O	-2.768646	2.412882	-1.940903
H	-1.389909	2.829820	-0.439348
H	-0.416096	3.572815	-2.792377
H	0.547964	2.300694	-1.997551
H	-0.591434	1.882676	-3.290102
C	-3.819595	2.489361	-0.996592
H	-3.882349	1.580318	-0.383044
H	-4.748563	2.605766	-1.560292
H	-3.692196	3.354258	-0.327615

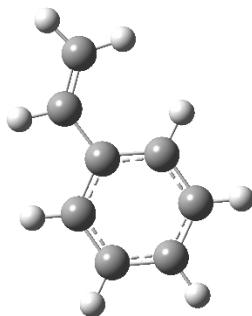
Enthalpy = -577.795959 Hartree

$\langle S^2 \rangle = 0.775906$

Imaginary frequency = i397 cm⁻¹

UB3LYP/6-31G(d)

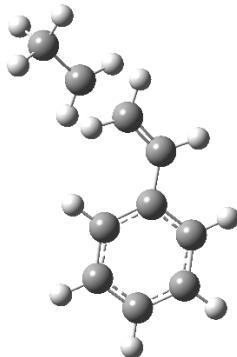
AT_STY



C	0.003836	0.000000	-0.039118
C	-0.039884	0.000000	1.358531
C	1.137659	0.000000	2.100057
C	2.392574	0.000000	1.463459
C	2.417763	0.000000	0.058298
C	1.239307	0.000000	-0.686791
H	-0.917597	0.000000	-0.615090
H	-0.997893	0.000000	1.872084
H	1.082238	0.000000	3.184901
H	3.378101	0.000000	-0.452666
H	1.287117	0.000000	-1.772600
C	3.669445	0.000000	2.196530
H	4.553838	0.000000	1.558832
C	3.852602	0.000000	3.522818
H	4.851915	0.000000	3.947145
H	3.030335	0.000000	4.233210

Sum of electronic and thermal Enthalpies = -309.511901 Hartree

AT_AE-STY_ts1



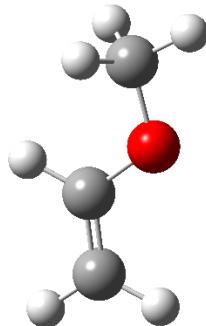
C	-0.002349	-0.002578	-0.002103
C	-0.001231	0.000201	1.396471
C	1.197866	0.000320	2.101783
C	2.437364	-0.004058	1.428245
C	2.414720	-0.001633	0.019154
C	1.214306	-0.003113	-0.687091
H	-0.941032	-0.002089	-0.549402
H	-0.942965	0.004384	1.939683
H	1.174784	0.008017	3.187754
H	3.358379	-0.001275	-0.522126
H	1.228410	-0.003118	-1.774043
C	3.724106	-0.008428	2.120310
H	4.595370	0.069863	1.470404

C	3.934341	-0.051202	3.462576
H	4.941187	-0.146935	3.854571
H	3.133403	-0.254970	4.166112
C	3.914656	2.227727	4.386373
H	4.757231	2.597466	3.808716
H	2.935710	2.482438	3.990230
C	4.076249	2.046960	5.861478
H	4.077391	3.013509	6.395485
H	3.260631	1.453397	6.292706
H	5.022628	1.551284	6.111006

Sum of electronic and thermal Enthalpies = -388.601518 Hartree
 $\langle S^2 \rangle = 0.781131$

Imaginary frequency = i294 cm⁻¹

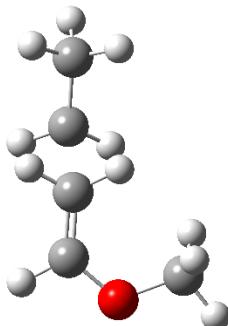
AT_VE2



C	0.018707	0.000002	0.002823
H	0.041110	-0.000133	1.087729
H	0.959079	0.000088	-0.534866
C	-3.472569	-0.000103	-0.907142
O	-2.344885	-0.000078	-0.044810
C	-1.132886	0.000055	-0.668354
H	-1.169550	0.000175	-1.758817
H	-3.492299	-0.894845	-1.544573
H	-4.355930	-0.000540	-0.265411
H	-3.492764	0.895039	-1.543998

Sum of electronic and thermal Enthalpies = -193.023658 Hartree

AT_AE-VE_ts2



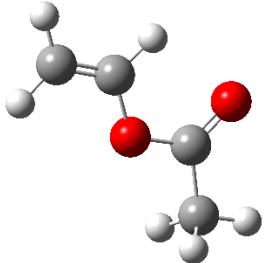
C	-0.007280	0.012286	0.005744
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H	-0.001871	-0.006276	1.089571
C	2.626916	0.004999	1.100039
O	2.415017	-0.153556	-0.293796
C	1.124072	-0.205975	-0.723405
H	1.099955	-0.351691	-1.798998
H	2.200293	0.948292	1.464779
H	3.708820	0.013975	1.245868
H	2.188476	-0.827642	1.666901
H	-0.954972	-0.217844	-0.467654
C	-0.616575	2.246741	0.077834
H	0.280890	2.669973	0.525172
H	-0.699872	2.426261	-0.991889
C	-1.877302	2.280615	0.889016
H	-1.717513	1.899134	1.905972
H	-2.278726	3.303087	0.996135
H	-2.671773	1.678502	0.429829

Sum of electronic and thermal Enthalpies = -272.109622 Hartree
 $\langle S^2 \rangle = 0.776574$

Imaginary frequency = i419 cm⁻¹

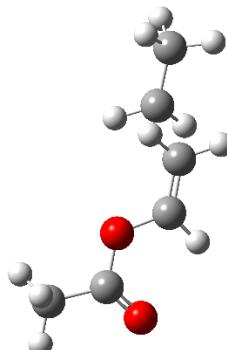
AT_VAC4



C	0.013022	-0.097960	0.004193
H	0.005988	0.039436	1.080526
H	0.948189	0.038875	-0.526333
C	-4.586084	-1.086342	0.170359
H	-5.459214	-1.355160	-0.424646
H	-4.771196	-0.147805	0.703247
H	-4.395640	-1.857161	0.924449
C	-3.389390	-0.940477	-0.734301
O	-3.378384	-1.092888	-1.931964
O	-2.283473	-0.602320	0.002510
C	-1.084396	-0.425715	-0.668455
H	-1.144616	-0.577245	-1.739823

Sum of electronic and thermal Enthalpies = -306.371838 Hartree

AT_AE-VAC_ts2

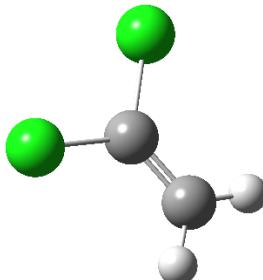


C	-0.002150	-0.002421	-0.000764
H	-0.002608	0.002519	1.083780
H	0.960054	0.001851	-0.499118
C	-4.578945	-1.117805	0.176994
H	-5.455920	-1.380955	-0.415080
H	-4.758814	-0.182470	0.717044
H	-4.389448	-1.894961	0.925164
C	-3.385494	-0.974035	-0.733777
O	-3.376294	-1.154237	-1.928959
O	-2.283328	-0.607531	-0.010536
C	-1.084112	-0.438873	-0.684733
H	-1.136805	-0.599779	-1.753988
C	0.054167	2.354145	0.085212
H	-0.913826	2.485771	0.562385
H	0.060456	2.546714	-0.984822
C	1.283228	2.690006	0.871399
H	1.406590	3.779792	0.995012
H	1.251516	2.261991	1.881174
H	2.194056	2.325502	0.380167

Sum of electronic and thermal Enthalpies = -385.458385 Hartree
 $\langle S^2 \rangle = 0.777704$

Imaginary frequency = i374 cm⁻¹

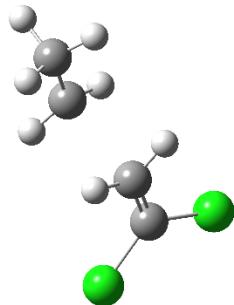
AT_VDC



C	0.002775	0.000000	0.001602
H	0.013247	0.000000	1.085371
H	0.946582	0.000000	-0.531214
C	-1.148287	0.000000	-0.662964
Cl	-2.699641	0.000000	0.134725
Cl	-1.233145	0.000000	-2.405320

Sum of electronic and thermal Enthalpies = -997.7375 Hartree

AT_AE-VDC_ts2

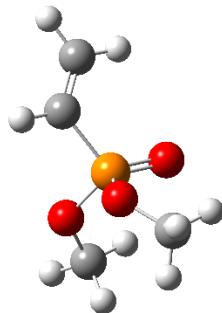


C	0.004499	0.011547	0.002750
H	0.005448	-0.000660	1.085823
H	0.959069	-0.000840	-0.508951
C	-1.114192	-0.339311	-0.666150
Cl	-2.660580	-0.504295	0.122003
Cl	-1.151687	-0.504579	-2.401373
C	0.203759	2.421298	0.121629
H	-0.746807	2.585242	0.622151
H	0.194844	2.585066	-0.952650
C	1.468996	2.670135	0.878148
H	1.431469	2.248745	1.890211
H	1.664610	3.750083	0.994997
H	2.342750	2.248578	0.366199

