Supporting Information for

In Situ and Real-Time Visualization of Mechanochemical Damage in Double-Network Hydrogels by Prefluorescent Probe via Oxygen-Relayed Radical-Trapping

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1. Supplementary Text

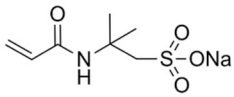
1.1 *Materials.*

2-Acrylamido-2-methylpropanesulfonic acid sodium salt (NaAMPS; Toagosei Co., Ltd.), 2-acrylamido-2-methyl-1-propanesulfonic acid (AMPS; Toagosei Co., Ltd.), 2-(acryloyloxy)ethyl trimethyl ammonium chloride (ATAC; Osaka Organic Chemical Co., Ltd.), and acrylamide (AAm; Junsei Chemical Co. Ltd.) are used as monomers. *N*,*N*′-methylenebis(acrylamide) (MBAA; Wako Pure Chemical Industries, Ltd.), 2,4-divinylbenzenesulfonic acid sodium salt (DVBS; Tosoh Finechem Corporation) and Poly(ethylene glycol) diacrylate ($PEGDA_{250}$; number average molecular weight M_n 250; Sigma-Aldrich Co., LLC.) are used as crosslinkers. *α*-ketoglutaric acid (*α*-keto; Wako Pure Chemical Industries, Ltd.) and Benzophenone (BP; KANTO Chemical Co., Inc.) are used as radical initiators. *N*-methyl formamide (NMF; Fujifilm Wako Pure Chemical Industries, Ltd.) and tetrahydrofuran (THF; Wako Pure Chemical Industries, Ltd.) are used as the organic solvents. All the chemicals are used as received. Milli-Q water (resistivity: 18.3 MΩ·cm) is used in experiments for synthesis and swelling equilibrium.

1.2 *Gel Synthesis.*

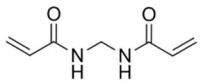
DN gels consisting of different first network and the same PAAm as the second network are synthesized by a two-step sequential network formation technique as previously reported.[1] The first network gels are denoted as X-Y (*m*-*c*-*i*) according to the polymers (X) and crosslinkers (Y), where *m* represents the monomer concentration (M), *c* represents the crosslinker concentration (mol%) and *i* represents the initiator concentration (mol%), respectively (**Figure 2a**). The first network gels of **DN1**, **DN2**, **DN3** and **DN4** are prepared from aqueous solutions containing certain amount of the corresponding monomer, crosslinker and *α*-keto initiator; because the crosslinker of $PEGDA_{250}$ is hydrophobic, the first network gel of **DN5** is prepared from the NMF organic solution containing certain amount of the AMPS monomer, $PEGDA_{250}$ crosslinker and BP initiator. To perform the polymerization, the first network precursor solutions are purged in an argon atmosphere to remove dissolved oxygen, and poured into glass molds consisting of two pieces of glass plates separated by a silicone rubber spacer. The glass molds are afterward irradiated with UV light (365 nm) for 8 h. The synthesized first network gels are then immersed in aqueous solutions of 2.0 M AAm monomer, containing 0.01 mol% MBAA and 0.01 mol% *α*-keto, for one day until swelling equilibrium was reached. The polymerization for the second network is then performed again by 365 nm UV irradiation for 8 h. The as-prepared DN gels are then immersed in pure water to reach equilibrium to obtain the virgin DN gels.

1.



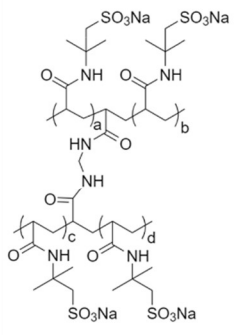
1.0 M NaAMPS
(monomer)

+



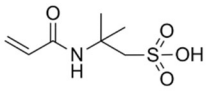
3 mol% MBAA
(crosslinker)

1 mol% *α*-keto initiator
UV irradiation (365 nm) for 8 h



1st network for **DN1**

2.



1.0 M AMPS
(monomer)

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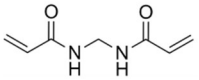
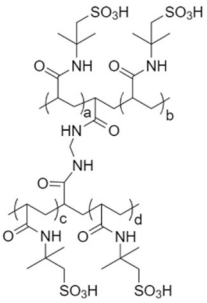


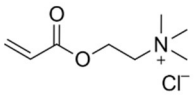
3 mol% MBAA
(crosslinker)

1 mol% *α*-keto initiator
UV irradiation (365 nm) for 8 h



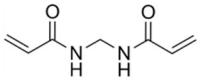
1st network for **DN2**

3.



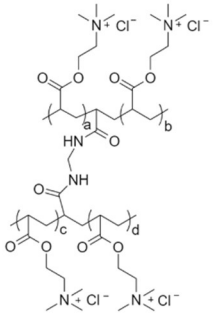
2.0 M ATAC
(monomer)

+



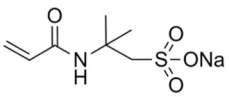
0.75 mol% MBAA
(crosslinker)

1 mol% *α*-keto initiator
UV irradiation (365 nm) for 8 h



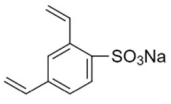
1st network for **DN3**

4.



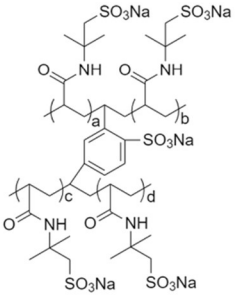
1.0 M NaAMPS
(monomer)

+

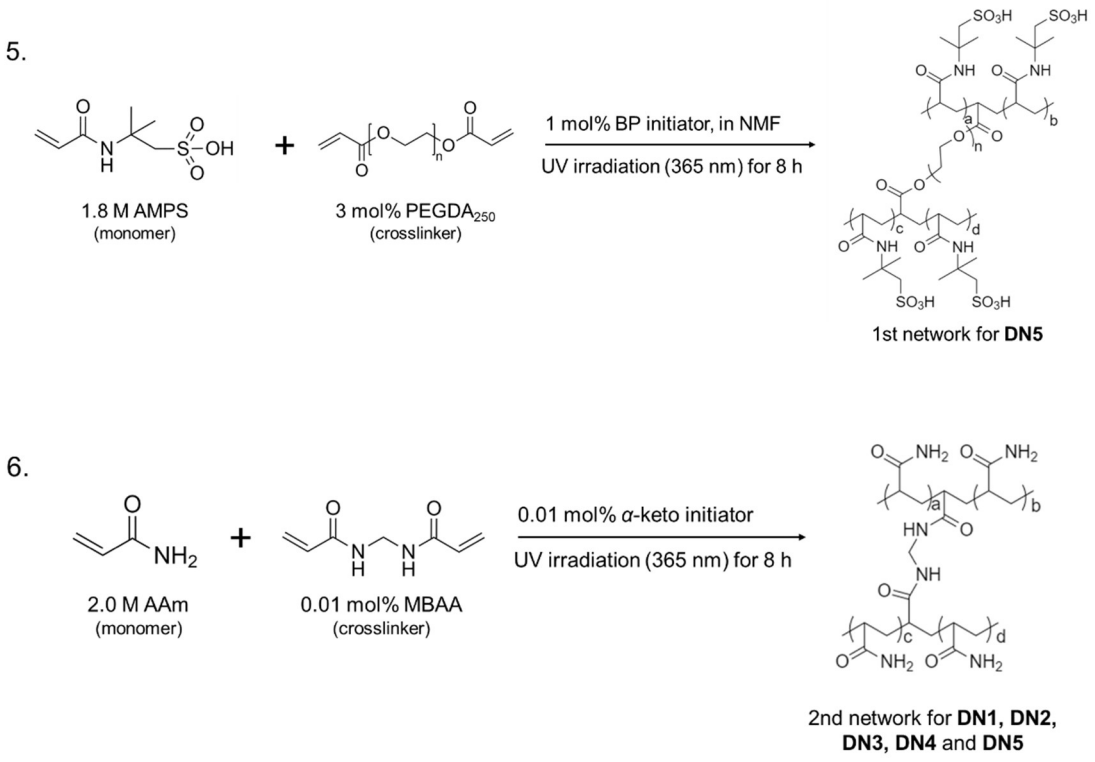


4 mol% DVBS
(crosslinker)

1 mol% *α*-keto initiator
UV irradiation (365 nm) for 8 h



1st network for **DN4**



1.3 ***Procedure for the prefluorescent molecule P treatment.***

The hydrophobic prefluorescent molecule **P** is dissolved in THF solvent in different concentrations $\mathbf{c_p}$ (0.01, 0.1, 0.4 and 1.0 mg/mL). We then immerse the DN virgin gels into the **P**/THF solutions for 24 hours. After that, the DN gels are directly immersed back into pure water, and the final gels are denoted as **DN-P-$\mathbf{c_p}$** gels according to various concentration $\mathbf{c_p}$ (**Figure 4c**).

1.4 ***Mechanical Tests.***

Uniaxial tensile tests are performed on samples cut into dumbbell shapes (gauge length: 12 mm and width: 2 mm) using a commercial tensile tester (Instron 5965, Instron Co.). The nominal stress σ-tensile strain ε curves are recorded while the sample gels are stretched at a constant velocity of 100 mm/min (strain rate of 0.14 s^{-1}). To reveal the energy dissipation behaviors, the cyclic tensile tests are next conducted using the same experimental setup of tensile tests. The samples are stretched to a pre-set stretch ratio, followed by unloading at the same strain rate, and the sequential loading–unloading cycles with increased stretch ratios are performed without waiting time.

1.5 ***Preparation of deoxygenated DN hydrogels.***

The deoxygenated DN hydrogels are prepared by putting the DN hydrogels into a negative-pressure vacuum chamber and performing 10 times vacuum cycling (at -80% vacuum degree) and Argon gas backfilling. After that, these deoxygenated DN hydrogels are transferred into glove box filled with Argon gas for at least 2 hours before using.

1.6 *Fluorescence measurements.*

Fluorescence microscopic spectra were recorded on a Photonic Hamamatsu PMA-12 Multichannel Analyzer at room temperature. The excitation light having 365 nm of maximum intensity.

1.7 *Spatial visualization by CLSM.*

Fluorescence microscopic measurements are carried out using a laser scanning confocal microscope (Nikon A1 Rsi and Ti-E, Nikon Co.). The excitation laser wavelength was 402.5 nm. Fluorescence emission is measured within a wavelength range of 451–471 nm. The excitation laser intensity is tuned to appropriate values to obtain clear images.

1.8 *DFT calculations for bond rupture under force and the probe-radical coupling reaction.*

All of the calculations were performed at the DFT level of theory with the B3LYP hybrid functional[2] as implemented in Gaussian 16.[3] To describe the dispersion properly, an explicit dispersion correction term developed by Grimme and co-workers,[4] was also employed in the DFT calculations. The Def2SVP basis set[5] was used for all the atoms involved in this study during both the geometry optimization and the single-point calculation processes. To describe the open-shell singlet species involved in the bond homolysis process, the unrestricted DFT, as well as the procedure to test and optimize the wavefunction were used in this work.[6] To properly simulate the solvation environment, the implicit solvation model, IEFPCM,[7] is applied to all the calculations involved in this study with water as the solvent (ε = 78.3553). For the mechanoradicals formation process, all of the structures were fully optimized with the constraint of external tensile force. The electronic energies (E_F), as well as the Gibbs free energies (G_F), were also computed with the consideration of force. The external tensile force is properly simulated through our AFIR method. For the probe-radical coupling reaction, since it is conducted under force free conditions, all of the minima and transition states were fully optimized without any constraints. The electronic energies and free energies associated with this process are labelled as E_0 and G_0. All the geometries shown in this article is visualized by the CYLview software.[8]

The first step of our theoretical study for the probe-mechanoradical interaction is to pinpoint the mechanoradical species that might be generated from the DN-hydrogel system once treated with external force. Three model molecules with different cross-linker molecules (MBAA, PEG and DVBS) were constructed to represent the DN-hydrogels used in our experiments. Note that the -NHR groups on the PAMPS chains were simplified to -NH_2 groups (which is equivalent to PAAm) to reduce the computational costs. The tensile force up to 4000 pico-Newton, which is simulated by our AFIR method,[9] is added diagonally to stretch both the PAAm chain and the cross-linker molecule (**Figure S2** to **Figure S4**).[10]

In MBAA case, three possible cleavage sites (as labelled A, B and C in **Figure 2b(i)** and **Figure S2**) were considered. Our calculations suggested the C-C bond near the joint area (which connects the polymer chain and the cross-linker molecule) is prone to break under tensile force. Similar situation was also found in the PEG case (see **Figure 2b(ii)** and **Figure S3**). However, it is changed in the case of DVBS, as the degradation of DVBS molecule was found. Interestingly, the electronic effect of $-SO_3H$ group on the benzene ring cannot be neglected. While the breaking of $C(sp^2)$-$C(sp^3)$ bond para to the $-SO_3H$ has a Gibbs barrier of +107.2 kJ/mol, the $C(sp^2)$-$C(sp^3)$ bond next to it has a barrier of only +56.5 kJ/mol under the force of 4000 pN. Thus, the homolytic cleavage of C-C covalent bond is expected to offer a secondary carbon radical and a phenyl radical in this case (**Figure 2b(iii)** and **Figure S4**).

Table S1a. Computed free energy barriers of bond cleavage in **PAAm-MBAA** at F_τ = 4000 pN

Cleavage Site	C-C (**A**)	C-C (**B**)	N-C (**C**)
Barrier $\Delta G^{\ddagger}_{F4000}$	+51.7 kJ·mol^{-1}	+68.1 kJ·mol^{-1}	+69.8 kJ·mol^{-1}

Table S1b. Computed free energy barriers of bond homolysis in **PAAm-PEG** at F_τ = 4000 pN

Cleavage Site	C-C (**A**)	C-C (**B**)	O-C (**C**)	O-C (**D**)
Barrier $\Delta G^{\ddagger}_{F4000}$	+49.4 kJ·mol^{-1}	+60.9 kJ·mol^{-1}	+61.9 kJ·mol^{-1}	+94.9 kJ·mol^{-1}

Table S1c. Computed free energy barriers of bond homolysis in **PAAm-DVBS** at F_τ = 4000 pN

Cleavage Site	C-C (**A**)	C-C (**B**)	C-C (**C**)
Barrier $\Delta G^{\ddagger}_{F4000}$	+61.0 kJ·mol^{-1}	+56.5 kJ·mol^{-1}	+107.2 kJ·mol^{-1}

Since the possible mechanoradicals were all located, we then started the calculations concerning the coupling reaction between the NO-luminophore probe and the radicals. As what are shown from **Figure S5** to **Figure S9**, all of the probe-radical coupling reactions were found having very little barrier or even barrierless. Meanwhile, it was revealed that the coupling reaction between two NO-probe radicals is not energetically favoured. Therefore, it is theoretically proved that, once the mechanoradicals is formed in the DN-hydrogel system, it will immediately react with the probe to trigger the luminescence.

1.9 *Comparison between our proposed OH radical generation mechanism and the generation mechanism of H_2O_2 proposed by Grzybowski et al.*

Grzybowski and co-workers proposed that hydrogen peroxide (H_2O_2) is formed on squeezing polymers (*Angew. Chem., Int. Ed.*, **2012**, *51*, 3596–3600.). In fact, there is no contradiction between the Angewandte paper by Grzybowski et al. and ours. Moreover, the Angewandte paper can be treated as the experimental proof to support our findings that hydroxyl radicals (·OH) are formed through the reaction between mechanoradical and O_2 molecule. Grzybowski et al. proposed independently in their pioneering work that the mechanoradicals would generate ·OH radicals through reactions with oxygen, and these ·OH radicals would eventually produce H_2O_2 (see Figure S1 in the supporting information from Grzybowski, B. A et al., *Angew. Chem., Int. Ed.*, **2012**, *51*, 3596–3600.). In our calculations (see **Figure 3** in the manuscript), we also found that ·OH radical can been formed via a series of intramolecular reactions. It should be noted that the C-O bond formed is very strong and the dissociation after the initial HAT reaction to generate an ·OOH radical is not possible. We hereby discuss the difference between our work and Grzybowski's work as follows.

1. As we can see from **Figure S10**, once the ·OH radical is formed, it can readily react with the C-H bonds from the polymer chain and eventually leaves a carbon-centered radical and a water molecule. In our case, this carbon-centered radical can react with the NO-probe to trigger the fluorescence change. That is, the relayed carbon-centered radical is eventually consumed by the NO-probe to terminate the ·OH radical. However, in Grzybowski's work, no NO-probe exists in the reaction system, which means the carbon-centered radical, even if generated (e.g., in the PVC case in Grzybowski's work), will have to react with another O_2 and finally deliver another ·OH radical. Therefore, it is expected that the equilibrium concentration of ·OH radical is generally much higher in Grzybowski's reaction system.

2. We notice that the polymer used in our case and Grzybowski's work are completely different. In our case, it is PAMPS while they were PDMS and PVC in Grzybowski's work. We have computed the energy change following the H_2O_2 formation process using different polymers. For the possible pathway for the formation of H_2O_2, generally, it is the carbon-centered radical reacting with water and another ·OH radical to deliver a H_2O_2 molecule. It is clear from **Figure S11** that the barrier of PDMS is the lowest and then it comes PVC. The polymer we used in our experiments, PAMPS, has the largest barrier of 102.8 kJ/mol, implying a very slow reaction under room temperature. Such calculation results are also consistent with Grzybowski's experimental observations that PDMS is a better polymer to efficiently generate H_2O_2 than PVC.