Sum of electronic and thermal Enthalpies = -1076.827239 Hartree
 $\langle S^2 \rangle = 0.776146$

Imaginary frequency = i310 cm⁻¹

AT_VP1

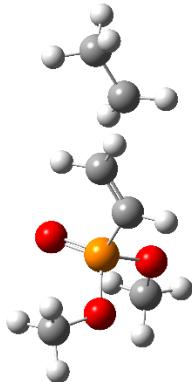


C	0.040570	-0.002003	-0.092838
H	0.003985	-0.002890	0.993806
H	1.023550	-0.002940	-0.556447
C	-1.070157	0.000272	-0.831988
H	-2.061713	0.001296	-0.384580
P	-0.956024	0.000991	-2.621302
O	-1.869366	-1.286495	-3.001281
O	-1.864991	1.292508	-2.996824
O	0.404843	-0.001363	-3.220585
C	-1.622580	-2.023123	-4.210568

H	-0.551768	-2.068973	-4.424693
H	-2.148150	-1.558181	-5.052355
H	-2.018329	-3.028062	-4.050184
C	-1.635171	2.013069	-4.219054
H	-2.028142	3.020198	-4.065963
H	-0.567365	2.055779	-4.448521
H	-2.172793	1.537814	-5.047430

Sum of electronic and thermal Enthalpies = -724.752298 Hartree

AT_AE-VP_ts4

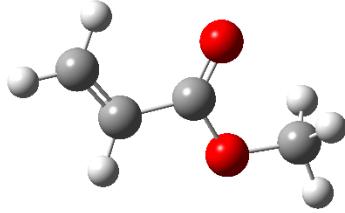


C	-0.035359	-0.001632	-0.027945
H	-0.057680	-0.000682	1.057061
C	1.153811	0.004001	-0.685413
H	1.206567	0.109751	-1.766495
P	2.677168	-0.240324	0.208414
O	3.393177	-1.396240	-0.665424
O	3.651685	1.016949	-0.158866
O	2.521505	-0.481565	1.668754
C	4.690197	-1.869231	-0.262501
H	5.444602	-1.093111	-0.424176
H	4.910989	-2.735747	-0.888483
H	4.681641	-2.165181	0.790914
C	3.573396	2.203833	0.644065
H	4.403788	2.842828	0.336450
H	2.627356	2.729000	0.465805
H	3.660417	1.960311	1.706588
H	-0.957566	0.260904	-0.538636
C	-0.867164	-2.229936	0.156638
H	-0.027847	-2.572111	0.755083
H	-0.819060	-2.482916	-0.899117
C	-2.206732	-2.092973	0.805246
H	-2.910070	-1.527520	0.181906
H	-2.667044	-3.079848	0.984665
H	-2.138365	-1.597479	1.781105

Sum of electronic and thermal Enthalpies = -803.842666 Hartree
 $\langle S^2 \rangle = 0.772527$

Imaginary frequency = i290 cm⁻¹

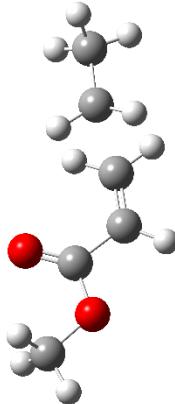
AT_MA1



C	-0.011652	-0.000067	-0.001569
H	-0.054536	-0.000021	1.083937
H	0.967329	-0.000134	-0.471152
C	-1.135718	-0.000042	-0.721008
H	-1.131997	-0.000087	-1.806960
C	-2.462684	0.000048	-0.054264
C	-4.787477	0.000177	-0.435075
H	-4.953363	0.889337	0.179416
H	-5.453973	0.000312	-1.298133
H	-4.953562	-0.889040	0.179282
O	-2.657029	0.000125	1.144787
O	-3.457249	0.000065	-0.973991

Sum of electronic and thermal Enthalpies = -306.367997 Hartree

AT_AE-MA_ts3

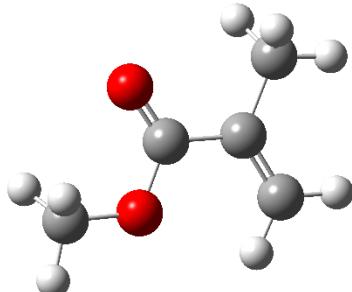


C	-0.001014	-0.001452	-0.000722
H	-0.001108	0.000100	1.084071
H	0.960678	0.000764	-0.502500
C	-1.123408	-0.290128	-0.702025
H	-2.090273	-0.407935	-0.222722
C	-1.078251	-0.400752	-2.168246
C	-2.349617	-0.872943	-4.095848
H	-3.381246	-1.141126	-4.327672
H	-1.664726	-1.654693	-4.436755
H	-2.078908	0.067251	-4.585015
O	-0.097748	-0.218062	-2.869107
O	-2.295948	-0.737433	-2.670278
C	0.312416	2.430874	0.062146
H	-0.657000	2.673836	0.488188
H	0.379310	2.489999	-1.019982
C	1.541396	2.645017	0.882953
H	2.410664	2.128233	0.459178
H	1.807074	3.715240	0.936682
H	1.409755	2.303325	1.916791

Sum of electronic and thermal Enthalpies = -385.459344 Hartree
 $\langle S^2 \rangle = 0.772073$

Imaginary frequency = i247 cm⁻¹

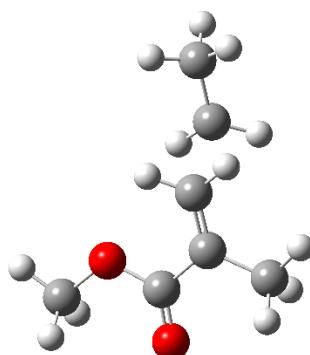
AT_MMA2



C	-0.027147	0.015268	0.041254
H	-0.170308	0.072520	1.126187
H	1.055646	-0.011210	-0.125209
H	-0.432596	0.921957	-0.416634
C	-0.688513	-1.213870	-0.524461
C	-0.196772	-2.505882	0.043871
C	-0.359858	-4.854124	0.041871
H	-0.945498	-5.611414	-0.480547
H	0.707608	-4.994172	-0.149452
H	-0.534975	-4.908860	1.119849
O	0.668317	-2.577720	0.895814
O	-0.806618	-3.594717	-0.480140
C	-1.643623	-1.184247	-1.462349
H	-1.996762	-0.241249	-1.871496
H	-2.095884	-2.092280	-1.844598

Sum of electronic and thermal Enthalpies = -345.65833 Hartree

AT_AE-MMA_ts1



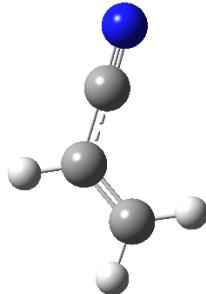
C	-0.000240	-0.000603	-0.000575
H	-0.000173	0.000413	1.082183
H	0.967503	0.000094	-0.493066
C	-1.127077	-0.296719	-0.700571
C	-2.437877	-0.438457	-0.028052
C	-3.640869	-0.331565	1.995475

H	-3.432092	-0.090105	3.038733
H	-4.012012	-1.356661	1.906982
H	-4.393294	0.349402	1.587618
O	-3.467689	-0.751114	-0.600512
O	-2.392822	-0.181286	1.307672
C	0.214420	2.433794	0.201671
H	0.172321	2.655772	-0.861062
H	-0.724468	2.532027	0.738279
C	1.497428	2.646847	0.936536
H	2.360648	2.276943	0.370082
H	1.681779	3.718613	1.126986
H	1.494472	2.151497	1.915017
C	-1.153406	-0.461428	-2.196536
H	-1.560383	-1.439935	-2.476375
H	-1.803580	0.285804	-2.668486
H	-0.148517	-0.365214	-2.618494

Sum of electronic and thermal Enthalpies = -424.74888 Hartree
 $\langle S^2 \rangle = 0.773944$

Imaginary frequency = i265 cm⁻¹

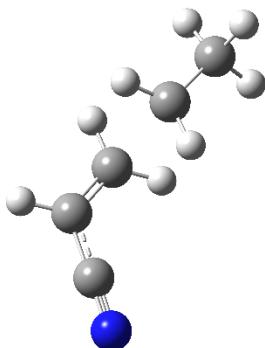
AT_AN



C	-0.016936	0.000000	0.009827
H	0.047998	0.000000	1.093387
H	0.914396	0.000000	-0.547346
C	-2.450058	0.000000	0.058431
N	-3.482559	0.000000	0.594790
C	-1.194059	0.000000	-0.627501
H	-1.247027	0.000000	-1.713688

Sum of electronic and thermal Enthalpies = -170.777421 Hartree

AT_AE-AN_ts1

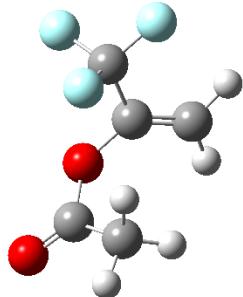


C	-0.006512	-0.011810	-0.006378
H	-0.004581	0.000975	1.077764
H	0.957621	0.000838	-0.502122
C	-2.401106	-0.479022	-0.086299
N	-3.450178	-0.604779	0.406922
C	-1.128170	-0.329034	-0.703658
H	-1.102895	-0.438555	-1.784866
C	0.229666	2.447531	0.170249
H	0.287536	2.625585	-0.900061
H	-0.750872	2.590842	0.614979
C	1.448275	2.652582	1.008444
H	2.345467	2.228823	0.541247
H	1.651455	3.726687	1.161296
H	1.339028	2.210541	2.005893

Sum of electronic and thermal Enthalpies = -249.869539 Hartree
 $\langle S^2 \rangle = 0.775047$

Imaginary frequency = i239 cm⁻¹

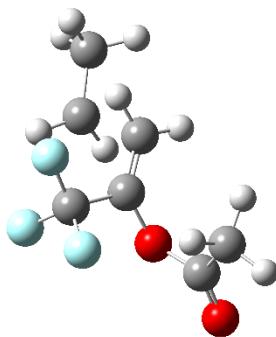
AT_FVAC1



C	0.047094	-0.050586	-0.049178
H	0.060004	-0.091448	1.034606
H	0.991971	-0.038583	-0.577626
C	-2.376513	2.331582	0.235594
H	-3.079388	3.086546	0.587962
H	-1.465552	2.370614	0.840975
H	-2.095899	2.538074	-0.800539
C	-3.047232	0.983014	0.353016
O	-4.130980	0.785670	0.825008
O	-2.338106	-0.126385	-0.107146
C	-1.103839	-0.030049	-0.713553
C	-1.197208	-0.042344	-2.222234
F	-1.954688	0.990970	-2.666711
F	-1.773684	-1.172868	-2.664151
F	0.015300	0.062719	-2.796598

Sum of electronic and thermal Enthalpies = -643.385521 Hartree

AT_AE-FVAC_ts4

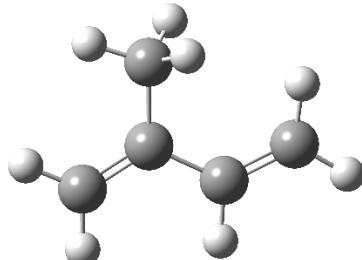


C	-0.011438	-0.001469	-0.000934
H	-0.006848	-0.009237	1.082696
C	3.511356	0.001551	0.241402
H	4.525091	-0.029579	0.641212
H	2.876498	-0.701282	0.789821
H	3.517466	-0.306807	-0.807790
C	2.998364	1.416985	0.376106
O	3.613948	2.333998	0.845156
O	1.702355	1.666612	-0.059491
C	0.929644	0.695939	-0.673484
C	0.985767	0.752750	-2.173691
F	2.263492	0.755600	-2.624814
F	0.402143	1.874376	-2.653964
F	0.353922	-0.300700	-2.731525
H	-0.589629	-0.759971	-0.512122
C	-2.007148	1.354600	0.097500
H	-1.578981	2.106076	0.755575
H	-2.000283	1.609837	-0.958537
C	-3.083360	0.460460	0.621756
H	-4.042223	0.999376	0.711726
H	-3.266053	-0.394035	-0.040915
H	-2.847040	0.075095	1.621052

Sum of electronic and thermal Enthalpies = -722.476023 Hartree
 $\langle S^2 \rangle = 0.774088$

Imaginary frequency = i291 cm⁻¹

Isoprene

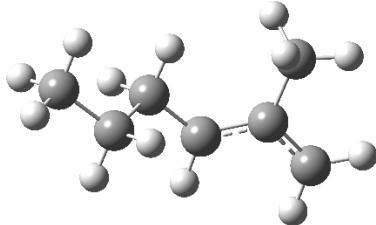


C	0.583816	-0.310213	0.972654
C	-0.566827	-0.805864	0.495775
H	1.384927	-0.965330	1.301884
H	-0.688450	-1.887857	0.442493
C	-1.715545	-0.023522	0.022926
C	-2.811268	-0.654682	-0.432938
H	-3.680072	-0.109340	-0.790835
H	-2.872094	-1.739864	-0.461920

C	-1.632167	1.483361	0.062964
H	-1.468438	1.844146	1.086353
H	-0.793511	1.850199	-0.542305
H	-2.550532	1.940611	-0.315960
H	0.770668	0.757050	1.052525

Sum of electronic and thermal Enthalpies = -195.193965 Hartree

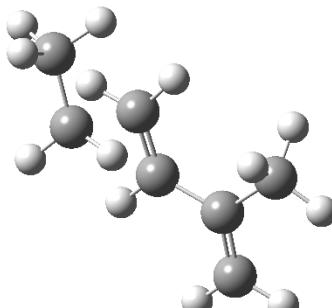
Iso-eth



C	0.073871	-0.069004	0.008830
C	-0.079690	-0.177416	1.528879
H	1.071425	-0.387225	-0.314765
H	-0.660599	-0.696917	-0.510602
H	0.686871	0.435534	2.022560
C	-1.474969	0.264769	2.024063
C	-1.610302	0.223952	3.515425
H	-1.648634	1.294402	1.667930
H	-0.918528	0.856017	4.073519
C	-2.510505	-0.545935	4.261112
C	-2.510382	-0.487063	5.646641
H	-3.200614	-1.075135	6.243044
H	-1.815500	0.153795	6.182243
H	-0.074216	0.963161	-0.332185
H	0.102763	-1.211217	1.850342
C	-3.507389	-1.457242	3.565137
H	-4.185991	-0.891698	2.915274
H	-3.004562	-2.201510	2.936038
H	-4.119080	-1.997458	4.293542
H	-2.240205	-0.355717	1.542708

Sum of electronic and thermal Enthalpies = -274.339251 Hartree
 $\langle S^2 \rangle = 0.780238$

Iso-eth-ts



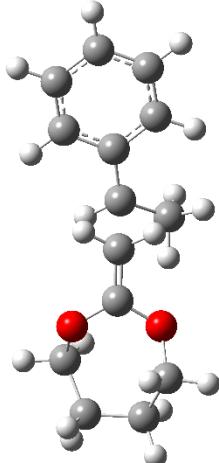
C	0.015246	0.007051	-0.029707
C	0.060701	0.003442	1.464949
H	1.027231	0.010676	-0.471408
H	-0.495300	-0.879709	-0.425215
H	0.338977	0.917858	1.981559
C	-2.289218	0.029606	2.155602

C	-2.386894	0.028579	3.513966
H	-2.359071	0.959237	1.600944
H	-2.372096	0.985724	4.034868
C	-2.461949	-1.149411	4.365906
C	-2.521862	-1.016243	5.708175
H	-2.587358	-1.877136	6.367317
H	-2.509666	-0.038228	6.182845
H	-0.499065	0.893949	-0.420179
H	0.334783	-0.914471	1.977817
C	-2.478730	-2.515773	3.719510
H	-3.334631	-2.624555	3.041238
H	-1.574742	-2.684009	3.120487
H	-2.539652	-3.308379	4.470745
H	-2.408057	-0.879273	1.574606

Sum of electronic and thermal Enthalpies = -722.476023 Hartree
 $\langle S^2 \rangle = 0.788268$

Imaginary frequency = i291 cm⁻¹

MDO-STYea



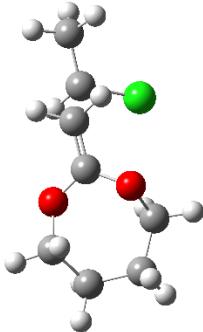
C	0.005086	-0.002648	-0.005682
C	-0.003243	0.007099	2.399762
C	2.340161	-0.003444	1.905485
H	-0.728950	-0.390565	-0.717617
H	-0.133662	1.082604	0.078891
H	3.186118	0.398896	2.470205
O	-0.330476	-0.639023	1.245382
O	1.184454	0.677067	2.436756
H	2.263531	-1.078031	2.114206
C	-0.908580	0.125023	3.427881
H	-0.517918	0.342828	4.415531
H	-1.790280	-0.502654	3.380095
C	-2.073862	1.971881	3.325766
C	-3.076177	1.794086	4.360550
C	-1.022040	3.046469	3.421755
C	-2.911721	2.275656	5.681214
C	-4.259147	1.065568	4.082620
H	-0.461522	2.997581	4.362816
H	-0.293046	2.950765	2.611725
H	-1.464857	4.052894	3.361006
C	-3.875654	2.044007	6.658747

H	-2.022509	2.843443	5.939008
C	-5.218609	0.835430	5.061110
H	-4.415143	0.685620	3.074695
C	-5.035490	1.323157	6.360224
H	-3.722555	2.432309	7.663047
H	-6.118039	0.277252	4.811876
H	-5.786071	1.146062	7.125645
H	-2.440781	1.786155	2.317166
C	1.420982	-0.352369	-0.458996
H	1.545093	-0.022309	-1.498994
H	1.513213	-1.446462	-0.460044
C	2.517794	0.268781	0.413747
H	2.541036	1.357151	0.270041
H	3.499729	-0.112984	0.103836

Sum of electronic and thermal Enthalpies = -694.980547 Hartree
 $\langle S^2 \rangle = 0.781096$