Concisely speaking, in our case, it is the existence of the NO-probe and the polymer used to prevent the formation of H_2O_2 from ·OH radicals in a short timescale of several seconds (our experimental timescale). However, both our theoretical calculations and the experimental work conducted by the Grzybowski group support

the formation of ·OH radical in the system from the addition of oxygen to mechanoradicals, which is a key species considered to promote the fluorescence change in our work.

1.10 *The promoted mobility of ·OH radical via huge hydrogen-bond network with water molecules.*

We show in this section that the water molecules can promote the mobility of ·OH radicals via a hydrogen transfer mechanism. The water molecules play a critical role in the mobility of OH radicals, thus enhancing the reaction probability between the probe **P** and the relayed carbon-centered radicals. Shown in **Figure S12** is our calculated barrier for the moving of ·OH radical via the rearrangement of hydrogen bonds, as well as a hydrogen atom transfer (HAT) reaction of hydroxyl radical to abstract the H atom from water. These barriers are as low as only +15.2 kJ/mol and +19.1 kJ/mol respectively, suggesting a super rapid reaction with the timescale of pico-seconds under room temperature. Based on the literature (Codorniu-Hernández, E. et al., *JACS*, 2012, 134 (1), 532-538.) and our calculations shown in **Figure S12**, it is known that water promotes the diffusion of ·OH radical in the aqueous solution via its huge hydrogen-bond (HB) network. The ·OH can be either moved via the rearrangement of hydrogen bonds or HAT reaction. The promoted mobility of ·OH radical makes it possible to travel a considerably long distance in a relatively short period of time, and eventually trigger the fluorescence at remote area where the probe P stays.

1.11 *The discussion on that the direct coupling between ·OH and TEMPO cannot compete with the coupling reaction between TEMPO and the carbon-centered radical.*

We discuss in this section that the direct coupling between ·OH radical and TEMPO cannot compete with the coupling reaction between TEMPO and the carbon-centered radicals. The prefluorescent probes bearing 2,2,6,6-tetramethylpiperidine 1-oxyl (TEMPO) moiety with free NO-radical have been well studied, and there is an enhancement of the fluorescence when the NO- radical is quenched by some alkyl-radicals generated from the reaction between the hydroxyl radical and organic compounds rather than the hydroxyl radical itself (*J. Am. Chem. Soc.* **2012**, 134, 4721–4730.; *TrAC-Trends Anal. Chem.* **2016**, 85, 181–202.; *J. Fluoresc.* **2014**, 24, 313–318.). These studies experimentally suggested that the direct coupling between ·OH radical and TEMPO cannot compete with that of TEMPO and the carbon-centered radicals.

To confirm this feature on the prefluorescent probe used in our study, further DFT calculations have been conducted to investigate whether there is a bond interaction between ·OH radical and the NO probe. As shown in **Figure S13**, the fully optimized structure of the resultant compound suggests a O-O bond length up to 1.77 A, being much longer than that of the O-O bond in HOOH (i.e., 1.47 A, experimental data).

As shown in **Figure S14**, further calculations also point out that, the O-O bond, if formed, is very weak. The change of free energy concerning the O-O bond formation is only -5.1 kJ/mol, which strongly suggests it is a fast equilibrium and therefore reversible. Additionally, it should also be noted that the concentration of polymer (PAMPS) which contains numerous C-H bonds is much higher than the NO-probe in the DN-gel system. Instead of reacting with the NO-probe, the highly reactive ·OH radical will react with the C-H bond from PAMPS and such a reaction is barrierless and highly exergonic (thus irreversible).

Furthermore, we have found a paper published in *J. Org. Chem.* in 2019 which claimed that the coupling between ·OH and TEMPO cannot compete with the coupling reaction between TEMPO and the carbon-centered radical, as the latter is much faster. It is consistent to our computational results. (please see Moores, L.C.; Kaur, D.; Smith, M. D.; Poole, J. S. Regioselectivity of Hydroxyl Radical Reactions with Arenes in Nonaqueous Solutions. *J. Org. Chem.* **2019**, 84, 3260−3269.)

2. Supplementary Figures

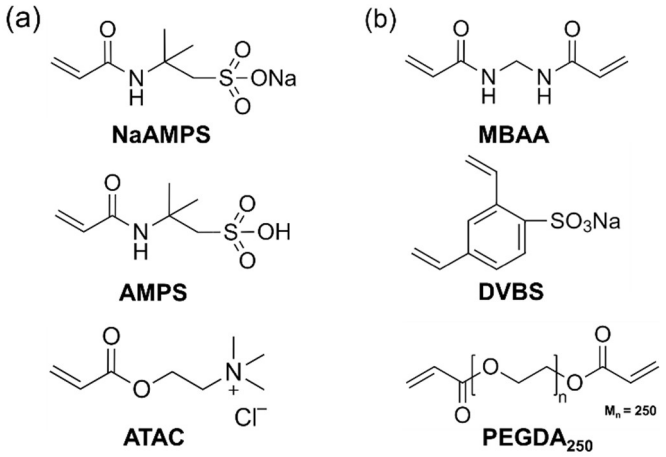


Figure S1. Chemical structure of various (a) monomers and (b) crosslinkers used for the first network of DN gels.

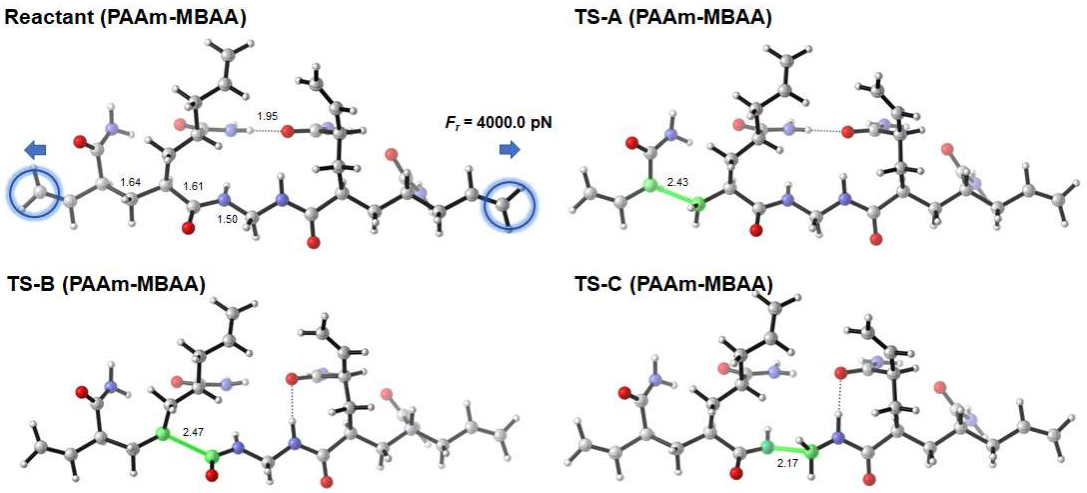


Figure S2. Three different cleavage patterns for PAAm-MBA system at F_τ=4000 pN.

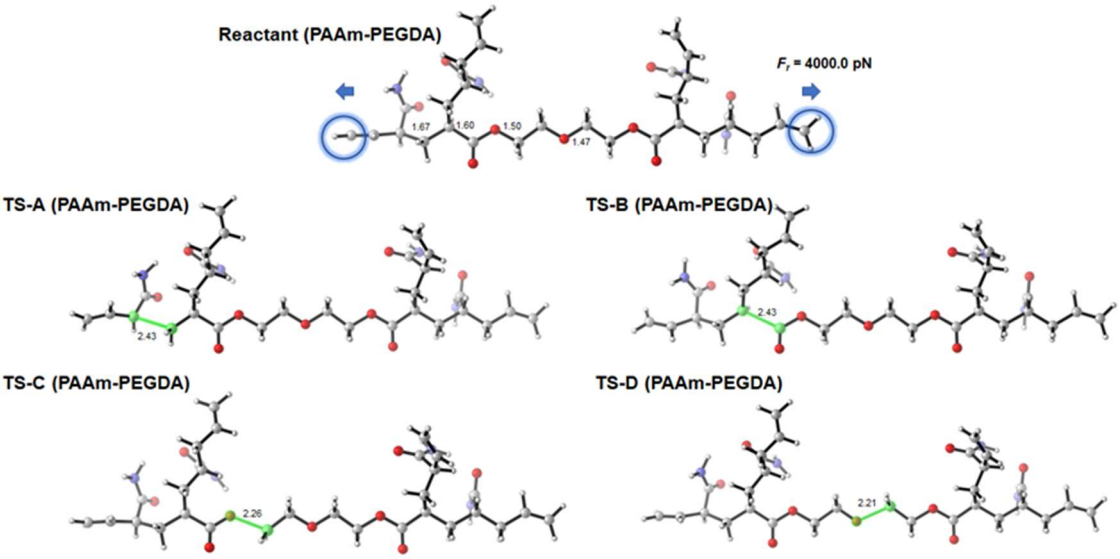


Figure S3. Four different cleavage patterns for PAAm-PEGDA system at F_τ=4000 pN.

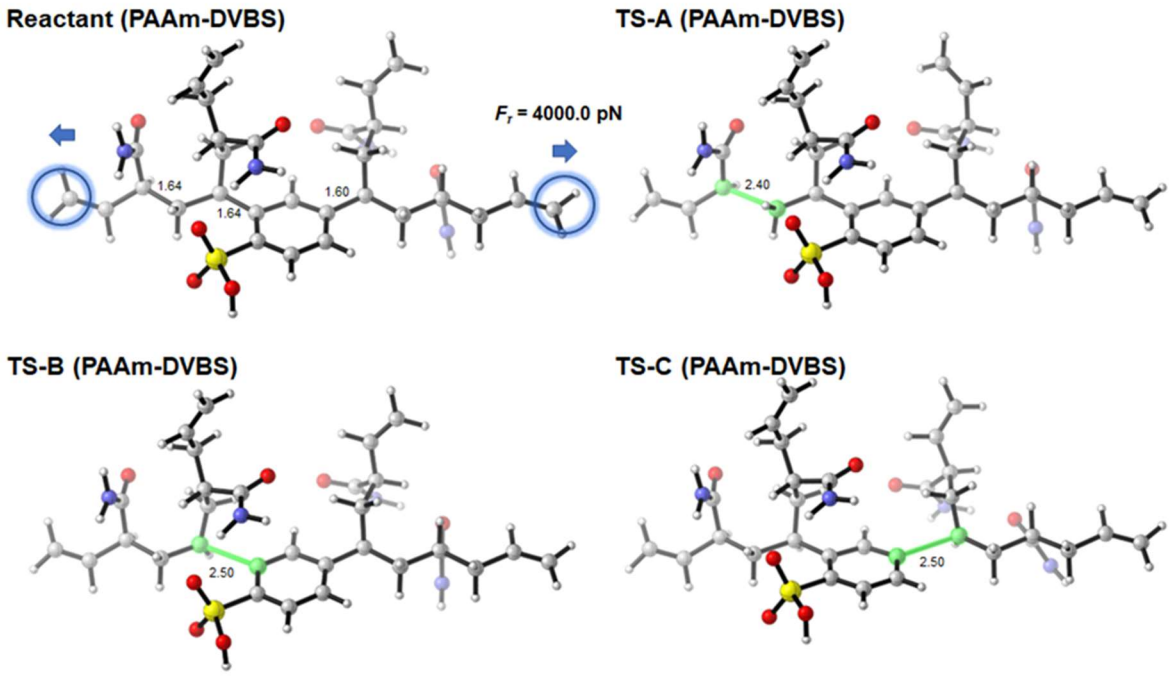


Figure S4. Three different cleavage patterns for PAAm-DVBS system at F_τ=4000 pN.

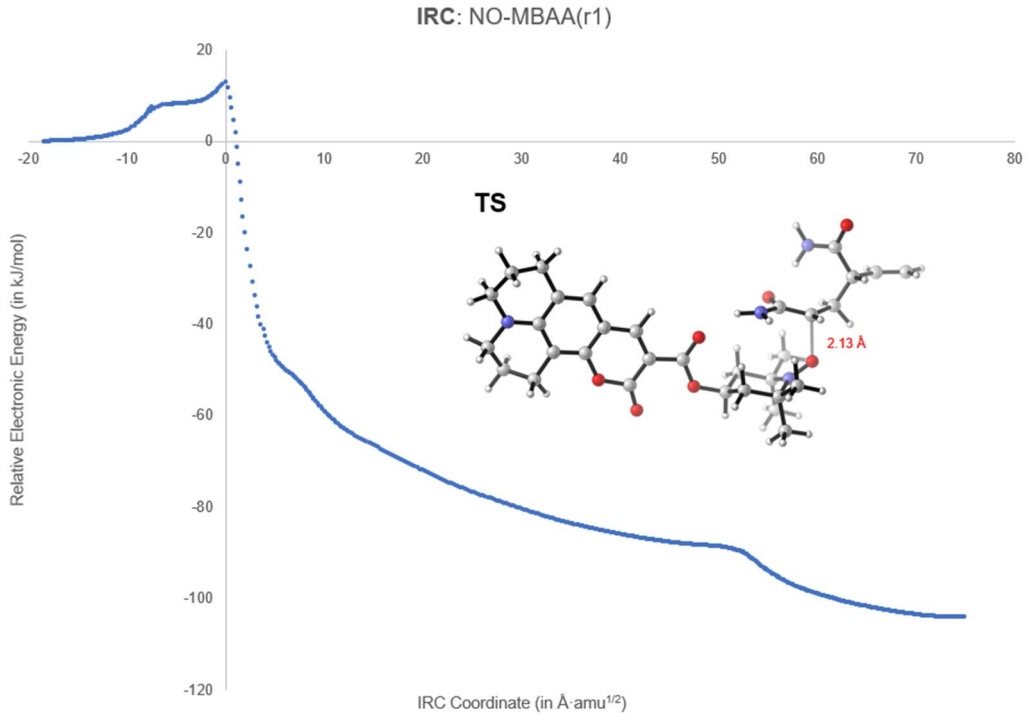


Figure S5. IRC pathway of the coupling reaction between the probe and the MBAA radical r1.

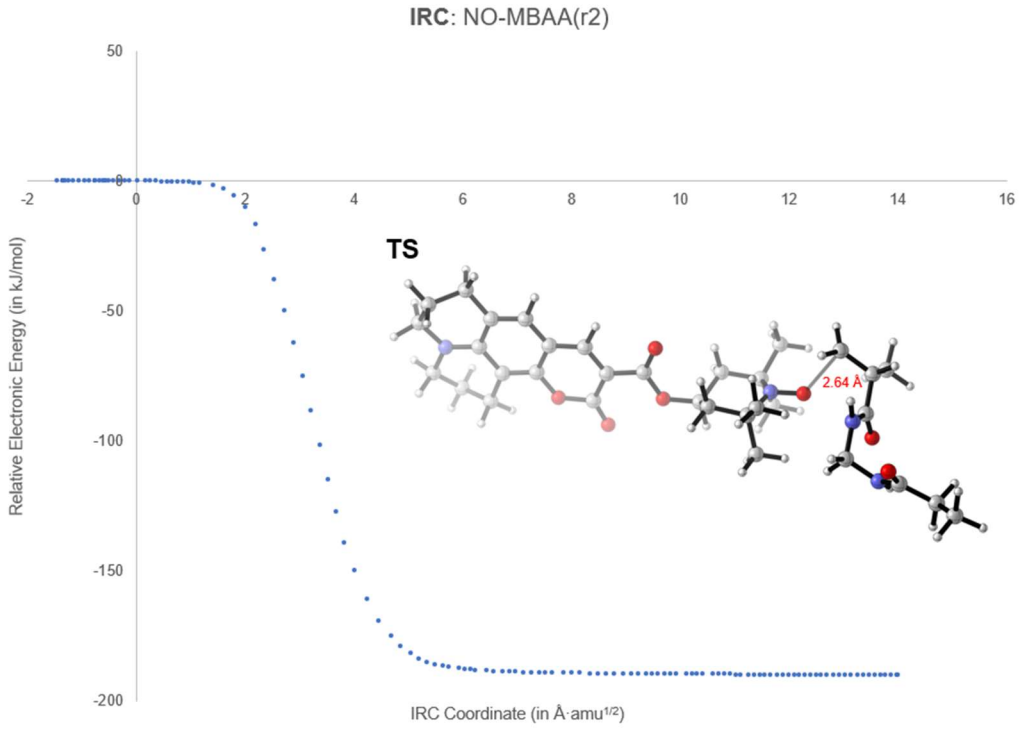


Figure S6. IRC pathway of the coupling reaction between the probe and the MBAA radical r2.