Imaginary frequency = i507 cm⁻¹

MDO-VCeA

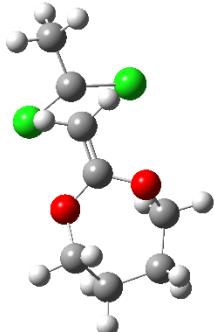


C	0.001409	-0.000366	-0.000126
C	0.000880	-0.000053	1.532971
C	1.399612	-0.000546	2.143560
C	0.862777	1.102381	-0.611893
C	2.817537	1.346692	0.755210
H	0.369070	-0.963623	-0.377508
H	-0.533230	0.882956	1.908251
H	2.009191	-0.833645	1.776208
H	0.587653	2.090876	-0.223136
H	-1.025616	0.115310	-0.371505
H	-0.541337	-0.880138	1.903569
H	1.343121	-0.070531	3.233142
H	0.749338	1.115226	-1.699614
O	2.087171	1.248210	1.894904
O	2.269034	0.867852	-0.396173
C	4.099912	1.803849	0.766550
H	4.498904	2.185940	1.697259
H	4.534725	2.152426	-0.162224
C	5.583489	0.024605	0.783627
H	5.268467	-0.439272	-0.146843
C	6.943274	0.646063	0.840087
H	7.081961	1.222415	1.762156
H	7.750528	-0.101662	0.793756
H	7.069773	1.325225	-0.012080
Cl	5.187055	-1.037120	2.151511

Sum of electronic and thermal Enthalpies = -923.607576 Hartree
 $\langle S^2 \rangle = 0.772107$

Imaginary frequency = i376 cm⁻¹

MDO-VDCea

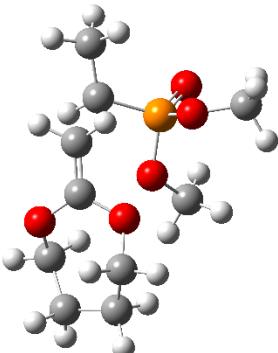


C	0.001410	-0.001769	0.003031
C	0.002101	0.002317	1.535742
C	1.401823	0.000868	2.141842
C	0.853936	1.106501	-0.609860
C	2.823960	1.329104	0.740809
H	0.374478	-0.962833	-0.373916
H	-0.531203	0.886227	1.909986
H	2.006346	-0.836680	1.776429
H	0.578658	2.091950	-0.213682
H	-1.026364	0.108525	-0.367531
H	-0.538732	-0.876915	1.910035
H	1.351167	-0.059971	3.231974
H	0.734524	1.124042	-1.696359
O	2.097781	1.245208	1.881617
O	2.264675	0.879444	-0.409951
C	4.116257	1.766237	0.755591
H	4.561508	2.088255	-0.177516
H	4.503430	2.170246	1.682126
C	5.578374	-0.002311	0.919235
C	6.933490	0.643477	0.844457
H	7.042323	1.368500	1.657557
H	7.745271	-0.092360	0.927045
H	7.039006	1.165661	-0.111987
Cl	5.252739	-0.769645	2.495926
Cl	5.240180	-1.097082	-0.438251

Sum of electronic and thermal Enthalpies = -1383.2117113 Hartree
 $\langle S^2 \rangle = 0.768794$

Imaginary frequency = i345 cm⁻¹

MDO-VPea

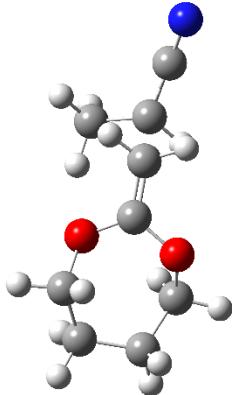


C	0.011119	0.006754	-0.004541
C	-0.002642	-0.002688	2.389941
C	2.342077	-0.008163	1.901963
H	-0.182398	1.077509	0.121143
H	-0.713927	-0.402828	-0.713461
H	3.188662	0.368335	2.482550
O	-0.273178	-0.676141	1.242330
O	1.192638	0.628623	2.492177
H	2.279807	-1.094394	2.044483
C	-0.943477	0.117769	3.373028
H	-0.622240	0.431135	4.357433
H	-1.832728	-0.493026	3.289321
C	-2.350891	1.928139	3.137611
C	-3.237509	1.757504	4.345142
P	-1.396112	3.417382	3.027702
H	-2.683361	1.932304	5.274211
H	-4.083054	2.461171	4.332268
H	-3.656221	0.744784	4.386022
O	-0.317470	3.229909	4.236613
O	-0.583551	3.181939	1.627328
O	-2.075136	4.747873	3.077170
C	0.273178	4.377838	4.860853
C	-0.058558	4.319135	0.928444
H	0.566767	4.073371	5.868501
H	-0.439060	5.205720	4.909321
H	1.166006	4.693588	4.308179
H	0.082544	4.014541	-0.111715
H	-0.752137	5.162444	0.980657
H	0.910058	4.613656	1.349814
H	-2.776682	1.632083	2.180829
C	2.506140	0.353244	0.427150
H	3.502444	0.027329	0.099791
H	2.485077	1.447578	0.344417
C	1.435458	-0.266211	-0.478038
H	1.573932	-1.354091	-0.533807
H	1.543302	0.120055	-1.500417

Sum of electronic and thermal Enthalpies = -1110.219162 Hartree
 $\langle S^2 \rangle = 0.769689$

Imaginary frequency = i335 cm⁻¹

MDO-ANea

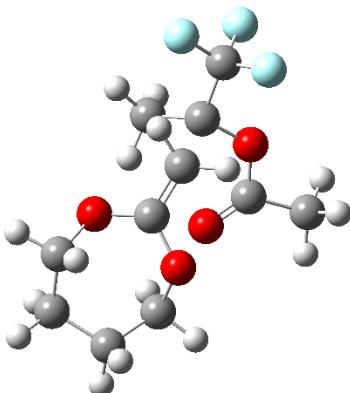


C	-0.002255	-0.001084	0.000901
C	-0.000913	0.001221	2.398705
C	2.351895	0.004819	1.891138
H	-0.732102	0.405989	-0.703867
H	-0.188674	-1.076283	0.112495
H	2.296365	1.090136	2.041817
O	-0.290538	0.668161	1.250235
O	1.197688	-0.628955	2.488141
H	3.198818	-0.382013	2.463692
C	-0.837241	0.082573	3.483567
H	-0.596771	-0.524135	4.347493
H	-1.883057	0.298557	3.302770
C	-0.505689	1.992560	4.581444
C	-0.941742	3.075908	3.623217
C	-1.262480	1.779482	5.757098
H	-2.024917	3.052333	3.465111
H	-0.685584	4.075791	4.002777
H	-0.453187	2.946216	2.652724
N	-1.917144	1.545758	6.699229
H	0.566959	1.866300	4.713427
C	2.498575	-0.348259	0.413527
H	2.477350	-1.442128	0.322987
H	3.491119	-0.021140	0.077113
C	1.419504	0.278126	-0.476732
H	1.520055	-0.097924	-1.503311
H	1.554629	1.366748	-0.523430

Sum of electronic and thermal Enthalpies = -556.252884 Hartree
 $\langle S^2 \rangle = 0.77462$

Imaginary frequency = i435 cm⁻¹

MDO-FVACea

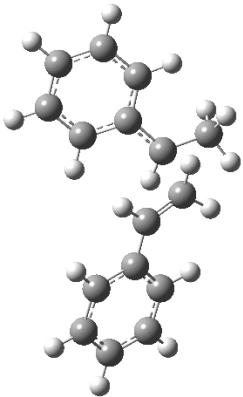


C	-0.000673	-0.007077	0.009046
C	0.000834	0.001708	1.541353
C	1.401173	0.013044	2.147570
C	0.822996	1.120883	-0.603474
C	2.727742	1.509743	0.797120
H	0.399084	-0.960119	-0.361257
H	-0.546284	0.876899	1.916500
H	2.032916	-0.787015	1.754305
H	0.494874	2.103213	-0.240503
H	-1.029896	0.073850	-0.365417
H	-0.526718	-0.886059	1.914546
H	1.348187	-0.093717	3.233991
H	0.739842	1.110260	-1.693752
O	2.236532	0.962416	-0.345011
O	2.064777	1.286693	1.954674
C	3.903555	2.209244	0.774871
H	4.198446	2.667881	-0.159516
H	4.236829	2.673369	1.694249
C	5.772920	0.883199	0.699930
C	6.801375	1.937544	0.398029
O	6.053378	0.442706	2.006329
C	5.318131	-0.504672	2.638311
C	5.880763	-0.750903	4.018815
H	6.924356	-1.075194	3.950893
H	5.865321	0.175865	4.601735
H	5.286569	-1.515563	4.520204
O	4.356952	-1.070459	2.164441
F	6.549088	2.527634	-0.795523
F	6.831919	2.908784	1.335186
F	8.064218	1.432894	0.320109
C	5.563700	-0.151990	-0.368424
H	4.638170	-0.703589	-0.206059
H	5.514143	0.342105	-1.342070
H	6.397632	-0.870250	-0.391659

Sum of electronic and thermal Enthalpies = -1028.867914 Hartree
 $\langle S^2 \rangle = 0.76938$