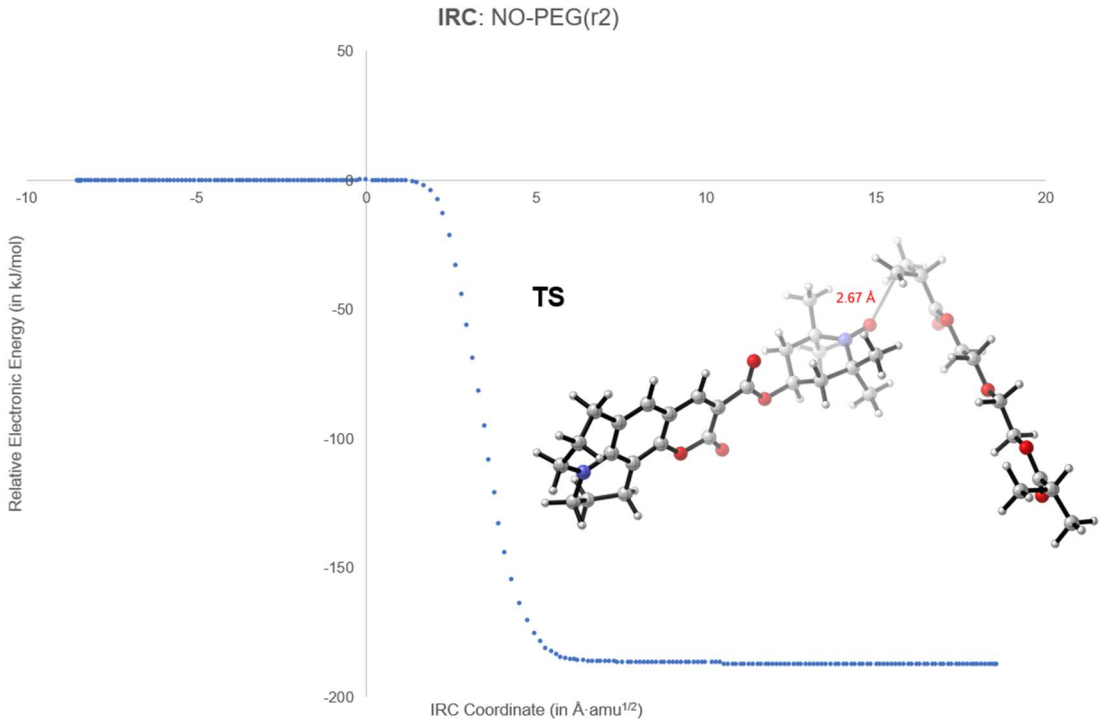


Figure S7. IRC pathway of the coupling reaction between the probe and the PEG radical r2.

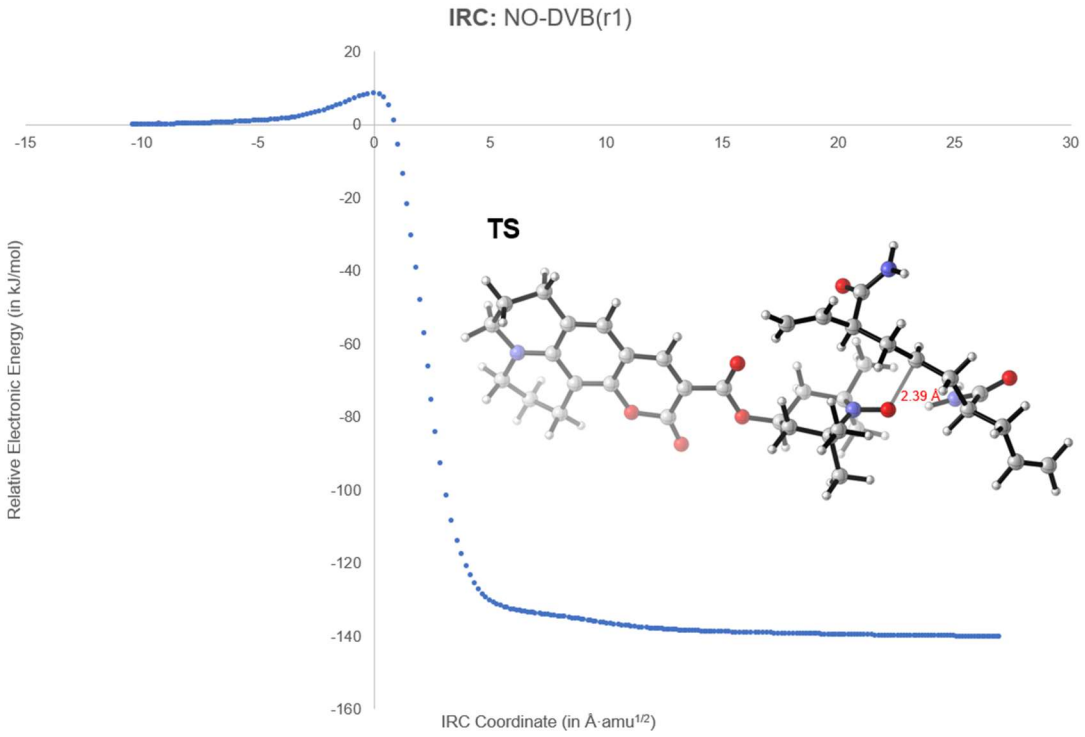


Figure S8. IRC pathway of the coupling reaction between the probe and the DVB radical r1.

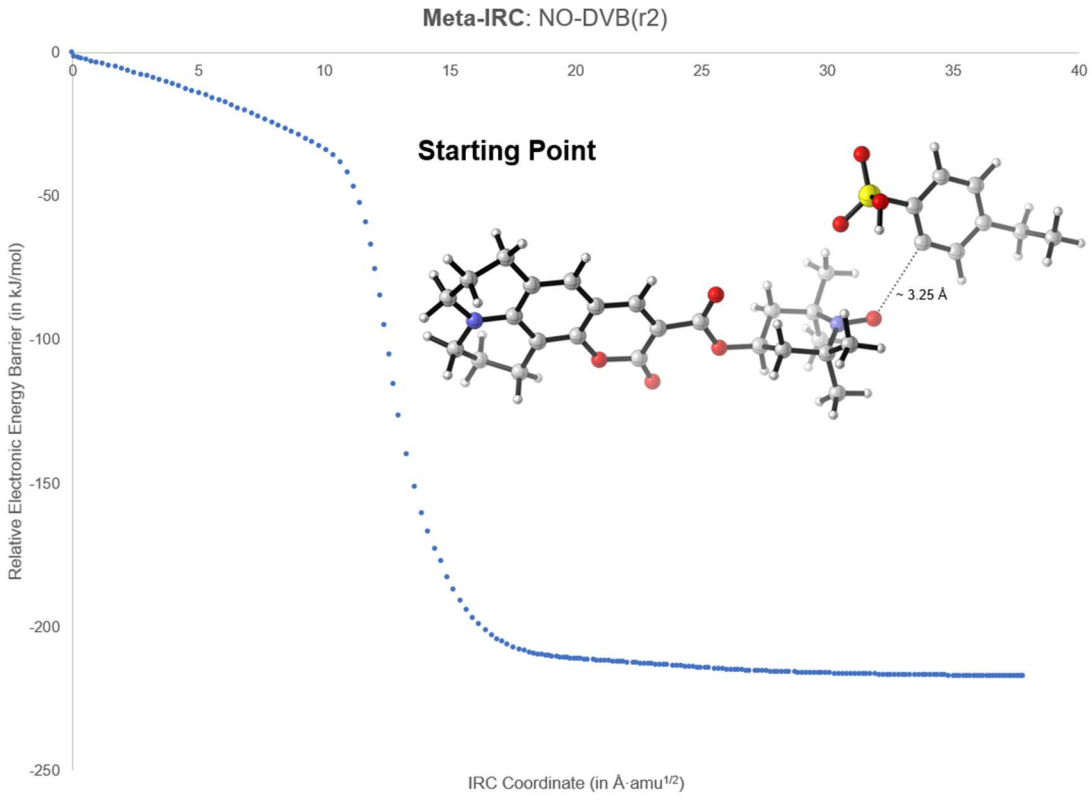


Figure S9. Meta-IRC pathway (steepest descent pathway) of the coupling reaction between the probe and the DVB radical r2, which clearly shows there is no obvious barrier due to the high reactivity of phenyl radical.

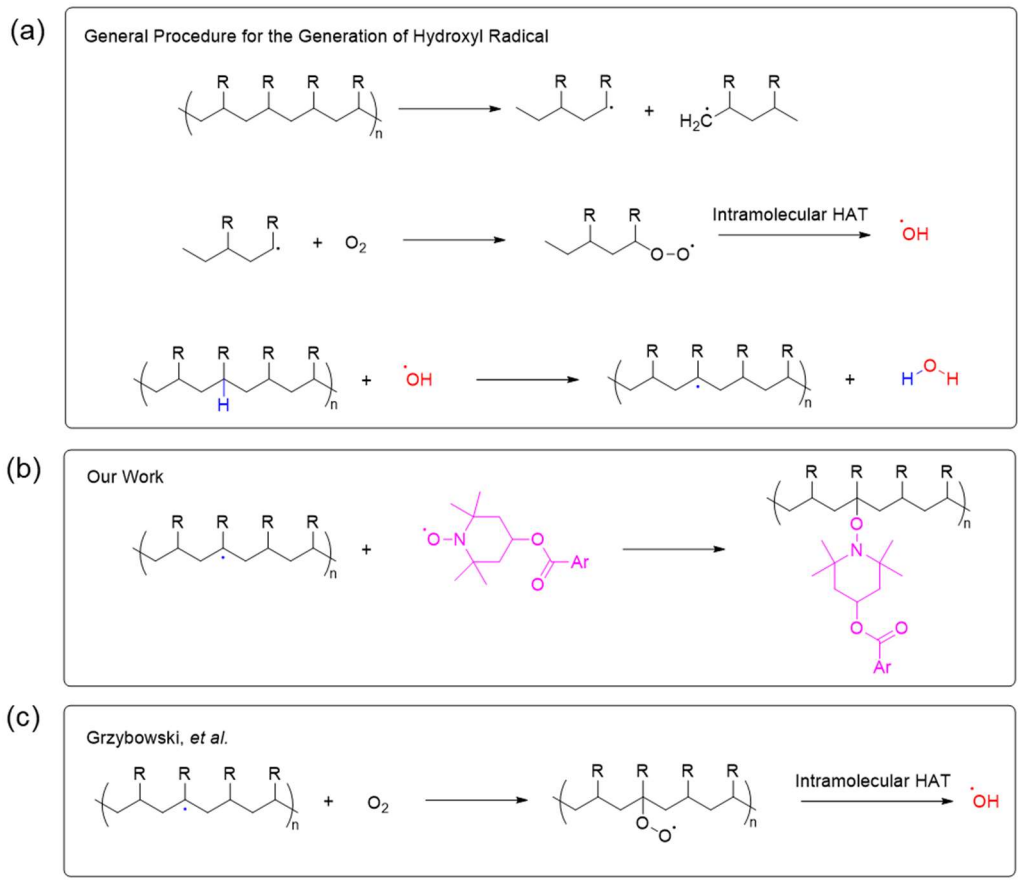


Figure S10. Generation mechanism of hydroxyl radical and termination of the carbon-centered radical by the NO-probe. (a) General procedure for the generation of hydroxyl radical from the addition of oxygen to mechanoradicals; (b) generation of hydroxyl radical and the termination of the carbon-centered radical by the NO-probe in our work; (c) in Grzybowski's work, no NO-probe exists in the reaction system, which means the carbon-centered radical, even if generated (e.g., in the PVC case in Grzybowski's work), will have to react with another O_2 and finally deliver another OH radical.

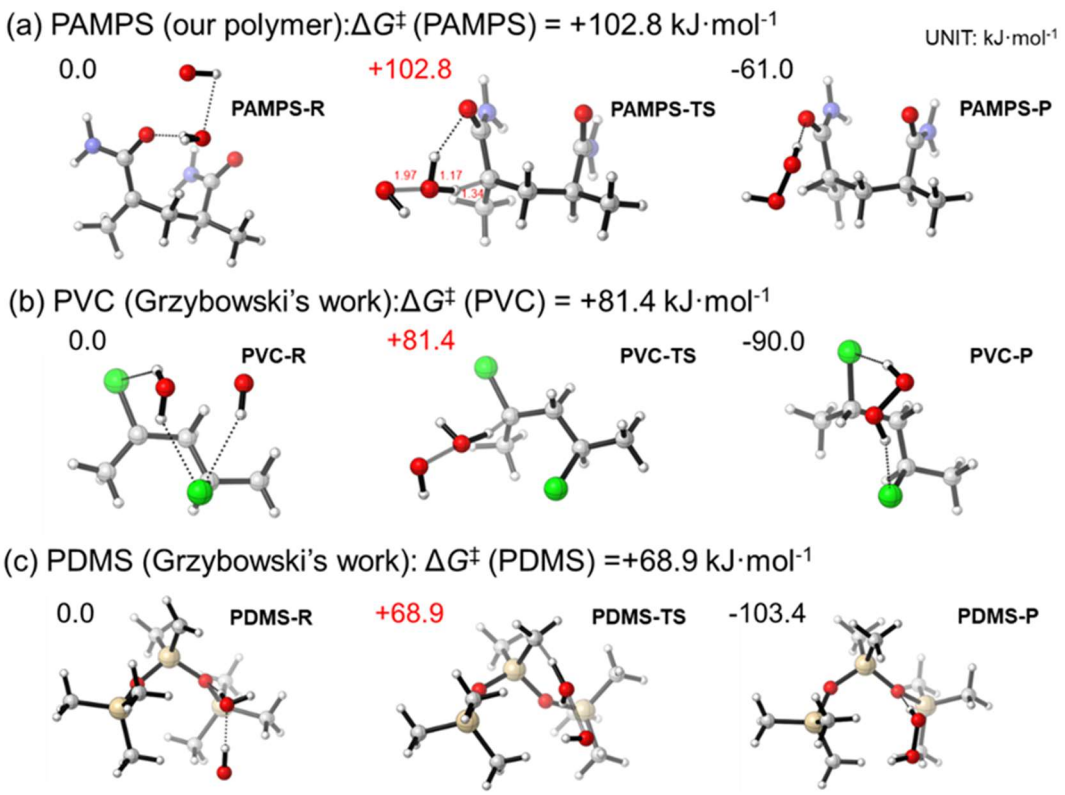


Figure S11. The energy barrier for the formation of H_2O_2 from three different polymers: (a) PAMPS has the highest $\Delta G^{\ddagger}$ (PAMPS) = +102.8 kJ·mol^{-1}; (b) PVC has the moderate $\Delta G^{\ddagger}$ (PVC) = +81.48 kJ·mol^{-1}; (c) PDMS has the lowest $\Delta G^{\ddagger}$ (PDMS) = +68.9 kJ·mol^{-1}. (Calculations done at UB3LYP-D3/Def2SVP//UB3LYP-D3/Def2SVP level of theory with the IEFPCM (solvent=water) solvation model). The notations "polymer-R", "polymer-TS" and "polymer-P" represent the reactants, the transition state and products in the reaction, respectively.

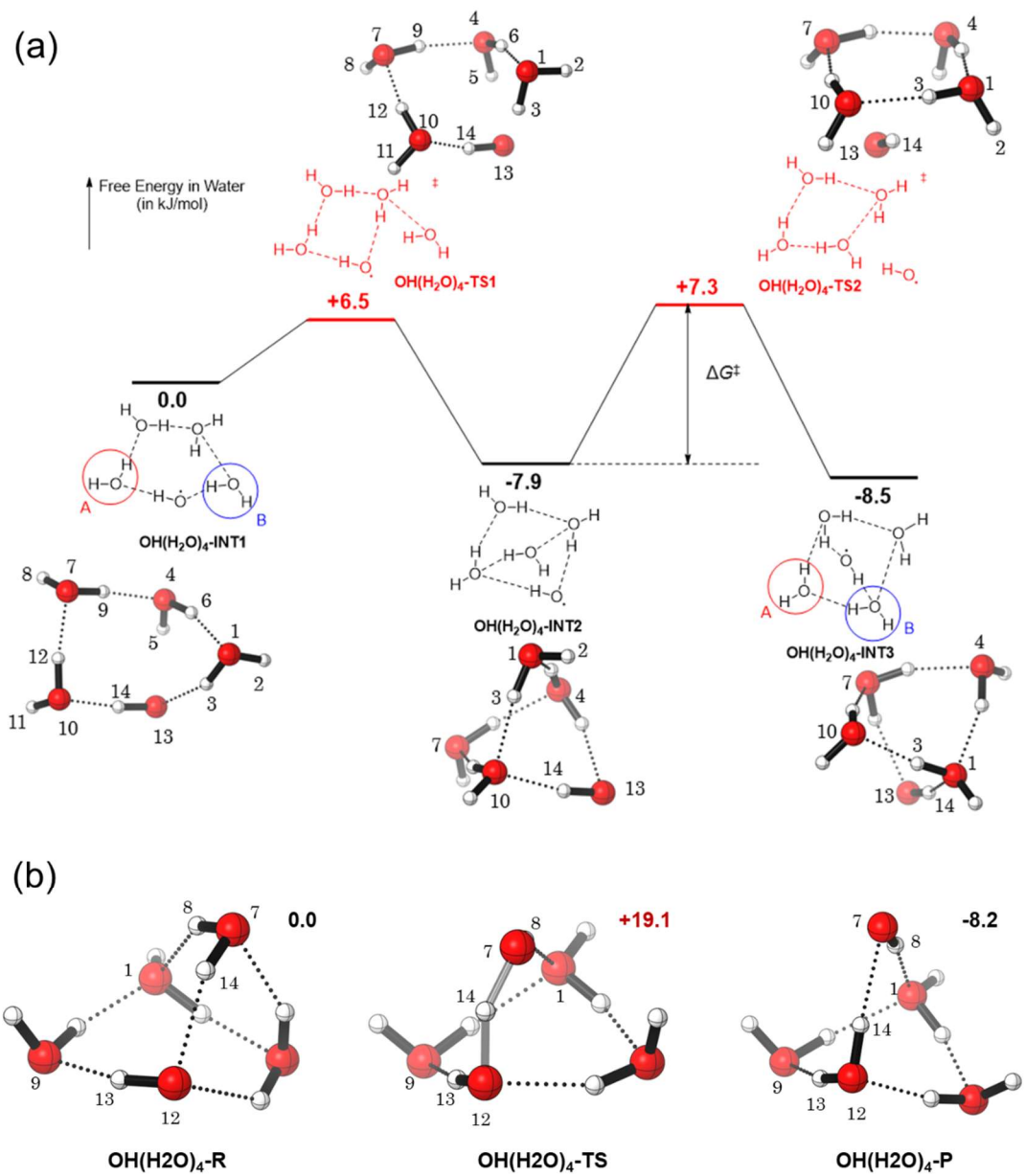


Figure S12. Delivering ·OH radical to the remote area via the HB network in aqueous system. (a) physical process to move the OH radical via the rearrangement of hydrogen bonds, from which we can see a water molecule B inserting to the space between water molecule A and the ·OH radical; (b) chemical process to move the ·OH radical via an HAT reaction. (Calculations done at UB3LYP-D3/Def2SVP//UB3LYP-D3/Def2SVP level of theory with the IEFPCM (solvent=water) solvation model)

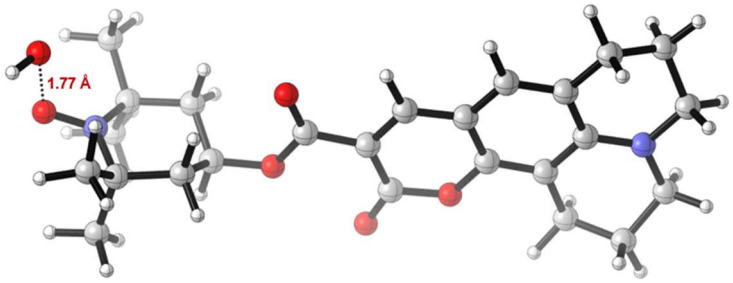


Figure S13. Optimized geometry of the proposed coupling product of ·OH radical and the NO-probe. (Calculations done at UB3LYP-D3/Def2SVP//UB3LYP-D3/Def2SVP level of theory with the IEFPCM (solvent=water) solvation model)

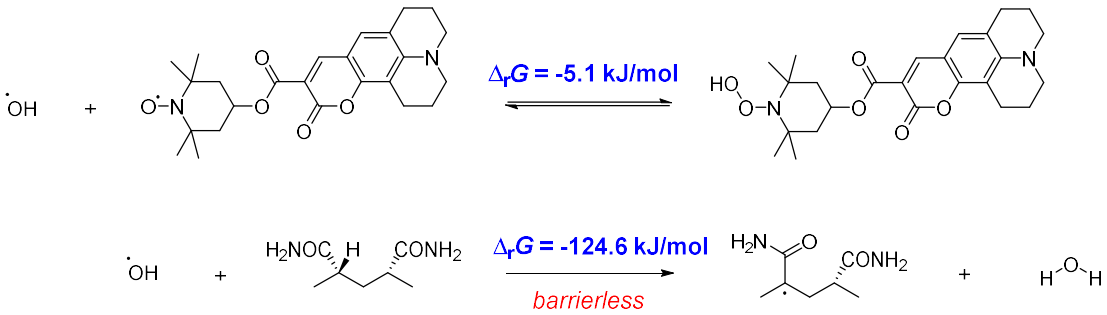


Figure S14. Energy change for the formation of the NOOH species and the hydrogen abstraction of ·OH radical from PAMPS. (Calculations done at UB3LYP-D3/Def2SVP//UB3LYP-D3/Def2SVP level of theory with the IEFPCM (solvent=water) solvation model)

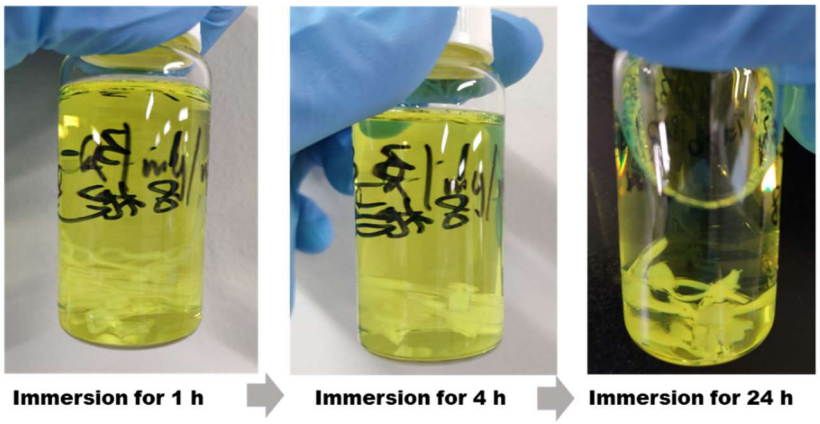


Figure S15. Photographs of **DN1** gel samples immersed in **P**/THF solution (c_p = 1.0 mg/mL) for different immersion time.

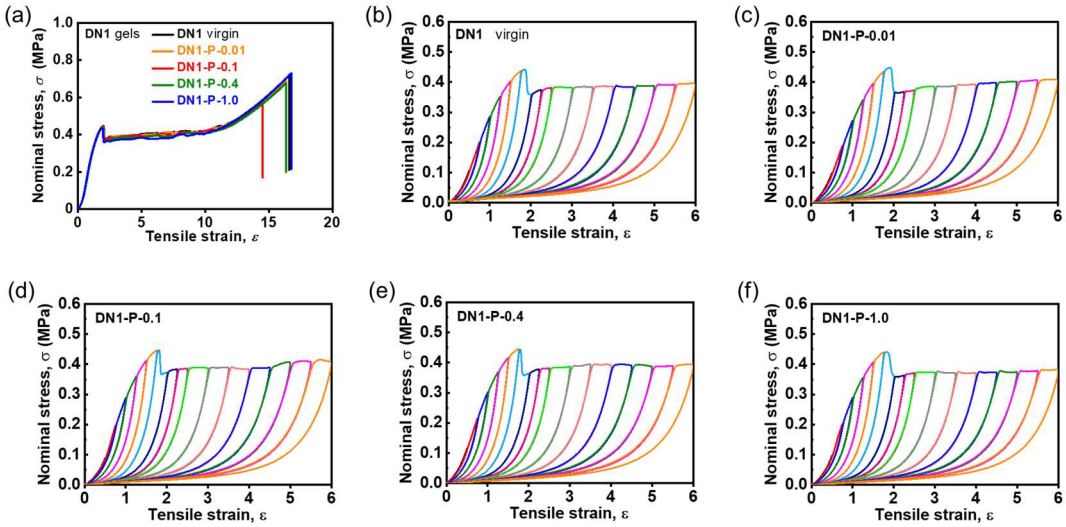


Figure S16. (a) The nominal stress σ-tensile strain ε curves for **DN1** virgin and **DN1-P-c_p** gels with varied concentration c_p. (b-f) The sequential loading–unloading cycles for (b) **DN1** virgin, (c) **DN1-P-0.01**, (d) **DN1-P-0.1**, (e) **DN1-P-0.4**, and (f) **DN1-P-1.0** gels.

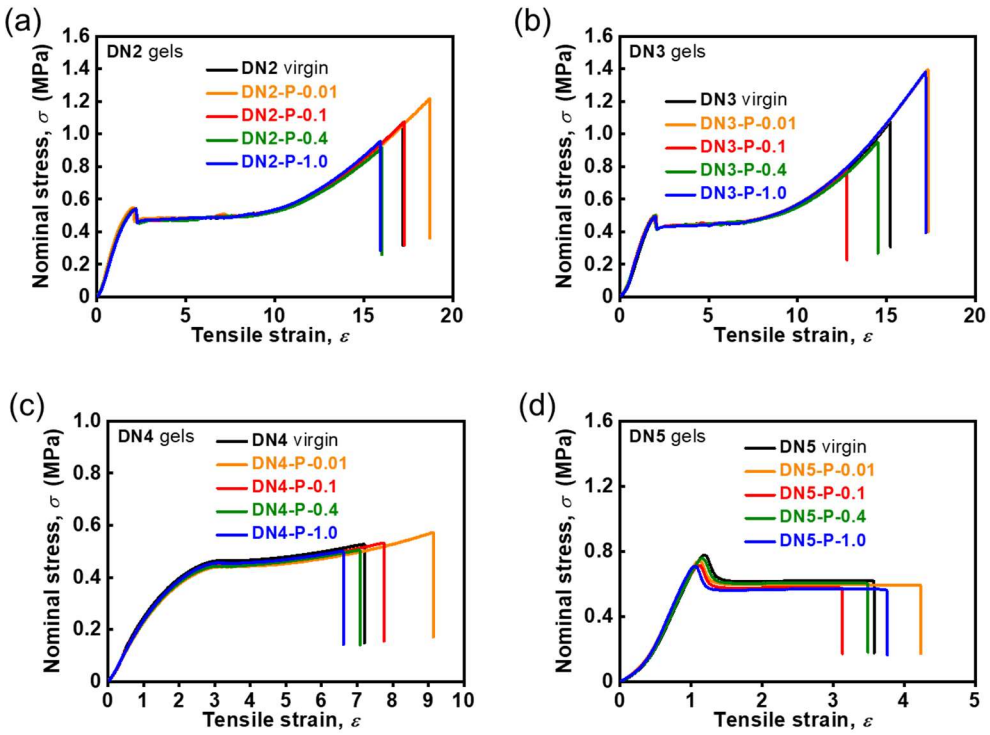


Figure S17. (a) The nominal stress σ-tensile strain ε curves for **DN2** virgin and **DN2-P-c_p** gels with varied concentration $\boldsymbol{c_p}$. (b) The nominal stress σ-tensile strain ε curves for **DN3** virgin and **DN3-P-c_p** gels with varied concentration $\boldsymbol{c_p}$. (c) The nominal stress σ-tensile strain ε curves for **DN4** virgin and **DN4-P-c_p** gels with varied concentration $\boldsymbol{c_p}$. (d) The nominal stress σ-tensile strain ε curves for **DN5** virgin and **DN5-P-c_p** gels with varied concentration $\boldsymbol{c_p}$.

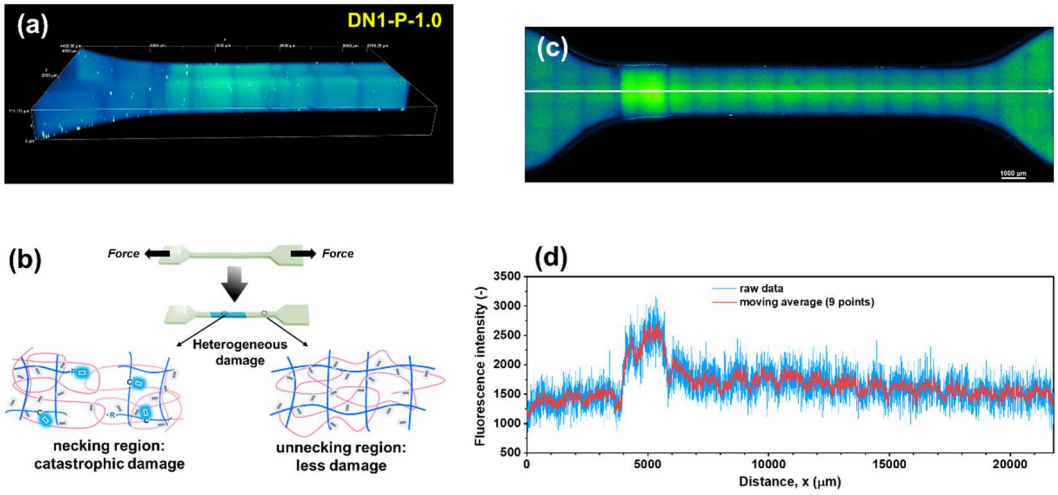


Figure S18. Visualization of stretching- damages in DN gels using prefluorescent reagent **P.** Spatial visualization of heterogeneous damage in **DN1-P-1.0** gel by CLSM. (a) 3D fluorescence image captured by CLSM, (b) illustration of the structure in DN gels, and (c) 2D fluorescence image and (d) line profiles of fluorescence intensity. The 3D images have been automatically constructed by the integration of a stack of scanned small original images captured by CLSM, which are shown as the mesh-like patterns in the integrated images. The weak intensity in the boundary area of these mesh-like patterns is caused by the CLSM microscope itself and therefore does not reveal any internal information

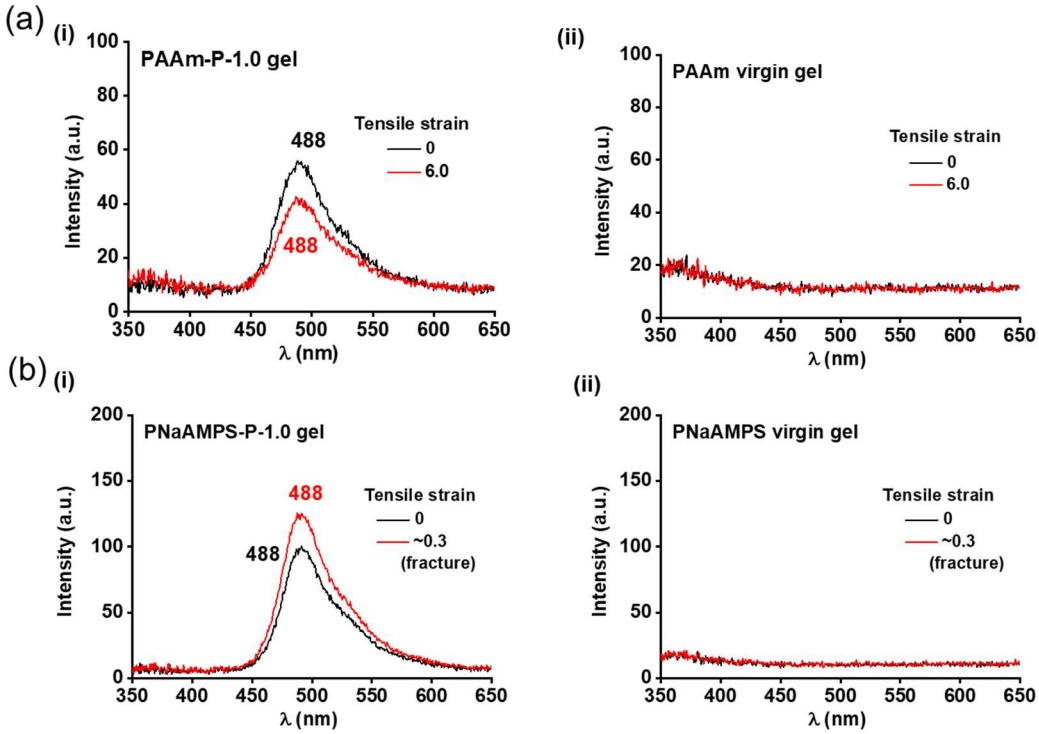


Figure S19. (a) The fluorescence spectra (λ_{ex} = 365 nm) of PAAm-P-1.0 (i) and PAAm virgin (ii) gels under various tensile strains. The PAAm virgin gel means the second network gel with the same composition as in **DN1** gels. The PAAm-P-1.0 gel corresponds to the second network gel under the same preparation protocol as illustrated in Figure. 2a. (b) The fluorescence spectra (λ_{ex} = 365 nm) of PNaAMPS-P-1.0 (i) and PNaAMPS virgin (ii) gels. The PNaAMPS virgin gel means the first network gel with the same composition as in **DN1** gels. The PAAm-P-1.0 gel corresponds to the second network gel under the same preparation protocol as illustrated in Figure 2a.