Imaginary frequency = i309 cm⁻¹

AT_H-STYts

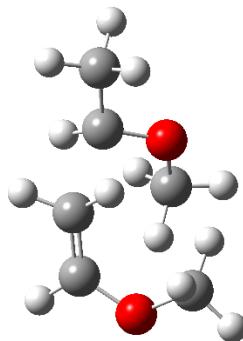


C	-0.003606	-0.000208	-0.002538
C	-0.004014	0.000380	1.394710
C	1.198347	-0.002107	2.095152
C	2.441237	-0.009759	1.424394
C	2.418725	-0.008976	0.011141
C	1.216197	-0.004144	-0.687379
H	-0.940822	0.003035	-0.552198
H	-0.944873	0.004219	1.939192
H	1.189707	-0.001101	3.182881
H	3.353277	-0.012696	-0.542628
H	1.227613	-0.003119	-1.774502
C	3.668270	-0.016411	2.203569
H	3.533732	0.046459	3.282311
C	4.954483	-0.001802	1.719749
H	5.162208	-0.242229	0.681080
C	5.655108	2.135040	1.358085
C	5.704804	2.747205	2.668736
C	6.901205	1.871591	0.556213
C	4.522902	3.269742	3.247543
C	6.894301	2.828061	3.430216
H	7.614709	1.229660	1.087456
H	6.662561	1.382769	-0.393687
H	7.429483	2.808098	0.319357
C	4.530772	3.840502	4.514456
H	3.595688	3.218796	2.681781
C	6.897986	3.402202	4.698302
H	7.823481	2.443719	3.019511
C	5.719066	3.911302	5.250568
H	3.608648	4.237216	4.931998
H	7.827528	3.456160	5.259698
H	5.725781	4.360081	6.240074
H	4.763166	2.360680	0.778515
H	5.778524	-0.165742	2.406497

Sum of electronic and thermal Enthalpies = -274.283078 Hartree
 $\langle S^2 \rangle = 0.792785$

Imaginary frequency = i311 cm⁻¹

AT_H-VETs

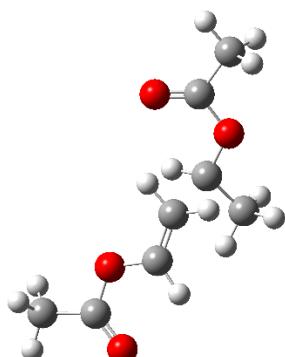


C	0.004755	-0.010920	-0.001842
H	0.002435	0.004287	1.082986
C	2.618775	-0.002600	1.136470
O	2.433917	-0.222578	-0.255386
C	1.143663	-0.310282	-0.700169
H	1.134723	-0.523955	-1.764547
H	2.172974	0.948507	1.453179
H	3.698193	0.022986	1.299857
H	2.180394	-0.818968	1.726721
H	-0.936912	-0.285061	-0.467555
C	-0.562953	2.185859	0.028137
C	-1.711310	2.223529	0.989359
O	0.506487	2.932768	0.472718
H	-2.127231	3.237761	1.096310
H	-2.516022	1.562464	0.649994
H	-1.395774	1.896255	1.987865
C	1.499409	3.211423	-0.504710
H	2.203836	3.910357	-0.046571
H	2.031562	2.302798	-0.807605
H	1.053586	3.681410	-1.393878
H	-0.795890	2.332196	-1.031552

Sum of electronic and thermal Enthalpies = -386.601053 Hartree
 $\langle S^2 \rangle = 0.776203$

Imaginary frequency = i424 cm⁻¹

AT_H-VACts1



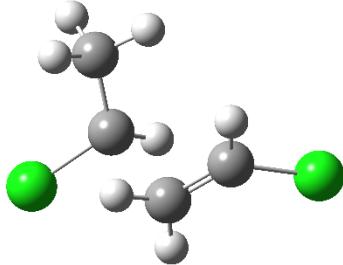
C	-0.046671	-0.027278	-0.151062
H	-0.110216	-0.166378	0.922709
C	2.430850	0.123219	-4.160517
H	3.411756	0.320199	-4.594044
H	2.085746	-0.871586	-4.462440
H	1.701274	0.848102	-4.535734
C	2.523253	0.202250	-2.657659

O	3.529614	0.388259	-2.013979
O	1.286202	0.025128	-2.099977
C	1.182890	0.034444	-0.718509
H	2.120004	0.168134	-0.193130
C	-1.001976	2.065820	0.080798
O	-2.123863	1.835984	0.875501
C	-3.235755	1.299975	0.289557
C	-4.341615	1.141962	1.303506
O	-3.298333	1.008918	-0.883782
H	-5.196613	0.655599	0.832856
H	-3.995079	0.548777	2.155865
H	-4.641916	2.122298	1.689433
H	-0.913522	-0.301165	-0.742629
C	0.005153	2.932837	0.755176
H	-0.345219	3.972336	0.855309
H	0.234267	2.564933	1.762057
H	0.931965	2.942899	0.172961
H	-1.235126	2.209534	-0.969595

Sum of electronic and thermal Enthalpies = -613.299467 Hartree
 $\langle S^2 \rangle = 0.775874$

Imaginary frequency = i370 cm⁻¹

AT_H-VCTs

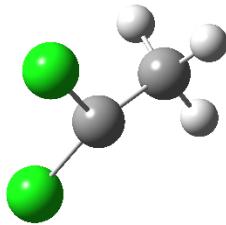


C	0.003075	0.010571	0.000390
H	0.005258	-0.001173	1.084596
H	0.970272	0.001824	-0.493064
C	-1.083386	-0.383468	-0.704596
H	-1.098469	-0.525336	-1.778559
Cl	-2.657251	-0.584585	0.030471
C	0.088471	2.330693	0.120356
C	0.087354	2.832629	-1.286009
Cl	1.529208	2.682162	1.071836
H	-0.799687	2.452922	-1.805240
H	0.059030	3.931925	-1.325876
H	0.979738	2.505164	-1.830829
H	-0.810878	2.445990	0.718065

Sum of electronic and thermal Enthalpies = -1076.837311 Hartree
 $\langle S^2 \rangle = 0.77729$

Imaginary frequency = i368 cm⁻¹

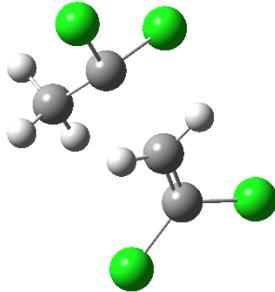
AT_VDC



C	-0.044870	-0.023870	0.001246
H	0.028800	0.019101	1.092240
H	0.974733	-0.102415	-0.407336
H	-0.485372	0.909675	-0.362060
C	-0.899336	-1.178628	-0.403796
Cl	-0.613148	-2.716559	0.358089
Cl	-1.463965	-1.242901	-2.048383

Sum of electronic and thermal Enthalpies = -998.308955 Hartree
 $\langle S^2 \rangle = 0.753615$

AT_H-VDCts

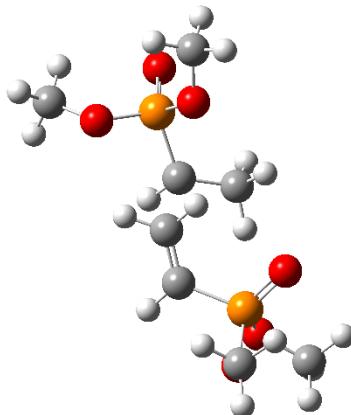


C	-0.000217	0.022793	0.006973
H	-0.011445	0.006262	1.090702
H	0.963721	-0.004046	-0.487258
C	-1.098396	-0.405837	-0.667838
Cl	-2.638768	-0.628751	0.115675
C	0.159059	2.320733	0.069345
C	-1.176056	2.813350	0.543924
Cl	0.580776	2.805570	-1.571895
H	-1.186115	3.908167	0.631808
H	-1.952654	2.514239	-0.165408
H	-1.406024	2.385075	1.523868
Cl	-1.103696	-0.656625	-2.385536
Cl	1.482744	2.553835	1.220961

Sum of electronic and thermal Enthalpies = -1996.038118 Hartree
 $\langle S^2 \rangle = 0.777135$

Imaginary frequency = i386 cm⁻¹

AT_H-VPts

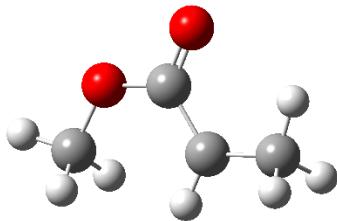


C	0.020835	0.014130	-0.005083
H	0.028056	-0.008769	1.080410
H	0.988672	-0.004226	-0.496113
C	-1.104561	-0.323698	-0.701590
H	-2.066981	-0.429033	-0.205025
P	-1.056020	-0.578313	-2.467853
O	-1.776231	-2.015334	-2.740800
O	-2.229865	0.412634	-2.976421
O	0.282938	-0.434619	-3.099844
C	-0.970699	-3.204423	-2.759468
H	-0.093828	-3.068953	-3.398295
H	-1.603694	-4.001579	-3.154586
H	-0.648028	-3.467010	-1.745151
C	-2.540843	0.459553	-4.381335
H	-3.238062	1.288429	-4.515178
H	-1.635579	0.636946	-4.969628
H	-3.011894	-0.476735	-4.695283
C	0.137876	2.314220	0.105367
C	0.151727	2.795983	-1.317812
P	1.563725	2.615817	1.144382
H	-0.761510	2.494239	-1.838268
H	0.211757	3.894609	-1.348103
H	1.010119	2.400143	-1.869096
O	1.311446	1.728586	2.489848
O	2.703234	1.764598	0.377625
O	1.895650	4.040278	1.430689
C	0.986824	2.370884	3.734999
C	4.071837	1.880545	0.805490
H	1.435388	3.365443	3.787539
H	1.381066	1.735802	4.531665
H	-0.100849	2.451664	3.841565
H	4.672343	1.358316	0.059018
H	4.369946	2.931264	0.859430
H	4.203681	1.405562	1.783311
H	-0.801744	2.430921	0.644733