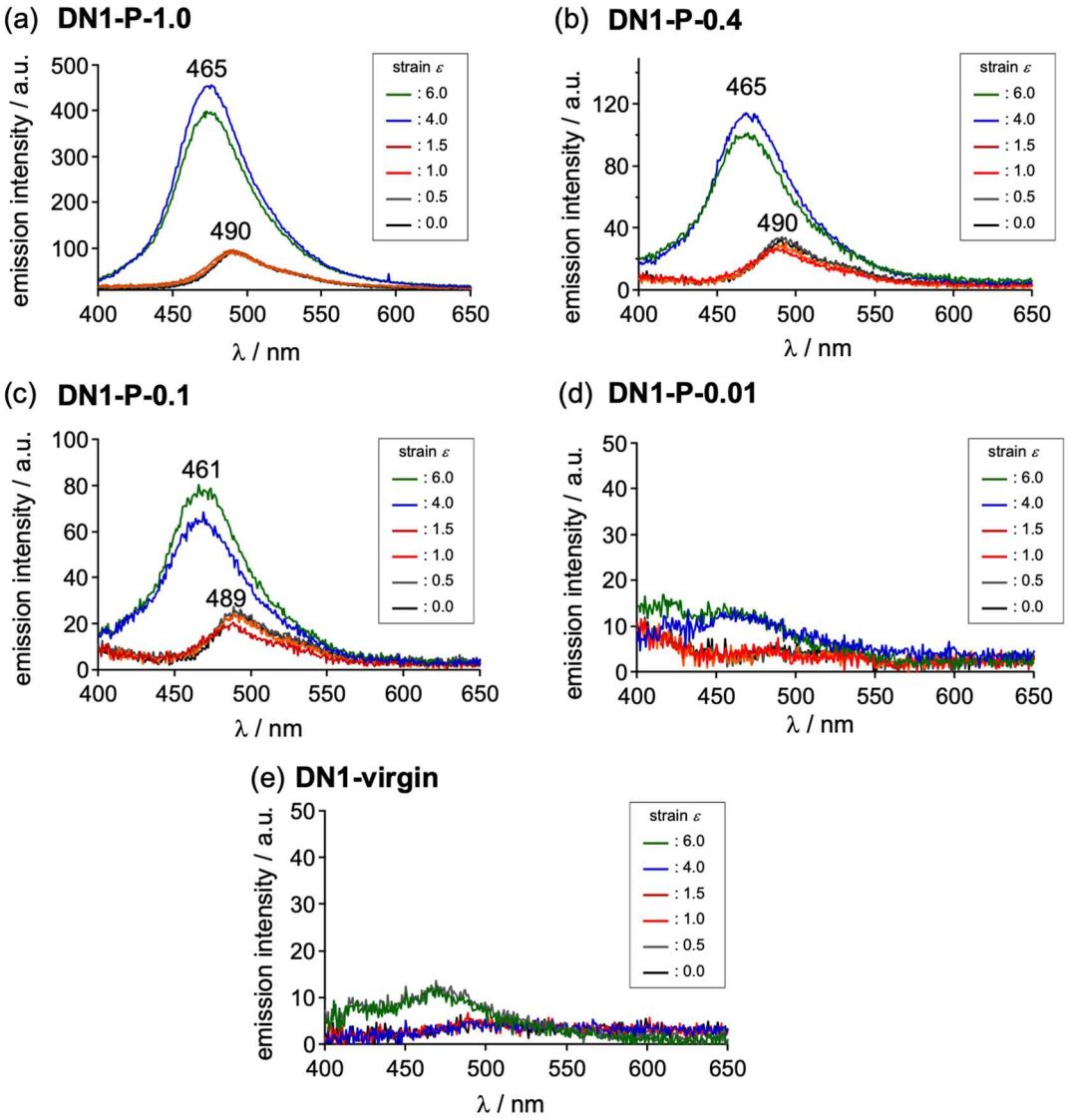


Figure S20. Emission spectra of DN1 under mechanical stress with various probe concentration.

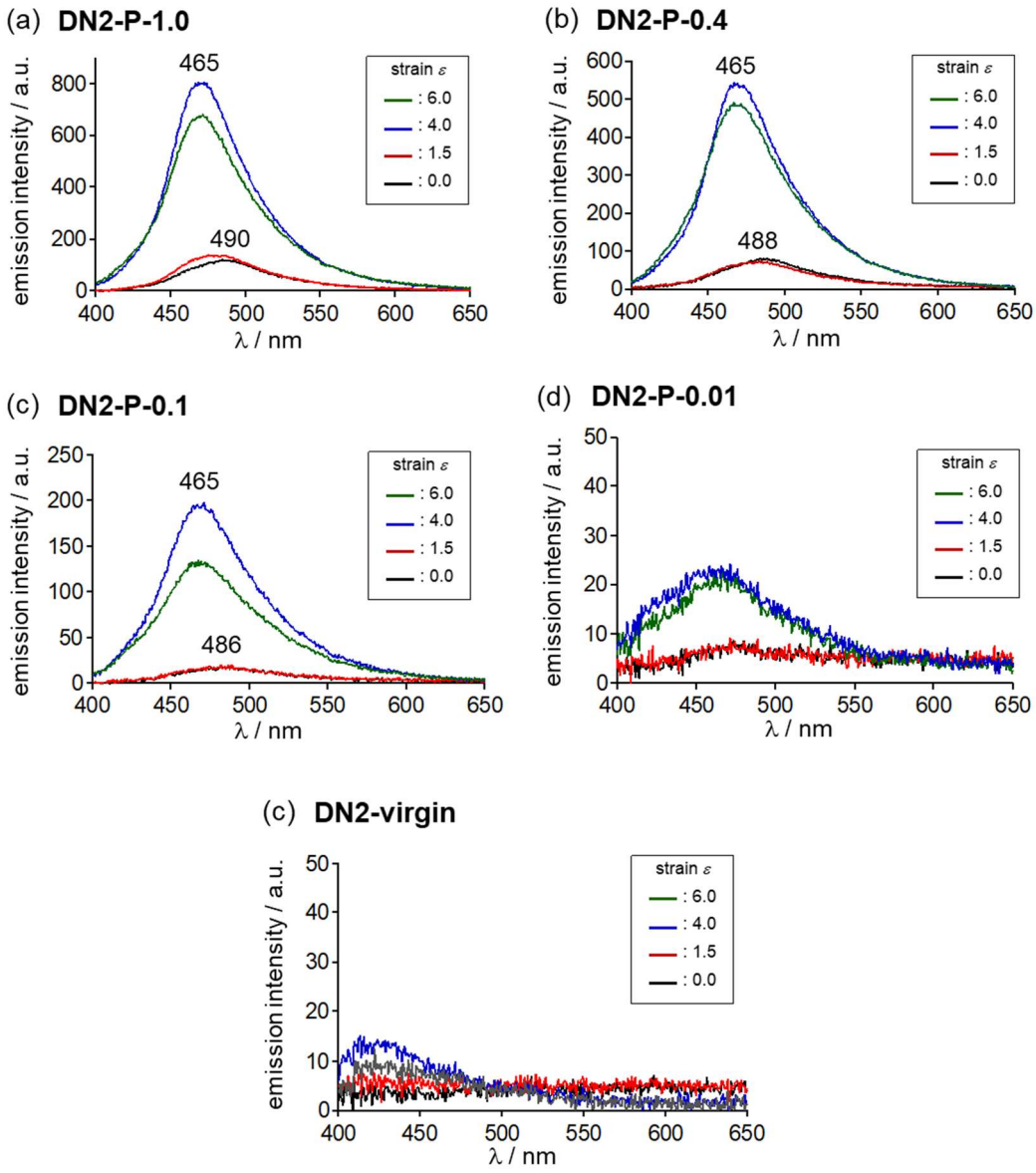


Figure S21. Emission spectra of DN2 under mechanical stress with various probe concentration.

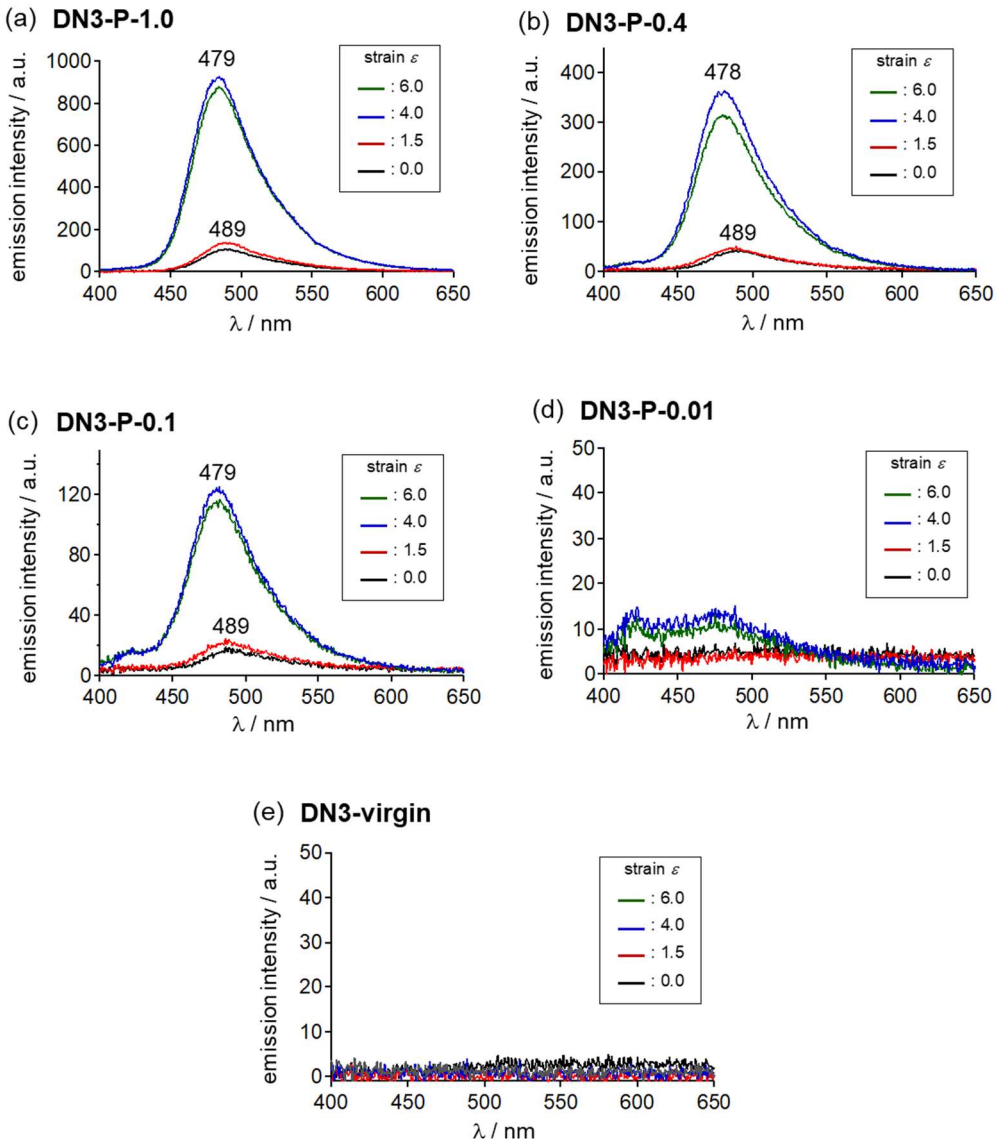


Figure S22. Emission spectra of DN3 under mechanical stress with various probe concentration.

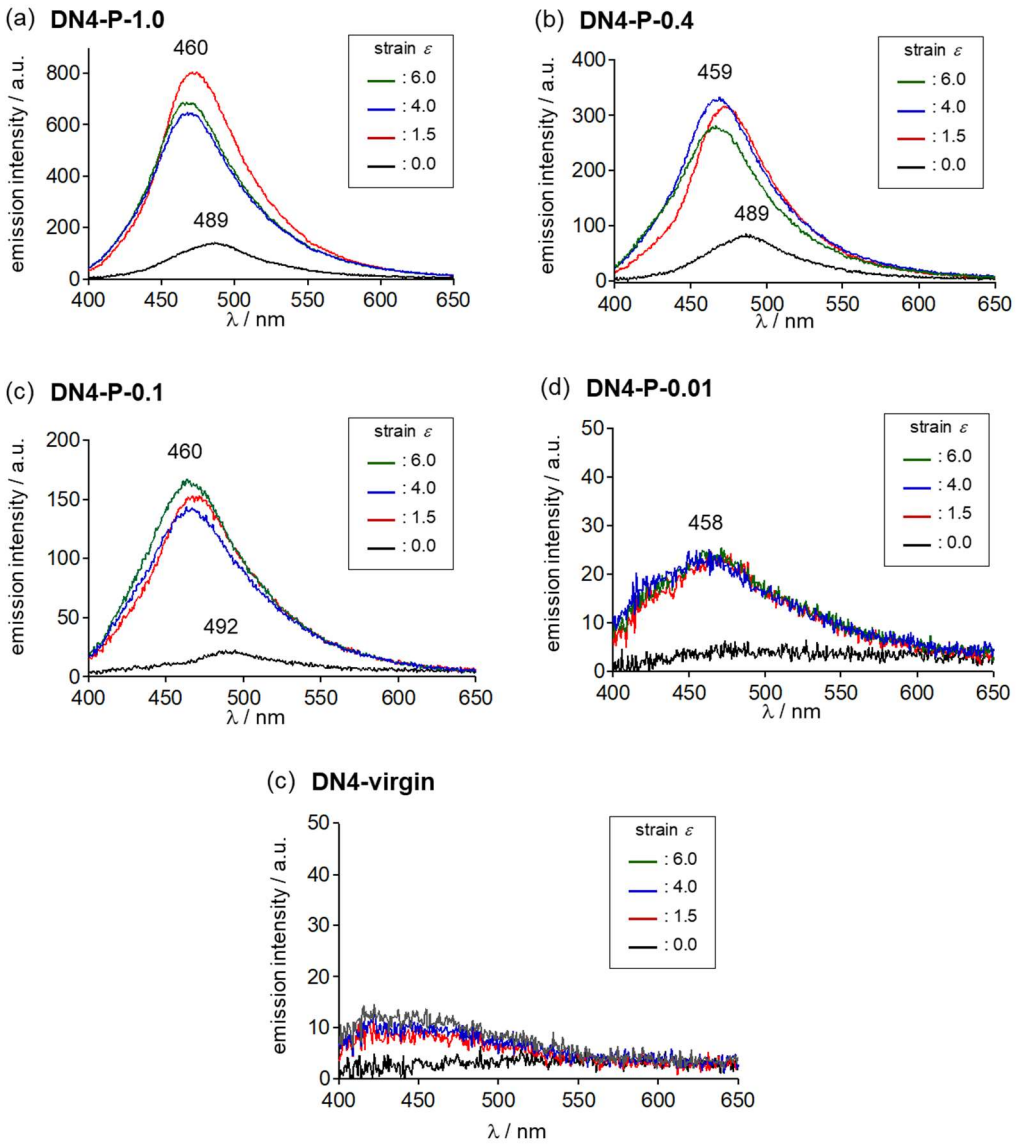


Figure S23. Emission spectra of DN4 under mechanical stress with various probe concentration.

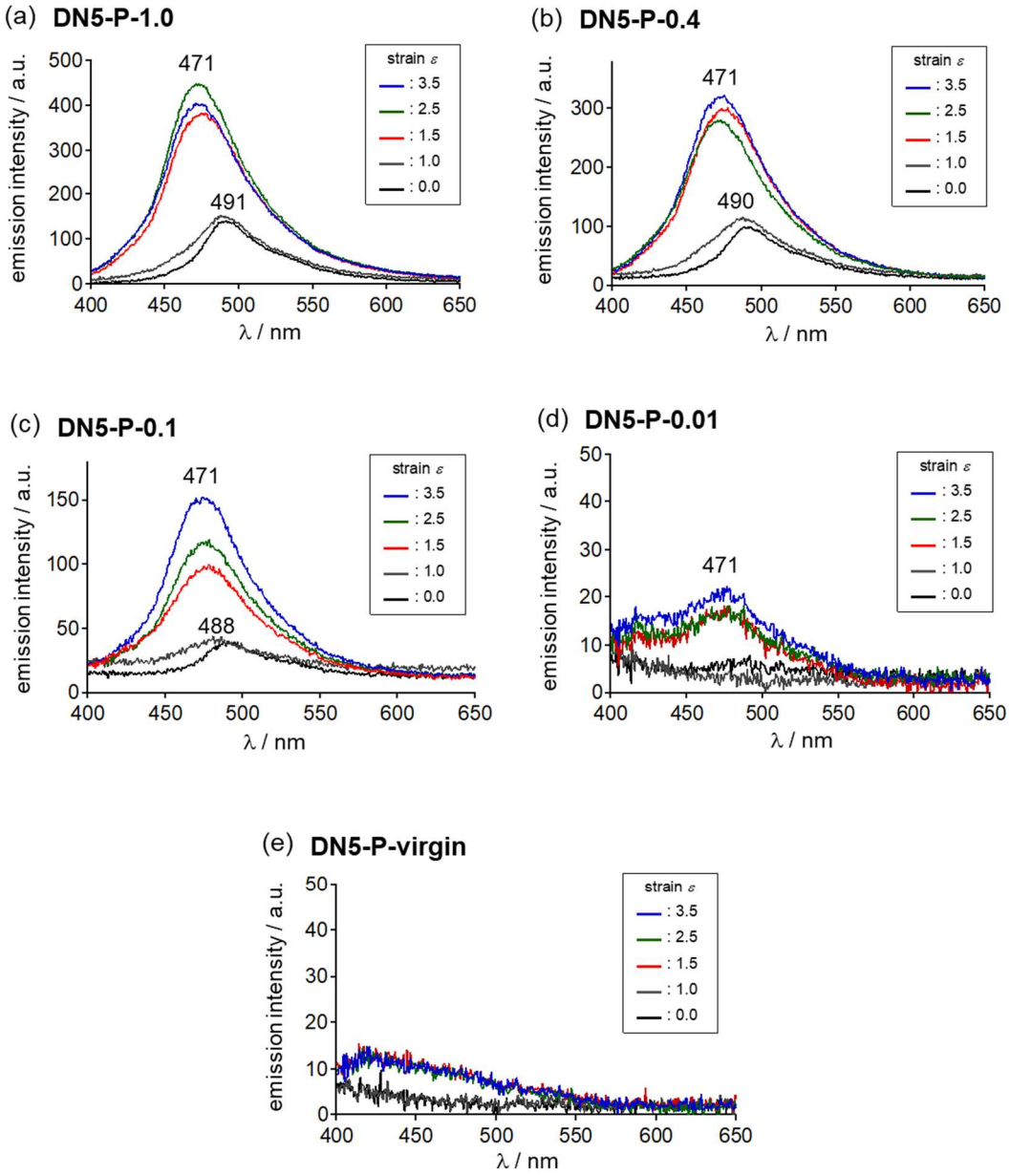


Figure S24. Emission spectra of DN5 under mechanical stress with various probe concentration.