Sum of electronic and thermal Enthalpies = -1450.062508 Hartree
 $\langle S^2 \rangle = 0.775847$

Imaginary frequency = i356 cm⁻¹

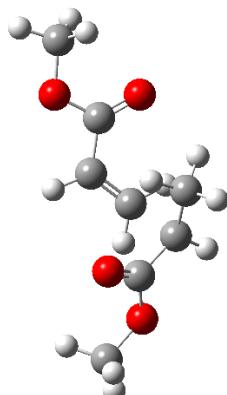
AT_MA



C	-0.619607	0.287086	0.167379
H	-1.342150	0.138882	0.971945
H	0.092349	1.071841	0.463435
H	-1.143771	0.670855	-0.720516
C	0.087328	-0.983386	-0.140469
H	0.837864	-0.983008	-0.923791
C	-0.221878	-2.198987	0.593503
C	1.431114	-3.401301	-0.724583
H	1.786314	-4.433131	-0.746335
H	1.016304	-3.146993	-1.707713
H	2.276149	-2.738775	-0.500387
O	-1.061657	-2.235155	1.482090
O	0.438508	-3.358781	0.296807

Sum of electronic and thermal Enthalpies = -306.926512 Hartree
 $\langle S^2 \rangle = 0.75956$

AT_H-MAts



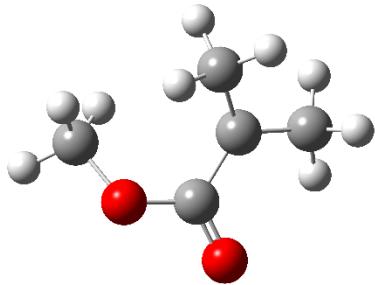
C	0.012031	0.007060	0.000509
H	0.009842	-0.010634	1.084863
C	1.188250	0.007137	-0.695861
H	2.137255	-0.221568	-0.221877
C	1.196585	0.260337	-2.144451
C	2.571802	0.509138	-4.041768
H	2.154764	1.487077	-4.298277
H	3.639426	0.478048	-4.261785
H	2.040226	-0.260118	-4.608939
O	0.210562	0.449903	-2.838563
O	2.460992	0.265067	-2.632743
C	-0.868666	-2.103894	-0.018098
C	-0.813216	-2.560233	-1.439240
C	0.025979	-2.723816	0.963580
H	-1.486633	-3.418463	-1.588241
H	-1.124184	-1.770349	-2.129542
H	0.197677	-2.885936	-1.696848
O	0.995586	-3.415292	0.700185
O	-0.332321	-2.401858	2.239526

C	0.508157	-2.952198	3.262836
H	0.090090	-2.601145	4.207156
H	1.539290	-2.605761	3.147161
H	0.499722	-4.045112	3.223399
H	-0.883868	0.370286	-0.493638
H	-1.809274	-1.725308	0.372553

Sum of electronic and thermal Enthalpies = -613.298948 Hartree
 $\langle S^2 \rangle = 0.778372$

Imaginary frequency = i403 cm⁻¹

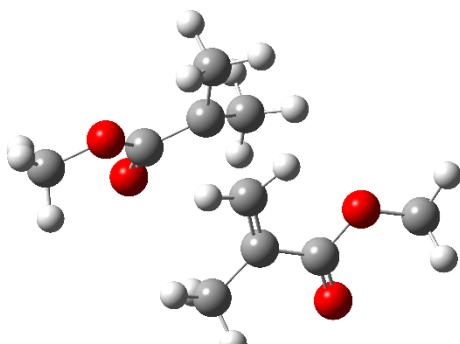
AT_MMA



C	-0.723808	0.290468	0.314995
H	-0.502970	0.277759	1.383522
H	-0.098947	1.047293	-0.180560
H	-1.766525	0.622650	0.190333
C	-0.518547	-1.055978	-0.301930
C	-0.368076	-2.201757	0.591232
C	1.235477	-3.375613	-0.808890
H	1.941118	-4.133053	-0.455834
H	0.912392	-3.636108	-1.822444
H	1.739776	-2.403520	-0.829646
O	-0.741552	-2.171408	1.753662
O	0.132427	-3.382542	0.099056
C	-0.673692	-1.188958	-1.786530
H	-1.514629	-0.572833	-2.132064
H	0.214137	-0.826931	-2.328955
H	-0.859529	-2.219987	-2.097029

Sum of electronic and thermal Enthalpies = -346.231305 Hartree
 $\langle S^2 \rangle = 0.759144$

AT_H-MMAts



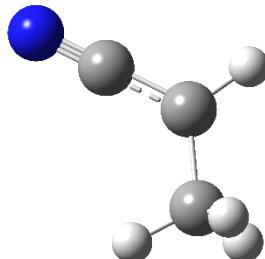
C	-0.001834	0.000357	-0.000008
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H	-0.006760	0.003663	1.097541
H	1.046770	-0.001844	-0.313820
H	-0.478315	0.924790	-0.339737
C	-0.722192	-1.205028	-0.534576
C	0.004024	-2.488130	-0.415096
C	-0.016442	-4.814091	-0.798990
H	-0.714213	-5.554351	-1.192888
H	0.252501	-5.051106	0.234117
H	0.895645	-4.788647	-1.401904
O	1.134886	-2.594242	0.027045
O	-0.705524	-3.558698	-0.869980
C	-1.995294	-1.148233	-1.055421
H	-2.404035	-2.014594	-1.561914
C	-3.569431	-1.376153	0.559531
C	-4.776057	-1.583853	-0.318361
C	-3.357458	-0.054526	1.181377
C	-3.097832	-2.550142	1.370505
H	-4.696155	-2.524643	-0.874134
H	-4.923486	-0.763855	-1.024744
H	-5.686733	-1.649368	0.297437
O	-2.643532	0.157641	2.148815
O	-4.024229	0.942601	0.533863
H	-2.919320	-3.422296	0.734759
H	-3.864269	-2.828414	2.110920
H	-2.185591	-2.310073	1.920098
C	-3.831695	2.255284	1.078446
H	-4.424534	2.922736	0.451569
H	-2.775328	2.537107	1.047859
H	-4.175216	2.297885	2.115715
H	-2.416538	-0.185008	-1.327440

Sum of electronic and thermal Enthalpies = -691.878201 Hartree
 $\langle S^2 \rangle = 0.778861$

Imaginary frequency = i437 cm⁻¹

AT_AN2

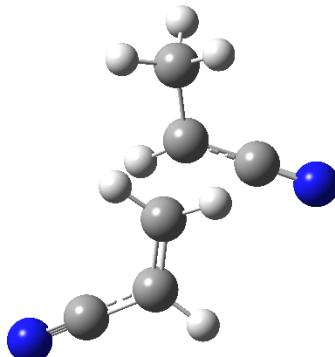


C	0.118701	0.287702	0.054572
C	0.014229	0.027775	1.524558
C	1.219262	-0.079238	-0.706251
H	0.901286	-0.479045	1.911566
H	-0.117593	0.969074	2.076370
H	-0.865794	-0.591835	1.747179
N	2.155249	-0.392693	-1.346787
H	-0.699145	0.787765	-0.457803

Sum of electronic and thermal Enthalpies = -171.35237 Hartree

$\langle S^2 \rangle = 0.766961$

AT_H-ANts

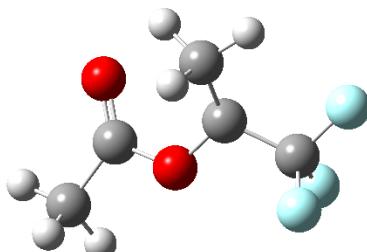


C	-0.002242	-0.016814	-0.007381
H	0.000934	0.006538	1.077648
H	0.963360	0.002773	-0.500850
C	-2.336592	-0.742064	-0.046229
N	-3.363020	-0.933920	0.474768
C	-1.091149	-0.507521	-0.682912
H	-1.053663	-0.667338	-1.757140
C	-0.080793	2.277559	-0.033838
C	0.966684	2.666772	0.976655
C	0.150594	2.540278	-1.403288
H	0.754126	2.216442	1.951038
H	1.969373	2.366077	0.657206
H	0.979270	3.757841	1.113738
N	0.365179	2.709353	-2.540175
H	-1.121023	2.321583	0.277958

Sum of electronic and thermal Enthalpies = -342.118447 Hartree
 $\langle S^2 \rangle = 0.789651$