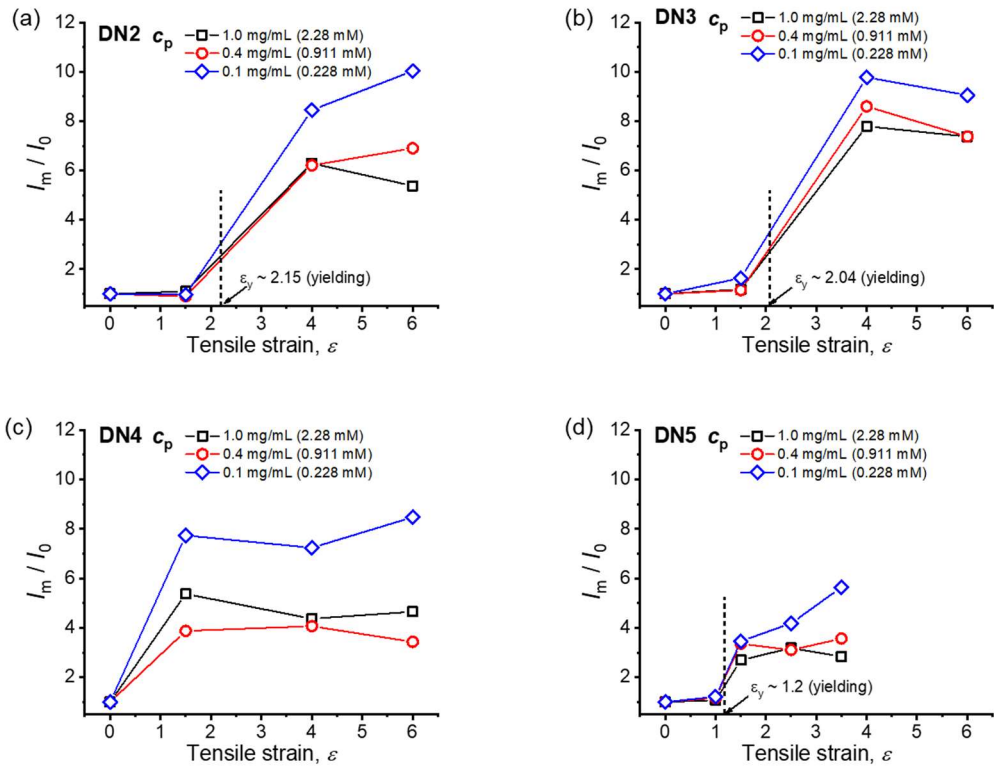


Figure S25. Emission intensity alternation ratio I_m/I_0 versus tension strain ε for various **DN1-P-*c*$_p$** gels: (a) **DN2**, (b) **DN3**, (c) **DN4**, (d) **DN5**. I_m and I_0 denote the peak intensity after stretching and before stretching, respectively.

3. SI References

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Cartesian coordinates of optimized geometries:

For the mechanochemical reactions, the force-coupled electronic energies and force-coupled free energies are labelled as E_F and $G_{F,298K}$. All the free energies were computed at 298.15 K and 1 atm.

I. FORMATION OF MECHANORADICALS

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E_{F4000} = -1834.648432437085 a.u. ($G_{F4000,298K}$ = -1834.048004032212 a.u.)

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H	-2.195086303307	0.341655408503	-4.632982208870
C	5.765635307955	-2.469273194960	-0.519516286609
H	5.710333511874	-1.951962876310	-1.490162166236
C	4.949891641114	-3.749264242427	-0.720667723213
O	3.940101483510	-3.756524683268	-1.432487809092
N	5.348443746056	-4.846986205094	-0.047553638686
H	6.178706376411	-4.865447790805	0.530108321375

C	4.958368941346	-1.542244140384	0.554771243954
H	5.551276118059	-0.622590529433	0.687739221644
H	4.968565030234	-2.062532379524	1.524916175737
C	3.436085363067	-1.115587166135	0.246857407091
H	2.885961859036	-2.056778645474	0.093130571715
C	2.570111375172	-0.942574789923	-2.218161801475
H	3.170341984360	-1.825946566109	-2.485710283154
C	1.200828635664	-1.433276333828	-1.750734730951
O	0.295166916329	-0.641752253596	-1.440535385527
N	1.072511514687	-2.765249173110	-1.651381476634
H	1.887423673412	-3.369588400635	-1.752580712564
C	-1.666707940337	2.050292472303	2.553700768111
O	-1.132851792704	2.973456358638	3.145973475863
N	-0.907704626158	0.970491875987	2.062773741400
H	-1.405091060271	0.145610367371	1.734168975028
C	0.566385948181	0.816600830875	2.297769510896
H	0.951275249195	1.840430133804	2.419906405411
H	0.749303173339	0.286517363838	3.245716666948
N	1.351298040303	0.082154883377	1.246841197083
H	0.979297915808	0.099723313973	0.295857537646
C	2.638294166219	-0.430528638558	1.472057317633
O	3.138027405710	-0.397119158128	2.588416076275
C	3.310939206189	-0.253214094035	-1.041918532564
H	4.315034664150	0.024643629683	-1.399484423529
H	2.805144230948	0.700538753754	-0.826602958172
C	7.337439312919	-2.728592104857	-0.223973032365
H	7.793485695759	-1.725676952290	-0.156801320324
H	7.455404500312	-3.150602080733	0.790105162765
C	8.201945410737	-3.571729572270	-1.255629871047
H	7.663825211278	-3.737966451261	-2.200645967241
C	9.482191312821	-4.077681198351	-1.222226432416
H	9.875779112799	-4.602605994745	-2.096521768429
H	10.137037606836	-3.982681913148	-0.348882563919
C	2.514404264382	-0.037746391169	-3.426480942845
H	3.503445291876	0.315418511739	-3.746076372776
C	1.439954262637	0.344693835706	-4.123645365253
H	0.428214259327	0.035596438243	-3.849715651417
H	1.544019716546	0.991785609351	-4.999037391992
H	-2.894251983743	-1.702809325312	-0.367172129029
H	-6.825969354613	2.277929245504	0.010348910312
H	0.217837004921	-3.151924822801	-1.262188176765
H	4.805140182530	-5.699507692413	-0.133119063664

MBAA_4000-TSB

E_{F4000} = -1834.616970236941 a.u. ($G_{F4000,298K}$ = -1834.022059747304 a.u.)

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C	-8.485477731984	4.776036079566	4.020637973911
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H	-9.182352560908	4.598080551069	3.196629888200
C	-7.199601627984	4.283776836778	4.023516190998
H	-6.599232579183	4.540910208225	4.907866278724
C	-6.406290982288	3.282461902388	3.082250390351
H	-6.611122716393	2.281595761303	3.501521224063
C	-6.971376178171	3.299072555477	1.655960917587
O	-7.407363060982	4.318750613239	1.135318508875
N	-6.980838600671	2.099386954937	1.009096166578
H	-6.374539106103	1.329430096144	1.281424653413
C	-4.741324454853	3.373363949735	3.076997519521
H	-4.477360716477	4.399296586868	2.773068151586
H	-4.456672149327	3.268212938901	4.136508297948
C	-3.900500199600	2.356104843138	2.206190182694
H	-4.170411068122	1.310765475259	2.383007504082
C	-3.760031189861	2.748397821317	0.752676497951
H	-4.769477512521	2.916476072514	0.338947311480
H	-3.259224481674	3.730381135148	0.692697526393
C	-3.022960825609	1.781884275753	-0.188943786521
H	-1.948256266603	1.813154807114	0.039576060347
C	-3.507312401121	0.340411442853	-0.025556786679
O	-4.674394517732	0.073563912314	0.258479251910
N	-2.568484159591	-0.627868638813	-0.202746733544
H	-1.660313585340	-0.456185146879	-0.637325158808
C	-3.190277972398	2.219353706554	-1.667913333147
H	-2.964001745999	3.300433422180	-1.710339242566
H	-4.243669916809	2.100810722721	-1.973002263050
C	-2.277941374799	1.492466250814	-2.616814244898
H	-1.209317043559	1.517456524791	-2.364377029867
C	-2.667398037536	0.823508788735	-3.706270588381
H	-3.723567951526	0.754820299984	-3.989600093826
H	-1.945492611758	0.320772928746	-4.356801637467
C	5.900271213847	-2.530565213306	-0.589262753284
H	5.854416185316	-1.997652325289	-1.552100500565
C	5.074887432773	-3.800229582876	-0.816923347940
O	4.052718884950	-3.778706313786	-1.510229854116
N	5.479337604872	-4.921892331389	-0.187277956023
H	6.322206425524	-4.966002409826	0.370348835504
C	5.093780162190	-1.614219341756	0.494005865116
H	5.687826381645	-0.696599571236	0.636051566484
H	5.103960225627	-2.144321991151	1.458858239769

C	3.571267747207	-1.183579762122	0.193698252730
H	3.020976807730	-2.123043673710	0.031315542368
C	2.644573010672	-0.959054596101	-2.249062296027
H	3.218136343449	-1.850675888981	-2.545687847284
C	1.274384658605	-1.429772740762	-1.759843354570
O	0.382240859256	-0.633361702790	-1.428659843848
N	1.131543146336	-2.762768143129	-1.668974130829
H	1.932926497083	-3.378614727432	-1.796611087873
C	-1.485895428885	2.000706179119	2.561922524607
O	-0.981638507832	2.937235553338	3.124391014116
N	-0.753853077373	0.933161360667	2.038396912730
H	-1.280322830639	0.128357745099	1.703616883396
C	0.731099708530	0.749964996278	2.271203453301
H	1.123792948955	1.769293417800	2.408679133795
H	0.899959708853	0.202674820501	3.211401014261
N	1.503827319199	0.027661363969	1.210986778449
H	1.131429616262	0.075169271238	0.260639492323
C	2.780306176936	-0.513791842335	1.429609329276
O	3.274566771781	-0.515696048699	2.548927204408
C	3.439098931777	-0.307484495850	-1.084619711839
H	4.441492133591	-0.061694861266	-1.469160558421
H	2.975049066406	0.662153315059	-0.846852392043
C	7.468290665970	-2.802491806697	-0.285903325190
H	7.927437365178	-1.802874028583	-0.194633179569
H	7.575127747691	-3.244827660049	0.720767164278
C	8.340491189957	-3.627368359862	-1.325889147036
H	7.812771516377	-3.769725111519	-2.280692114785
C	9.617874415221	-4.140359336744	-1.288542678750
H	10.019461742476	-4.647635641636	-2.169630001830
H	10.262615565819	-4.068124144040	-0.405464548531
C	2.586382159398	-0.030429406855	-3.439500926036
H	3.579865251692	0.256415942964	-3.808304717624
C	1.507150012327	0.450417333469	-4.064607102090
H	0.492690350202	0.213373842205	-3.735753103262
H	1.612382610985	1.108906244430	-4.931373741778
H	-2.896504057041	-1.589616732638	-0.216498289137
H	-7.211264544190	2.127636547545	0.019959162306
H	0.278505504923	-3.141308123303	-1.268582456733
H	4.931295722098	-5.768907740534	-0.294557305997

MBAA_4000-TSC

E_{F4000} = -1834.617304568980 a.u. ($G_{F4000,298K}$ = -1834.021437206414 a.u.)

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C	-8.288029493212	4.697749518534	4.112023255547

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H	-8.975254167319	4.564087522459	3.271269699809
C	-7.008287720634	4.190044978248	4.112010048391
H	-6.417877872719	4.403151349083	5.014835176143
C	-6.208571630901	3.218949039335	3.139006790480
H	-6.432638972866	2.206122934273	3.519935911111
C	-6.780940589495	3.304353128556	1.718074018774
O	-7.130815578226	4.366054248025	1.216805866878
N	-6.904217000577	2.119173236681	1.054518898279
H	-6.339403549676	1.309875926306	1.299730480671
C	-4.568174284729	3.304587037801	3.151267648369
H	-4.283008609144	4.327206598533	2.857117313954
H	-4.277894171814	3.199372371089	4.208567797651
C	-3.656551884540	2.279975106004	2.285294551536
H	-4.086138848935	1.269018697616	2.371678958014
C	-3.652920551487	2.707438223419	0.792458725171
H	-4.683953170350	2.837751303208	0.445690847329
H	-3.171789070268	3.697986111980	0.728973801418
C	-2.945922849772	1.776323172800	-0.209901692110
H	-1.870086866570	1.746405039994	0.012420996769
C	-3.497290501017	0.350781058447	-0.131540927636
O	-4.683607643364	0.126008144086	0.109914997439
N	-2.603017715618	-0.646330526082	-0.343046032779
H	-1.653864549369	-0.491201715340	-0.679946353843
C	-3.100675162347	2.305354224583	-1.659056365433
H	-2.839432459627	3.379124206628	-1.640491259839
H	-4.157262759505	2.238328180099	-1.968920065517
C	-2.210062517578	1.605156135732	-2.648011931166
H	-1.140472081715	1.593721290907	-2.397546387570
C	-2.615480476223	1.002027783312	-3.769600160340
H	-3.673127272894	0.972697499954	-4.054214117003
H	-1.905426951823	0.516273095164	-4.445728457497
C	5.859386723064	-2.554478649258	-0.524371961563
H	5.808663219568	-2.031903552371	-1.492375287747
C	5.049554899325	-3.836659370180	-0.740673350676
O	4.021417849456	-3.828617872958	-1.425305030555
N	5.475496618148	-4.951888832224	-0.116244363870
H	6.324815743134	-4.985355787595	0.432293728138
C	5.041656418621	-1.634217687705	0.548960242408
H	5.637857517113	-0.720693674457	0.704199906500
H	5.027836709061	-2.168895943585	1.511294270618
C	3.530607768941	-1.187199492477	0.207636905464
H	2.962993974952	-2.120229618138	0.057596219299
C	2.713056259384	-1.029774828701	-2.277650038852

H	3.315248014988	-1.910277083435	-2.546829723729
C	1.340109229199	-1.525311480953	-1.825987977801
O	0.445901019890	-0.737016393208	-1.471825893649
N	1.190990027391	-2.856718338448	-1.789335515869
H	1.999445225908	-3.467550303431	-1.899099988728
C	-2.065971575858	2.211280870406	2.671261507944
O	-1.563001895333	3.238103367100	3.137521314375
N	-1.323933458392	1.092293423931	2.370540345534
H	-1.826756748355	0.332241760846	1.915252889481
C	0.749573347604	1.130799411564	1.727997456737
H	0.402406440755	1.948572586941	1.100326306503
H	1.150929578289	1.386067755878	2.709388102107
N	1.426214879406	0.130639999688	1.051140016785
H	1.108654223509	-0.016423170750	0.082123745061
C	2.724996970033	-0.463341889485	1.393871278637
O	3.153907892358	-0.369642059135	2.515978335457
C	3.449330356861	-0.340561922232	-1.098094890573
H	4.467531116329	-0.096168084938	-1.437315661712
H	2.971611946855	0.632577380291	-0.910076467434
C	7.430718269591	-2.808566886457	-0.224188373523
H	7.881406943540	-1.804125563902	-0.145377917730
H	7.547842923835	-3.241866024888	0.785043000997
C	8.300783732575	-3.633022368507	-1.266318848771
H	7.774333798221	-3.765429555587	-2.223157910511
C	9.575588451916	-4.152081775907	-1.230473489249
H	9.976086530043	-4.654572890683	-2.114733662351
H	10.219084916923	-4.089442819415	-0.345850939314
C	2.663240745282	-0.112828033573	-3.478623159722
H	3.658468924796	0.160542250951	-3.852192384653
C	1.585549112449	0.376845173344	-4.099415817530
H	0.569835016871	0.153418120198	-3.763937571516
H	1.693300110450	1.029511862475	-4.970157627545
H	-2.959276358882	-1.596009787907	-0.393744183215
H	-7.127473964973	2.186902676563	0.065410461583
H	0.327937863495	-3.244283484790	-1.419530033980
H	4.939496084198	-5.806984416568	-0.221123127224

PEG_4000

E_{F4000} = -2067.771690080107 a.u. ($G_{F4000,298K}$ = -2067.120950438192 a.u.)