Imaginary frequency = i436 cm⁻¹

AT_FVAC2

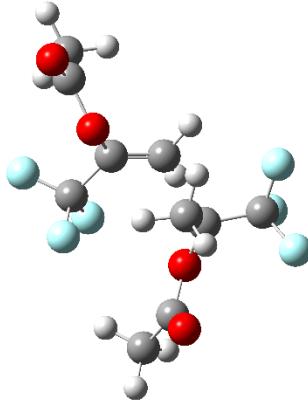


C	0.091471	0.179845	0.058270
C	0.074157	0.063903	1.543011
O	1.266047	0.084614	-0.655271
C	-0.902111	1.012098	-0.686271
H	0.723272	0.824522	2.006503
H	-0.942301	0.213262	1.912783
H	0.432630	-0.917975	1.861908
C	2.111865	-0.995610	-0.496478
F	-1.028507	0.610248	-1.966205
F	-0.557594	2.327871	-0.721154

F	-2.116040	0.938566	-0.099145
C	3.350879	-0.790238	-1.327918
O	1.862708	-1.941495	0.205721
H	3.079211	-0.611992	-2.373065
H	3.895280	0.093001	-0.976779
H	3.987301	-1.671944	-1.249447

Sum of electronic and thermal Enthalpies = -643.959989 Hartree
 $\langle S^2 \rangle = 0.753366$

AT_H-FVACts1

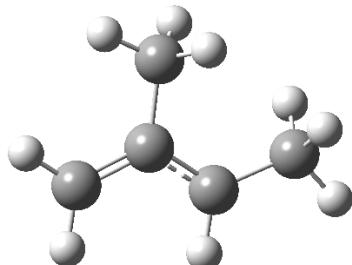


C	0.006916	-0.002224	-0.001692
H	0.000103	0.000428	1.083022
C	3.524816	-0.002705	0.397311
H	4.522524	-0.026193	0.835984
H	2.865602	-0.683558	0.945020
H	3.567994	-0.344833	-0.640532
C	3.015060	1.417299	0.467197
O	3.605889	2.348480	0.935935
O	1.737714	1.655546	-0.042360
C	0.989276	0.672108	-0.659215
C	1.105649	0.699495	-2.156697
F	2.398583	0.673088	-2.555706
F	0.566515	1.833223	-2.677939
F	0.472949	-0.342705	-2.728241
H	-0.516447	-0.804247	-0.505485
C	-1.888485	1.257337	-0.156696
C	-1.464161	2.637033	0.235855
O	-2.180044	0.955602	-1.477469
C	-2.786856	0.492653	0.781161
H	-2.315837	3.326690	0.246160
H	-1.013610	2.613608	1.231448
H	-0.725587	3.021141	-0.471767
C	-2.781615	1.855877	-2.345619
F	-2.886054	-0.808382	0.438606
F	-4.043128	0.998667	0.792100
F	-2.317019	0.552297	2.047997
C	-2.726979	1.299506	-3.743071
O	-3.257885	2.903851	-1.999976
H	-3.246166	1.975303	-4.422866
H	-1.680632	1.189072	-4.044415
H	-3.185702	0.306239	-3.773700

Sum of electronic and thermal Enthalpies = -1287.34092 Hartree
 $\langle S^2 \rangle = 0.777501$

Imaginary frequency = i387 cm⁻¹

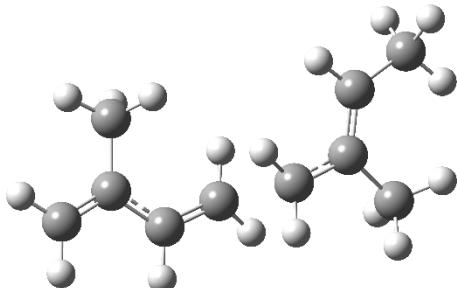
Radiso-conf1



C	-0.001579	-0.012390	-0.001581
H	0.005265	-0.017171	1.095725
H	1.047144	-0.017041	-0.324597
H	-0.459730	-0.946956	-0.337792
C	-0.743199	1.194229	-0.545535
C	-1.848449	1.006696	-1.358326
H	-2.203045	0.014808	-1.620021
H	-2.399019	1.851842	-1.762292
C	-0.296732	2.480755	-0.215951
H	-0.851072	3.324380	-0.622300
C	0.886777	2.778158	0.655081
H	1.817459	2.351467	0.251118
H	1.039684	3.856043	0.762037
H	0.773601	2.359378	1.666728

Sum of electronic and thermal Enthalpies = -195.769882 Hartree
 $\langle S^2 \rangle = 0.780829$

Iso-iso-3-add-ea



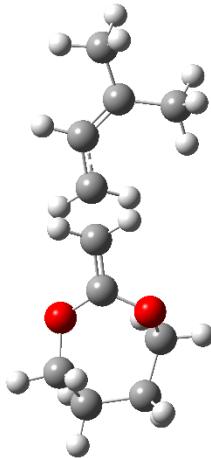
C	0.004109	0.003256	0.002197
H	0.006929	0.005431	1.102552
H	1.046933	0.006579	-0.326344
H	-0.440320	-0.956189	-0.299350
C	-0.785764	1.158132	-0.534394
H	-1.840754	1.165780	-0.256945
C	-0.345022	2.193547	-1.316791
C	1.098761	2.325057	-1.764109
H	1.159872	2.822572	-2.738242
H	1.601083	1.358148	-1.854407
H	1.682179	2.930480	-1.056632
C	-1.237813	3.248985	-1.685594
H	-2.300805	3.122985	-1.502048
H	-0.990663	3.881329	-2.532419
C	-0.947410	4.893430	-0.165240

H	0.101018	4.983400	-0.431476
H	-1.160161	4.198395	0.640544
C	-1.802949	5.936742	-0.443372
H	-1.470509	6.701626	-1.144976
C	-3.156112	6.081904	0.049992
C	-3.922850	7.126169	-0.345944
H	-4.934958	7.266036	0.022354
H	-3.550603	7.869547	-1.046384
C	-3.694012	5.058256	1.025606
H	-3.690980	4.050456	0.591531
H	-3.081006	5.014164	1.934734
H	-4.720186	5.294868	1.321130

Sum of electronic and thermal Enthalpies = -390.94843 Hartree
 $\langle S^2 \rangle = 0.812313$

Imaginary frequency = i515 cm⁻¹

MDO-iso-2-add-ea



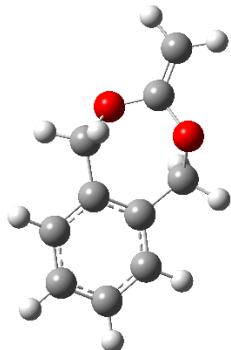
C	-0.002426	0.002513	-0.000032
C	-0.002206	0.001301	1.533311
C	1.396898	-0.001781	2.145842
C	0.865606	1.099884	-0.612251
C	2.793247	1.395376	0.776229
H	0.360844	-0.963039	-0.376171
H	-0.532818	0.884997	1.911694
H	2.004401	-0.828491	1.756708
H	0.583308	2.092800	-0.239547
H	-1.029252	0.121545	-0.371011
H	-0.546767	-0.878207	1.902132
H	1.335724	-0.099081	3.233628
H	0.766916	1.099244	-1.701793
O	2.078136	1.252304	1.928679
O	2.266469	0.868265	-0.366925
C	4.092195	1.849600	0.792564
H	4.493284	2.236206	-0.136628
H	4.441092	2.318210	1.704564
C	5.491112	0.201813	0.928425
H	5.130713	-0.321233	0.047485
H	5.117511	-0.202852	1.865050
C	6.816278	0.739028	0.878628
H	7.218269	0.901473	-0.123498
C	7.613154	1.134595	1.917833

C	8.973825	1.729281	1.665973
H	9.200340	1.794377	0.596548
H	9.056149	2.742137	2.089859
H	9.768153	1.135093	2.143370
C	7.228510	1.006528	3.368297
H	6.246745	0.548371	3.512557
H	7.964688	0.402506	3.919772
H	7.211852	1.990494	3.860643

Sum of electronic and thermal Enthalpies = -580.663245 Hartree
 $\langle S^2 \rangle = 0.790283$

Imaginary frequency = i570 cm⁻¹

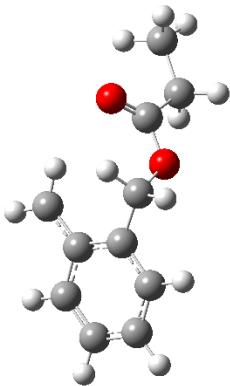
BMDO-conf1



C	-0.045459	-0.410962	0.041660
C	-0.005021	-0.375184	1.435018
C	1.191585	-0.066400	2.080886
C	2.357899	0.204581	1.357016
C	2.316713	0.170256	-0.047234
C	1.112184	-0.141262	-0.687369
H	-0.970037	-0.651068	-0.476005
H	-0.898947	-0.581924	2.016937
H	1.222631	-0.032764	3.168021
H	1.082856	-0.174462	-1.774561
C	3.524258	0.512589	-0.894828
H	3.449707	0.014525	-1.865391
H	3.578794	1.594301	-1.076418
O	4.774693	0.064578	-0.341043
C	3.640135	0.473751	2.116787
H	4.200688	-0.456927	2.277136
H	3.408248	0.896979	3.097973
O	4.501799	1.439944	1.488492
C	5.348173	0.926453	0.548643
C	6.642277	1.244165	0.502880
H	7.085795	1.835337	1.293381
H	7.255119	0.912371	-0.325024