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C	-12.046990414611	1.818497347212	0.469732040499
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H	-12.186513386652	2.901949864675	0.385442693101
C	-10.816667678959	1.212900549357	0.339527499966

H	-10.816628020964	0.118836043355	0.451607978557
C	-9.360621262061	1.799625323165	0.098283934526
H	-9.443960336759	2.583937372162	-0.667163527531
C	-8.787915252164	2.560397676851	1.305791910861
O	-8.024823069482	3.504885529092	1.126470957060
N	-9.089453633845	2.101330716144	2.544078931084
H	-9.668787613692	1.280986850792	2.675950675142
C	-8.164814091878	0.784385077172	-0.461073997481
H	-8.499355873060	-0.248927955605	-0.275746466693
H	-8.144809144287	0.907738883613	-1.552189826683
C	-6.637279095569	0.886811715200	0.078738717471
H	-6.418191004474	1.946591832670	0.278525272900
C	-6.537082271066	0.081678424190	1.400641347524
H	-7.457480641028	0.266991544137	1.971004210364
H	-6.540401236367	-0.994417313340	1.156932340501
C	-5.349578741987	0.368314935897	2.340644819368
H	-4.415192832561	0.129485307322	1.814135116728
C	-5.350085001664	1.854594785184	2.712151455642
O	-6.098905148713	2.312445116882	3.572350413367
N	-4.486894686229	2.619308849048	2.003622023958
H	-3.970092223784	2.229259918126	1.222083746073
C	-5.441617036335	-0.495785890401	3.612947090820
H	-5.612599272041	-1.541882944142	3.302782672516
H	-6.318509071433	-0.174273509642	4.196492608264
C	-4.197122925392	-0.424875104652	4.453545178389
H	-3.285114551262	-0.817706158138	3.983609594366
C	-4.122601248073	0.090177539689	5.684841982996
H	-5.006305092908	0.503952407823	6.182577621147
H	-3.179453556507	0.119720991982	6.238761909497
C	8.541327294208	-1.620878755630	-2.249068792829
H	8.668226995566	-2.031746903464	-1.238518162384
C	8.854411713017	-0.131201261757	-2.114323411375
O	9.236882417652	0.357704560973	-1.045335262881
N	8.688613441569	0.619809100714	-3.220672493569
H	8.393996992684	0.228112607952	-4.106697786746
C	6.982904039822	-1.836247997719	-2.664990788215
H	6.809620779794	-2.923962207377	-2.694847067526
H	6.835365073383	-1.480563277591	-3.696517339709
C	5.803540884660	-1.187951360948	-1.758654722578
H	5.968700223737	-0.095522490998	-1.722027643386
C	6.707633196116	-0.981735764659	0.690088089077
H	7.720773426686	-0.914520259721	0.270533647400
C	6.178137404128	0.443545049242	0.891711026121
O	5.061538600521	0.662143009086	1.357126229733

N	7.017896002449	1.425905305636	0.497267515248
H	7.911700770727	1.223461249322	0.046826197342
C	-5.500323587884	0.406317419516	-0.941183386142
O	-5.744666829276	-0.028718279049	-2.037421783450
C	4.331136587739	-1.303708926782	-2.388152283485
O	4.130055978188	-1.746162134941	-3.491875678195
C	5.788906616277	-1.729069614231	-0.307279626832
H	6.059158117967	-2.797984558480	-0.321597656790
H	4.771462337220	-1.662898221690	0.101838717584
C	9.699066529746	-2.324607025443	-3.152620538121
H	9.453121836059	-3.399560186559	-3.194482403706
H	9.608844414087	-1.961537792517	-4.190796456738
C	11.210298141513	-2.175343070632	-2.683409925150
H	11.288418840707	-1.653329641105	-1.718253798756
C	12.410902472406	-2.575864191117	-3.225710117564
H	13.339561766819	-2.363214053197	-2.689589031349
H	12.486434266942	-3.105066635488	-4.182244077492
C	6.820045543501	-1.771914497681	1.976854020014
H	7.375846863265	-2.711497042316	1.858199083766
C	6.323262124763	-1.467719404021	3.179696400073
H	5.743270520454	-0.557455174200	3.348778956502
H	6.479404873343	-2.135322653182	4.032043832645
O	-4.177734202353	0.506828983828	-0.487804607151
O	3.293807123666	-0.832130986039	-1.592191087617
C	-3.055198014167	0.019686985636	-1.362229399861
H	-3.065282168947	0.621025486467	-2.282873880260
H	-3.272491904671	-1.023725594585	-1.632236656895
C	-1.620194356991	0.110128626844	-0.681284856348
H	-1.629667723143	-0.491594857068	0.246179758427
H	-1.428252796289	1.161478152673	-0.397888884370
O	-0.553631004850	-0.365180580481	-1.568099928743
C	0.817289677919	-0.325444309308	-1.048189849842
H	0.884212868297	-0.933458499712	-0.127387654485
H	1.086425957212	0.713789725257	-0.784274209428
C	1.882244259022	-0.873475191811	-2.095996109448
H	1.835811079991	-0.274697430529	-3.017676865663
H	1.646126278980	-1.916332148508	-2.353967761890
H	-8.475377143630	2.387962067257	3.302910704735
H	-4.522642717355	3.627931177340	2.108614966490
H	8.897604280033	1.611874307738	-3.181744616485
H	6.704453001081	2.388058205083	0.573075932539

PEG_4000-TSA

E_{F4000} = -2067.750658188173 a.u. ($G_{F4000,298K}$ = -2067.102124093158 a.u.)

0 1

C	-12.648921700439	1.592997889475	0.759865420596
H	-13.424302257085	1.174220248905	1.406159058472
H	-12.951270034164	2.319560039831	-0.001807867054
C	-11.332775159233	1.198984981618	0.933760370647
H	-11.181487766108	0.481351837150	1.753617467741
C	-10.020473071419	1.690310704347	0.306808724083
H	-10.134651385925	2.160331940271	-0.674437267089
C	-9.073189003829	2.502114630811	1.140718922257
O	-8.357870363379	3.365650382774	0.627150413752
N	-9.015323460716	2.241645199123	2.479750302516
H	-9.497659539397	1.441160437583	2.870384290839
C	-8.066369977158	0.468496213365	-0.455771569804
H	-8.449470315156	-0.542898885161	-0.288231840597
H	-8.233742498941	0.833420012827	-1.471725633578
C	-6.619784996011	0.721044879501	0.095497165426
H	-6.494214817573	1.815927053715	0.180907735633
C	-6.483010550308	0.077782843192	1.494885235681
H	-7.419725316796	0.282580395811	2.032381004593
H	-6.419925919543	-1.017722056387	1.383980351916
C	-5.316114800673	0.551452575771	2.383828647305
H	-4.369632086585	0.255499885411	1.910126425986
C	-5.355504750839	2.077724987226	2.504459470571
O	-6.147112353687	2.654144143102	3.251834096212
N	-4.485207900804	2.740674165729	1.713578978682
H	-3.927317379603	2.245755540688	1.025199932592
C	-5.399512868514	-0.090629522178	3.782215816599
H	-5.531121023219	-1.178891788184	3.649516324021
H	-6.296579904628	0.292651141108	4.293473639270
C	-4.172000113108	0.167398827603	4.611290451143
H	-3.243478123765	-0.286190690769	4.238887642434
C	-4.132103124105	0.913770438870	5.719541997069
H	-5.033974373565	1.394795243553	6.113291587274
H	-3.200663798293	1.073981208350	6.270827989451
C	8.630044719314	-1.483903087874	-2.338257391049
H	8.740959415699	-2.058226410786	-1.408788413435
C	8.944221743294	-0.038596589895	-1.953641480599
O	9.295864090023	0.267843408396	-0.808920437735
N	8.813885837422	0.882391527644	-2.928395172283
H	8.545325144245	0.639557575099	-3.873977481232
C	7.076827559436	-1.616998818476	-2.805879272207
H	6.901671542266	-2.681533558517	-3.029492711948
H	6.945333831810	-1.083255260110	-3.759924395887
C	5.885490197413	-1.133334539053	-1.816399172840

H	6.046926732990	-0.063599649466	-1.589892294459
C	6.757358181112	-1.352658686302	0.643403872551
H	7.774762203345	-1.211138748163	0.253832468384
C	6.219621184366	0.015008720623	1.082243717169
O	5.098856727216	0.146868283948	1.569695907404
N	7.057151404723	1.053354582056	0.867157000286
H	7.954887704435	0.933428321882	0.395428308485
C	-5.432277250765	0.243567020271	-0.900570239325
O	-5.661008907881	-0.211884057628	-1.990896126063
C	4.420811737557	-1.147388565623	-2.473441573679
O	4.231304429238	-1.425073927706	-3.631598197740
C	5.853687982501	-1.917103726721	-0.480059841392
H	6.127193595428	-2.967306397727	-0.675337128910
H	4.830723648093	-1.923411188509	-0.079285204480
C	9.797926971205	-2.034223417415	-3.330498331853
H	9.550650090148	-3.087249960695	-3.549323123413
H	9.722194664034	-1.507857542931	-4.297534649546
C	11.302715548640	-1.970903469799	-2.822941359592
H	11.367359132067	-1.628875260169	-1.779325120613
C	12.510964715674	-2.271597618268	-3.410942356090
H	13.431975575387	-2.159270839293	-2.832845308698
H	12.600036217806	-2.623066085633	-4.444995647543
C	6.858720278178	-2.354410033764	1.774274527812
H	7.419024987136	-3.258021862518	1.499808990579
C	6.349133393923	-2.265331099462	3.006574929811
H	5.764020065140	-1.399726817918	3.325781705345
H	6.499373643953	-3.071031014065	3.731057082685
O	-4.118489856222	0.386855207822	-0.443832793793
O	3.374798516092	-0.796483453627	-1.627557339851
C	-2.982997275940	-0.064752052044	-1.329038961865
H	-3.012592352604	0.550210102836	-2.239969380577
H	-3.180978786531	-1.108093351646	-1.612202513873
C	-1.546138823123	0.047088247391	-0.655999336979
H	-1.530311532864	-0.581091231452	0.253467738688
H	-1.378992389893	1.094776899440	-0.344641736090
O	-0.477317970100	-0.373013368155	-1.567331803508
C	0.894815905752	-0.346628852484	-1.049105040456
H	0.977212034938	-1.024305965458	-0.179586578523
H	1.144179673869	0.673594562696	-0.704357156784
C	1.965649679785	-0.788803882135	-2.139921665463
H	1.922407307270	-0.105716464652	-3.000943655862
H	1.731735464942	-1.802965140388	-2.496240787974
H	-8.159280766572	2.536168631776	2.954668177775
H	-4.531098691263	3.753594368370	1.669346582844

H	9.022777758166	1.853941939974	-2.723908545838
H	6.738390492867	1.987385597249	1.103272684017

PEG_4000-TSB

E_{F4000} = -2067.743994657176 a.u. ($G_{F4000,298K}$ = -2067.097741884826 a.u.)

0 1

C	-12.666840347736	1.554056015146	0.696924018827
H	-13.574452083415	0.974284639576	0.510822477438
H	-12.773762787179	2.520606180845	1.200599997572
C	-11.447476001813	1.044442446305	0.305717231491
H	-11.481664345215	0.064463887793	-0.189489216078
C	-9.972922605891	1.633781531722	0.361596388608
H	-9.931339359946	2.443301147985	-0.382912333368
C	-9.613630479513	2.349546498096	1.669814439774
O	-8.812189415349	3.278277854284	1.665824788873
N	-10.158649078724	1.857752087772	2.805510361887
H	-10.869758639622	1.136596532785	2.788829440797
C	-8.706107270656	0.627383089842	-0.065918627269
H	-8.953978544934	-0.380082621238	0.302840991233
H	-8.726245987635	0.583062319770	-1.165897646916
C	-7.246007426696	0.978621104503	0.413337153754
H	-6.950679833261	2.013691166936	0.225036797682
C	-6.922158584001	0.441117408804	1.778868821154
H	-7.677767592478	0.870128745408	2.467575533303
H	-7.110347873328	-0.645891719574	1.792911921438
C	-5.528621628175	0.709148770542	2.368697894559
H	-4.788334377615	0.212815485517	1.725264382311
C	-5.237620921539	2.215286475307	2.396090583991
O	-5.707313104514	2.947153385082	3.262288081766
N	-4.451421104468	2.664944484927	1.392169591382
H	-4.080451089870	2.032584375856	0.686169654613
C	-5.414277826651	0.132495265837	3.793882477056
H	-5.797619026304	-0.903150779923	3.777481253220
H	-6.061869442060	0.718267136942	4.464724726907
C	-3.998654644602	0.129323706768	4.300505647171
H	-3.300436724582	-0.517025713119	3.751210642781
C	-3.540174568619	0.857413113902	5.323612713586
H	-4.200577852334	1.524750909263	5.887876229086
H	-2.491501473396	0.816084246138	5.633166795820
C	8.777023577177	-1.516509574032	-2.343227528420
H	8.887043377765	-2.083687006307	-1.409289563688
C	9.087261279713	-0.067703401340	-1.968740913285
O	9.434748615490	0.248222583720	-0.825351722196
N	8.958300523005	0.845479226630	-2.950961356336

H	8.693613713373	0.594773918648	-3.895565380861
C	7.225130455244	-1.656532473394	-2.813341440143
H	7.052964454912	-2.723006738070	-3.029832587552
H	7.094603207539	-1.129926060158	-3.771487602813
C	6.030270595402	-1.168942934296	-1.830090299374
H	6.187308352138	-0.097042070937	-1.611199818278
C	6.898037596911	-1.368403875034	0.633215982774
H	7.915775787277	-1.226765107931	0.244638564012
C	6.355763017793	0.000741870638	1.061584912277
O	5.234009622130	0.132851370247	1.546644255438
N	7.190556571639	1.039929670044	0.840116665160
H	8.089370947709	0.919170674824	0.370675783319
C	-5.335406772409	0.195711469655	-0.866532465360
O	-5.609539343835	-0.338324818535	-1.897201383113
C	4.566706613292	-1.195783098564	-2.489150369497
O	4.379333231585	-1.493580124283	-3.642656633268
C	5.998123868293	-1.943106286980	-0.488041386785
H	6.274758554646	-2.993939548076	-0.675307580908
H	4.974368840756	-1.949321364772	-0.089247013208
C	9.948371726700	-2.071622346672	-3.328663515571
H	9.704028776567	-3.126842275217	-3.540022023756
H	9.873613036573	-1.552826402812	-4.299845294855
C	11.451837046534	-2.000978684062	-2.818168292334
H	11.513224603540	-1.651366383660	-1.776882434419
C	12.662180962340	-2.302950194206	-3.401169553726
H	13.581562607882	-2.184266358558	-2.821755756888
H	12.754536118602	-2.661581405014	-4.432460546383
C	6.999805478481	-2.362232345204	1.771025618091
H	7.564563708508	-3.265368818622	1.504289502973
C	6.485660034957	-2.267239291292	3.000974011579
H	5.896077765725	-1.401899179123	3.312529334586
H	6.636668047945	-3.067620721135	3.731147572508
O	-3.983087547826	0.365282283386	-0.464955404498
O	3.518838685564	-0.834215811871	-1.650189546808
C	-2.849016753307	-0.134212323770	-1.350695081246
H	-2.896058276236	0.434539797330	-2.290563992504
H	-3.051711397996	-1.191594914738	-1.571724684577
C	-1.405939453704	0.019988911171	-0.700836597558
H	-1.376817013692	-0.563621348452	0.237500083839
H	-1.246614827591	1.082740903318	-0.440624008513
O	-0.336089922824	-0.432600604601	-1.597866295905
C	1.036839402957	-0.375115517382	-1.084748067146
H	1.127717414349	-1.019849429561	-0.191267285361
H	1.278149218610	0.659106356259	-0.777911660990

C	2.109121292163	-0.847371319476	-2.161542328400
H	2.063010897748	-0.192715111333	-3.044162787559
H	1.878832678635	-1.873437572543	-2.484747182818
H	-9.932178475731	2.301835716969	3.688890353926
H	-4.254029178602	3.658022270474	1.330142777243
H	9.164779664823	1.818955394699	-2.753360895028
H	6.868747700132	1.974686529699	1.069048258522

PEG_4000-TSC

E_{F4000} = -2067.744276068501 a.u. ($G_{F4000,298K}$ = -2067.097388779123 a.u.)

0 1

C	-12.509353092724	1.293485215311	0.796863048240
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H	-12.761408452337	2.296108846113	0.433874884398
C	-11.232144374224	0.780135973997	0.741559940214
H	-11.115317410609	-0.236587416943	1.144541736906
C	-9.857643167780	1.398671520807	0.240588214923
H	-10.062294618022	1.935536494734	-0.696298030206
C	-9.309366510128	2.507063751847	1.154909448039
O	-8.672668316839	3.440046357027	0.674921367514
N	-9.488682455850	2.369868799272	2.491421191849
H	-9.963646912996	1.564326973709	2.880510085545
C	-8.585179511292	0.378584786009	-0.128023474206
H	-8.821970588869	-0.607093987871	0.304039910724
H	-8.607284875424	0.246892256895	-1.218271470798
C	-7.065320526371	0.736023724126	0.299734094228
H	-6.937739541186	1.824034062613	0.219109237993
C	-6.864407860611	0.290473700300	1.766343015121
H	-7.772748125171	0.556912369099	2.325091419889
H	-6.804150040574	-0.811583427361	1.792796633763
C	-5.662469475436	0.863504542485	2.541822810520
H	-4.739707177596	0.524258848876	2.049875808313
C	-5.715939982071	2.393812224815	2.489430098986
O	-6.422826552088	3.051692684060	3.250946502144
N	-4.946262902383	2.950589925729	1.524526489365
H	-4.532094915050	2.353588992498	0.810041617503
C	-5.667559557235	0.376165654915	4.002737527780
H	-5.812188090216	-0.718835214810	3.996630405184
H	-6.530156911801	0.822574791164	4.521941250091
C	-4.392305693767	0.703906045820	4.728486550715
H	-3.488273820378	0.212880240842	4.342973955715
C	-4.282700779653	1.546103168346	5.760903267081
H	-5.157790559920	2.066460534323	6.164923105930
H	-3.318624780437	1.748916153414	6.237093254755