Sum of electronic and thermal Enthalpies = -537,307998 Hartree

radBMDO-conf1

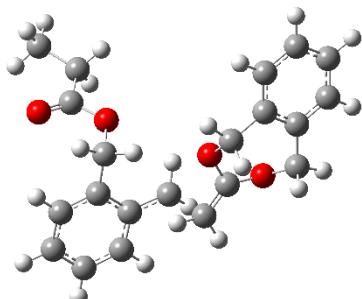


26

C	-0.117314	-0.331969	0.177220
C	-0.008213	-0.179010	1.565930
C	1.228151	0.057331	2.141791
C	2.419095	0.153295	1.359262
C	2.287897	-0.003109	-0.065084
C	1.032587	-0.240009	-0.615958
H	-1.083115	-0.519683	-0.282685
H	-0.893307	-0.247812	2.192933
H	1.312510	0.171734	3.219684
H	0.946787	-0.356877	-1.694138
C	3.650542	0.385827	1.996804
H	3.687157	0.487441	3.076996
H	4.588039	0.466062	1.460088
C	3.482045	0.084837	-0.977122
H	4.355974	-0.438408	-0.585578
H	3.236853	-0.323242	-1.961639
O	3.846609	1.477336	-1.203787
C	5.114566	1.858145	-0.928290
C	5.303564	3.330884	-1.240320
H	5.027445	3.487078	-2.290974
H	4.559942	3.889198	-0.657220
O	5.974242	1.122585	-0.487883
C	6.721254	3.822515	-0.955483
H	6.810407	4.887465	-1.193625
H	6.981846	3.680679	0.097499
H	7.455445	3.272365	-1.551508

Sum of electronic and thermal Enthalpies = -577,200122 Hartree
 $\langle S^2 \rangle = 0.784$

BMDO-BMDO-add-ea



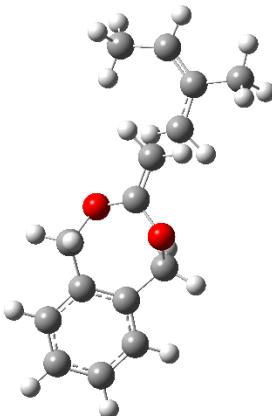
C	-0.004862	-0.029783	0.022153
C	0.004587	-0.025646	1.420814
C	1.211233	-0.008254	2.108487

C	2.454750	0.003288	1.430312
C	2.431005	0.019035	0.002999
C	1.208711	-0.009927	-0.670049
H	-0.944056	-0.051331	-0.523370
H	-0.931719	-0.041996	1.973295
H	1.213316	-0.013291	3.196403
H	1.212900	-0.030038	-1.756544
C	3.710043	0.067076	-0.794304
H	3.505516	0.324752	-1.834848
H	4.431195	0.772942	-0.377116
O	4.418366	-1.208624	-0.768384
C	4.079261	-2.109734	-1.717351
C	4.842151	-3.406887	-1.517774
H	5.907735	-3.162553	-1.425846
H	4.549038	-3.810637	-0.539557
O	3.277437	-1.900870	-2.603517
C	3.682637	0.046973	2.179025
H	3.631356	-0.171036	3.241844
H	4.604861	-0.259298	1.700417
C	4.214633	2.203824	2.424464
H	3.587955	2.513043	1.598346
H	3.796136	2.267031	3.420972
C	5.572115	2.329588	2.286387
C	7.148118	3.288464	0.735549
C	7.490709	2.935143	3.603797
C	8.502182	2.913753	1.289708
H	6.828817	4.273812	1.107349
H	7.184195	3.337098	-0.355298
C	8.667971	2.743164	2.676986
H	7.782153	2.724320	4.635553
H	7.122011	3.971428	3.562375
O	6.113429	2.330026	1.027285
O	6.391169	2.043063	3.342874
C	9.597813	2.745311	0.441390
H	9.466390	2.867520	-0.631286
C	9.925608	2.408271	3.181559
H	10.050690	2.266733	4.252624
C	10.856648	2.422856	0.954681
H	11.700293	2.296196	0.281906
C	11.020894	2.253927	2.327934
H	11.993860	1.994325	2.735822
C	4.590851	-4.420620	-2.632137
H	4.905641	-4.024666	-3.602593
H	5.145129	-5.345441	-2.440635
H	3.526849	-4.662735	-2.707611

Sum of electronic and thermal Enthalpies = -1114,488948 Hartree
 $\langle S^2 \rangle = 0.78745$

Imaginary frequency = i523 cm⁻¹

BMDO-iso-trans-add-ea

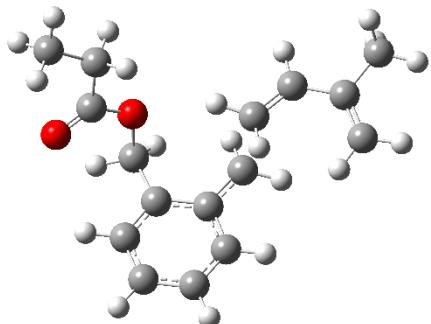


C	-0.013400	-0.022273	0.011384
C	-0.006787	-0.019602	1.405713
C	1.209292	-0.007937	2.087618
C	2.428086	-0.003455	1.399933
C	2.421646	-0.003678	-0.005724
C	1.196366	-0.016618	-0.681760
H	-0.952645	-0.032678	-0.534653
H	-0.940902	-0.022500	1.960601
H	1.214959	-0.000633	3.175701
H	1.192223	-0.023711	-1.769783
C	3.697013	0.067905	-0.819175
H	3.529419	-0.361826	-1.810509
H	4.013415	1.110839	-0.952505
O	4.792899	-0.688123	-0.265302
C	3.711035	-0.056835	2.204078
H	4.018330	-1.097760	2.374969
H	3.555726	0.410657	3.180440
O	4.808375	0.661892	1.614401
C	5.523470	-0.042470	0.688715
C	7.456553	1.952032	-0.356426
H	6.888422	2.599873	0.303022
H	6.971980	1.754267	-1.309428
C	8.892923	2.014677	-0.344820
C	9.603336	1.334463	-1.500147
H	9.308637	1.773835	-2.462307
H	10.691458	1.414766	-1.412325
H	9.350631	0.266378	-1.551815
C	9.633468	2.585784	0.651539
H	10.718682	2.542620	0.558249
C	9.127103	3.288562	1.877031
H	9.506136	4.319736	1.927448
H	8.035502	3.334432	1.923238
H	9.474929	2.789290	2.793309
C	6.888383	0.080495	0.607217
H	7.395469	-0.551733	-0.111815
H	7.427139	0.318577	1.516147

Sum of electronic and thermal Enthalpies = -733,057695 Hartree
 $\langle S^2 \rangle = 0.790479$

Imaginary frequency = 1558 cm⁻¹

BMDO-prop-iso-ea



C	0.011666	-0.011204	-0.007762
C	0.002446	-0.003028	1.391588
C	1.199034	0.009498	2.093226
C	2.455324	0.010743	1.431400
C	2.449194	-0.004323	0.001588
C	1.233552	-0.012044	-0.684790
H	-0.920394	-0.018292	-0.565442
H	-0.940826	-0.008799	1.931784
H	1.188011	0.012034	3.180868
H	1.250070	-0.007688	-1.771089
C	3.728780	-0.018940	-0.793440
H	4.496210	-0.641689	-0.329801
H	3.546695	-0.369967	-1.809961
O	4.345197	1.302321	-0.872788
C	3.985430	2.075639	-1.927323
O	3.229293	1.718698	-2.805008
C	4.658615	3.433146	-1.850608
H	4.283692	3.933642	-0.947501
H	5.729198	3.272130	-1.674018
C	3.653899	0.063487	2.212115
H	3.587136	-0.126795	3.278024
H	4.618513	-0.138018	1.763325
C	4.122972	2.310954	2.526904
H	4.334764	2.397941	1.467188
H	3.090581	2.481194	2.816108
C	5.139036	2.408523	3.441693
H	6.161149	2.403619	3.062178
C	5.009838	2.447330	4.894594
C	6.291056	2.699025	5.661919
H	7.040181	1.926728	5.442185
H	6.737922	3.661542	5.380664
H	6.120835	2.707306	6.742398
C	3.842360	2.262025	5.548997
H	3.790120	2.305683	6.632875
H	2.909328	2.066100	5.028727
C	4.414124	4.287082	-3.093361
H	3.344084	4.446227	-3.253970
H	4.898914	5.262976	-2.987071
H	4.811552	3.800695	-3.989461

Sum of electronic and thermal Enthalpies = -772,380367 Hartree
 $\langle S^2 \rangle = 0.804259$

Imaginary frequency = i434 cm⁻¹

² Gaussian 16, Revision A.03, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.

³ A. D. Becke, *Journal of Chemical Physics*, 1993, **98**, 5648-5652. R. Ditchfield, W. J. Hehre, and J. A. Pople, *Journal of Chemical Physics*, 1971, **54**, 724-728.