C	8.857732387394	-1.432816360976	-2.427070660295
H	8.955515540920	-2.127339022698	-1.581933320423
C	9.170088784757	-0.053918213814	-1.846781412154
O	9.512405284319	0.092266736267	-0.668009988061
N	9.049596091577	0.992374831216	-2.687108670164
H	8.789098770056	0.883657140372	-3.659514383734
C	7.310425272121	-1.496801051122	-2.927846604330
H	7.136189994270	-2.522039281114	-3.291931439467
H	7.191667730165	-0.841412561398	-3.804580421014
C	6.107720928736	-1.143338486117	-1.897410505543
H	6.271687356058	-0.114293407552	-1.528206940586
C	6.947154271411	-1.692303325132	0.520518948255
H	7.969920484060	-1.505997597302	0.165113846393
C	6.409531422289	-0.392252510681	1.131511996554
O	5.282180494983	-0.319633718663	1.616219899633
N	7.255288979440	0.659765342779	1.070474669128
H	8.159608375463	0.598337288807	0.600110004336
C	-5.846290951199	0.097432601359	-0.621327372415
O	-6.116197314216	-0.699055653313	-1.500343314442
C	4.653265961679	-1.051792916646	-2.570308791673
O	4.481085611398	-1.139526142773	-3.760358328364
C	6.054836179653	-2.097445252712	-0.678231018924
H	6.326129821903	-3.114021488791	-1.008046117550
H	5.027064842494	-2.150609080943	-0.293735360682
C	10.038040982158	-1.849101490843	-3.468965856150
H	9.793917067048	-2.863507818014	-3.828402260436
H	9.974011295898	-1.199257199068	-4.358607460686
C	11.536733544521	-1.853451974976	-2.939617308208
H	11.589890142376	-1.637071665757	-1.862291705650
C	12.751117450083	-2.086020782507	-3.545633913245
H	13.665666227605	-2.045490076013	-2.948107481744
H	12.851401481946	-2.313031041414	-4.612948173130
C	7.031033801607	-2.835443999173	1.509848344676
H	7.587173856826	-3.699657622599	1.122961963116
C	6.511810181212	-2.904880897298	2.739393343853
H	5.930345543004	-2.083941333463	3.165568469788
H	6.650002916009	-3.800061297919	3.352726850272
O	-4.614109726343	0.505022823102	-0.296081803765
O	3.593371687826	-0.832956904572	-1.695767793508
C	-2.730901392176	-0.115604385120	-1.377743565584
H	-2.918354944392	0.737371650070	-2.032588618659
H	-3.233760012779	-1.047065827787	-1.644036842273
C	-1.336556028567	-0.176615682190	-0.657824068216
H	-1.341744820586	-1.010132578713	0.064509121444

H	-1.185222607443	0.767464187024	-0.104065205521
O	-0.255674117870	-0.365174400606	-1.634649696940
C	1.110271776108	-0.491788575814	-1.087401872486
H	1.147158905123	-1.347070514557	-0.389783365597
H	1.364626716034	0.422044113081	-0.522031110071
C	2.198390242632	-0.710869938477	-2.226603567420
H	2.175471193339	0.136248112093	-2.927911810567
H	1.967221095258	-1.627522158478	-2.788708670796
H	-8.873268037746	2.906433710326	3.098179930762
H	-5.052209892071	3.941589256790	1.332557374598
H	9.258235297636	1.925860054088	-2.348689961379
H	6.937905721407	1.555425775457	1.426624783745

PEG_4000-TSD

E_{F4000} = -2067.730368998208 a.u. ($G_{F4000,298K}$ = -2067.084802492866 a.u.)

0 1

C	-12.440309770764	1.577651571470	0.677898418275
H	-13.284681524379	0.961744525205	0.998039753034
H	-12.637568637529	2.629072088938	0.441149057290
C	-11.185649185765	1.016191682994	0.588440751660
H	-11.125716632227	-0.047966228663	0.859883050804
C	-9.769989957081	1.627408382253	0.208611094619
H	-9.919783813827	2.299238062045	-0.648162774998
C	-9.190920072391	2.564984260251	1.281355055030
O	-8.488906054782	3.515220099315	0.948566750459
N	-9.415503339266	2.254007237345	2.580605045693
H	-9.945164903390	1.431330323098	2.842487451262
C	-8.546955855314	0.599890834925	-0.263921701038
H	-8.827492738733	-0.414575788338	0.062063728565
H	-8.567956280353	0.584693921163	-1.361820792122
C	-7.008661322358	0.832941070912	0.199531808293
H	-6.834390920272	1.917890975177	0.261002418323
C	-6.825946026714	0.202042248959	1.603932225377
H	-7.732963772884	0.420197370633	2.184059241545
H	-6.789852598598	-0.895298332536	1.494292116896
C	-5.619818524115	0.650154841141	2.452822175024
H	-4.695192244470	0.372962005637	1.927988742045
C	-5.661847911902	2.171994884878	2.623103558911
O	-6.397640145140	2.717638151069	3.442502527691
N	-4.850959660211	2.861036078128	1.786612268593
H	-4.350333460343	2.385040277406	1.042778571473
C	-5.638936584553	-0.037650091748	3.831374081109
H	-5.778281741877	-1.121234473808	3.669887913743
H	-6.509609156735	0.329095538106	4.397340702354

C	-4.373117149710	0.190068694270	4.610014873311
H	-3.462482670397	-0.239595325671	4.170702598709
C	-4.279998742925	0.881282257810	5.750399961573
H	-5.162366352605	1.337022815502	6.212543216798
H	-3.322523364025	1.019480446594	6.261668192969
C	8.894358069367	-1.532285831662	-2.400825906744
H	9.006096975630	-2.097386344357	-1.465867978111
C	9.210723241750	-0.083412421131	-2.031482910528
O	9.566523405625	0.233620160257	-0.890971272922
N	9.077896094445	0.828107655498	-3.014667410239
H	8.808001410295	0.576182626172	-3.957491573832
C	7.340316447417	-1.669558744079	-2.864924463403
H	7.164205817675	-2.736181215108	-3.077253908351
H	7.207139537436	-1.144972842691	-3.823796152260
C	6.151872962661	-1.175534323367	-1.876745578632
H	6.312340797863	-0.103287855647	-1.662281222634
C	7.030863787156	-1.370476281947	0.582037190655
H	8.047019887500	-1.233479724797	0.187757673277
C	6.495501014410	0.001820430277	1.009456778076
O	5.376448143500	0.138909890330	1.499231446984
N	7.332882749886	1.037469250186	0.781537748620
H	8.229788649493	0.912383095665	0.309565837906
C	-5.884330837668	0.286689778525	-0.802947347701
O	-6.148444820432	-0.267070947718	-1.839793673912
C	4.684708477810	-1.196693911810	-2.530082368851
O	4.486041934118	-1.488204624850	-3.681625891460
C	6.122849686460	-1.945785139591	-0.532378316033
H	6.394705605288	-2.998063283317	-0.718151925414
H	5.101267703076	-1.947059580726	-0.128134334618
C	10.060959672424	-2.093323411886	-3.388630650193
H	9.813182986017	-3.148481404770	-3.596235590630
H	9.984588979146	-1.576869909295	-4.360911260454
C	11.566025417796	-2.025163115101	-2.882477445557
H	11.631098960916	-1.673769332054	-1.842022894814
C	12.773983563026	-2.331062050448	-3.468336383774
H	13.695230195107	-2.213503978736	-2.891663157685
H	12.862611903949	-2.691781584909	-4.499230369799
C	7.135441200439	-2.361268226117	1.722314624288
H	7.694448416456	-3.267766398568	1.454899582224
C	6.630011432489	-2.259595781306	2.955329244468
H	6.046422566092	-1.390535781783	3.267858568356
H	6.782386199355	-3.058071055149	3.687308663977
O	-4.553539112693	0.482021658075	-0.410924383770
O	3.640993938693	-0.831574428924	-1.678890396868

C	-3.439135194585	-0.038154520530	-1.282492326420
H	-3.496789905640	0.494450884799	-2.242507306597
H	-3.633102771356	-1.104091221658	-1.466434231811
C	-1.949171460688	0.132318482973	-0.679505365129
H	-1.927272484873	-0.412384335110	0.285977643634
H	-1.809729990605	1.210568247990	-0.461094716033
O	-0.977064233945	-0.366175861293	-1.609885653108
C	1.182494277069	-0.382296837902	-1.123659898567
H	1.003308856736	-1.073664306289	-0.298130458014
H	1.163813965483	0.679514499724	-0.870372272067
C	2.221365239754	-0.830422946011	-2.200654295468
H	2.191230933127	-0.155365238880	-3.067259847505
H	1.999305942929	-1.851090478021	-2.543168335476
H	-8.787241624239	2.664565533802	3.267520097520
H	-4.918556951701	3.873112183641	1.758363734831
H	9.289413621152	1.801230770433	-2.820563353751
H	7.015883535430	1.973836579468	1.010664911403

DVB_4000

E_{F4000} = -2312.387884065114 a.u. ($G_{F4000,298K}$ = -2311.776547737118 a.u.)

0 1

C	-5.015102107998	-6.556347106858	0.368932390821
H	-5.730363983063	-7.028406529655	1.047009943060
H	-4.949901497628	-6.943796356000	-0.653581896905
C	-4.246711625611	-5.506980123912	0.819837597958
H	-4.403712956817	-5.213128479067	1.866928342569
C	-3.068081826914	-4.662243538315	0.144079055451
H	-2.156283328327	-5.265564676729	0.280795038325
C	-3.299451771489	-4.637897194467	-1.371397207852
O	-2.539742894805	-5.190881438647	-2.162501512514
N	-4.395748051945	-3.954473542928	-1.782224659333
H	-5.083823997650	-3.604453561499	-1.126884172583
C	-2.769614969650	-3.174038074903	0.754671561973
H	-3.624086434324	-2.560012976704	0.457430479798
H	-2.834935316766	-3.274808499725	1.845057762878
C	-1.378370771886	-2.352246309294	0.433544420059
H	-0.587239448282	-2.955795387987	0.907948920004
C	-1.053119197138	-2.354206889196	-1.081023048863
H	-0.023612179566	-2.002146809877	-1.248699951022
H	-1.069474027720	-3.397349422680	-1.424086323297
C	-1.993115543013	-1.522212967167	-1.979296828534
H	-3.024775741907	-1.609564475910	-1.608910362996
C	-1.576990131913	-0.045875993354	-1.993925037763
O	-0.487659159272	0.300431611309	-2.449075232889

N	-2.489734381071	0.835085296842	-1.529081665938
H	-3.299770558000	0.518555509781	-1.002048767601
C	-1.956916853450	-2.037375274514	-3.438607950065
H	-2.137249652156	-3.124867308952	-3.418195400604
H	-0.943481235116	-1.875034854413	-3.839633573709
C	-2.982118334820	-1.375421593288	-4.314119726406
H	-4.028863439500	-1.555316771500	-4.032509248716
C	-2.718283457666	-0.589117374008	-5.362648979697
H	-1.687768078219	-0.374366673804	-5.666524503583
H	-3.517120317945	-0.131319849871	-5.953872556720
C	3.954052005209	3.776952809500	1.044305831055
H	4.089907084753	3.757075479191	-0.046220650879
C	5.011347378468	2.817514321794	1.592287510681
O	5.651354070228	2.061973198253	0.853542358933
N	5.185073539301	2.816262863895	2.928988049666
H	4.672882284404	3.433334531799	3.546653135582
C	2.479916288331	3.154338878416	1.356302110501
H	1.749676695058	3.881122642027	0.964389659278
H	2.349347333356	3.136268314579	2.450485615688
C	2.090533887246	1.691437559908	0.769696665006
H	2.836742131513	0.987038416183	1.171408090867
C	3.465813388831	1.057872932268	-1.388550704564
H	4.341026338445	1.651036248318	-1.090650008691
C	3.628173834250	-0.368774715152	-0.844681790935
O	2.850363472725	-1.273329041729	-1.150436156075
N	4.662366146124	-0.538405526477	0.005907760513
H	5.212006779148	0.258729647323	0.331265381936
C	2.182469890062	1.685125501452	-0.787904931759
H	2.103431976922	2.718518344421	-1.163822375018
H	1.322528324931	1.150777986763	-1.215130430449
C	4.245215774415	5.305696623026	1.510286587796
H	3.473045877748	5.924287676631	1.021059459256
H	4.042831637422	5.404186875809	2.591069324904
C	5.661494108475	5.947652088482	1.186869916218
H	6.271399085046	5.294533528926	0.544689938227
C	6.249497977882	7.148601599349	1.515697040486
H	7.250619410728	7.376948432940	1.140941131081
H	5.758587922277	7.899227815649	2.145181216231
C	3.357860305494	1.021466656748	-2.891192450872
H	2.560644704325	0.376619706378	-3.279403757957
C	4.131962968278	1.718240698502	-3.728193778296
H	4.931971220482	2.369512875576	-3.358875013021
H	3.993902050432	1.666314363234	-4.812342400468
C	-1.061317013851	-0.844904894461	1.004357829098

C	-1.967751711087	0.068177027083	1.611947162657
C	0.257349511457	-0.284611955545	0.819222764657
C	-1.586632503280	1.362317833681	1.996512681641
C	0.672351256450	1.059732009876	1.158847054571
H	1.000979596059	-0.921073692903	0.330252275146
C	-0.299084786167	1.850146219595	1.778030196363
H	-2.319158488053	2.027737461859	2.447783500692
H	-0.079877194513	2.875412958647	2.079862434179
S	-3.719464124144	-0.300270135868	1.823502995464
O	-4.336232091926	-0.413146877683	0.494018459830
O	-3.933356699782	-1.345340405636	2.823730876126
O	-4.355308144669	1.073745456362	2.425621758884
H	-4.367396463414	1.016643198727	3.399836707668
H	-2.216932031529	1.809360547730	-1.448789755565
H	5.855422079593	2.175325236597	3.340114448576
H	4.778280017626	-1.441552105836	0.454326090011
H	-4.638945953643	-3.962856315519	-2.766594605422

DVB_4000-TSA

E_{F4000} = -2312.362156304666 a.u. ($G_{F4000,298K}$ = -2311.753326146608 a.u.)

0 1

C	-5.807164207577	-6.856678193469	-0.030034444720
H	-6.455798980600	-7.427899854392	0.638370576760
H	-5.942103734953	-6.980488466590	-1.109224234859
C	-4.856427325507	-6.007323458646	0.512359744438
H	-4.814932318941	-6.007517509301	1.610721049435
C	-3.688806203167	-5.202999119283	-0.096200401575
H	-2.732626701874	-5.670542948171	0.158154062361
C	-3.733326059672	-4.866104616433	-1.550577206925
O	-2.762921501972	-5.032204216185	-2.294780085190
N	-4.901469346094	-4.338644158115	-2.002042236910
H	-5.708760979775	-4.232361203346	-1.400236691051
C	-2.898075764001	-3.082057173049	0.708018835068
H	-3.762302979592	-2.593860875223	0.261977660265
H	-3.059229352020	-3.340902508855	1.754323653056
C	-1.492907016823	-2.385305256683	0.411939674030
H	-0.732471614171	-3.027888184149	0.884398038596
C	-1.188494290624	-2.396013091997	-1.107020485479
H	-0.136493553089	-2.123559496051	-1.284358351898
H	-1.313140106710	-3.431317012679	-1.452657487576
C	-2.074874079064	-1.483714560692	-1.979713571913
H	-3.108885294022	-1.505768853337	-1.602767359966
C	-1.555409274613	-0.040096603561	-1.967780930284
O	-0.434946541519	0.230215909016	-2.397259046761

N	-2.412549987109	0.899660599973	-1.511166368541
H	-3.251176960221	0.634261171105	-1.001355247107
C	-2.085462086299	-1.972506316607	-3.448708768680
H	-2.343928972182	-3.044292565612	-3.437009248958
H	-1.065891940239	-1.874082597150	-3.855504947385
C	-3.068716505750	-1.226705547666	-4.304141049267
H	-4.122866234122	-1.336548915011	-4.013384900892
C	-2.761189873640	-0.449459751281	-5.347758457998
H	-1.721360435422	-0.304819804539	-5.661536780605
H	-3.531763731645	0.069665157857	-5.925760598911
C	4.134172864242	3.462692494525	1.286517754862
H	4.282140147808	3.506802913012	0.198578888034
C	5.146268517955	2.429105976641	1.783954729186
O	5.846221933098	1.772394926884	1.005998738063
N	5.217620219450	2.258280710930	3.119233464330
H	4.657832254690	2.797013598478	3.768263367013
C	2.626221314170	2.903494023668	1.545914231228
H	1.941674505131	3.681082009906	1.169481804127
H	2.467569973575	2.849351941992	2.635235114152
C	2.172634225578	1.485610687121	0.895757922099
H	2.874941916609	0.727596946367	1.281011242493
C	3.594412845375	0.926437610031	-1.237497368329
H	4.449476462846	1.485787560761	-0.832118252082
C	3.721002365073	-0.527208953722	-0.774483183736
O	2.890095223423	-1.388894025036	-1.067412378874
N	4.790821261937	-0.778021971405	0.011623554282
H	5.381248123282	-0.020222815315	0.357092628672
C	2.289305505330	1.526058530776	-0.659185173379
H	2.194266001728	2.569308160933	-1.004815250241
H	1.454312570748	0.981283151182	-1.120693139444
C	4.506025335044	4.941681262259	1.850949908560
H	3.762974361183	5.631874878813	1.415521240067
H	4.321293479690	4.970531994713	2.938838493523
C	5.953169275549	5.527987377557	1.558779089407
H	6.534264736892	4.874237414785	0.891153567641
C	6.598405389245	6.680955645957	1.946783723016
H	7.612428814382	6.875622515557	1.587997187557
H	6.141269834152	7.425497238829	2.608126936114
C	3.612791037375	1.097292807424	-2.741268428688
H	3.790492589954	2.133572855093	-3.057679738272
C	3.406349106345	0.166090486909	-3.677759033830
H	3.199728865471	-0.874257302668	-3.415995400009
H	3.431116410828	0.427568351198	-4.739698391960
C	-1.097112753781	-0.894929379547	1.009929282719

C	-1.974118308615	0.042144062730	1.619406801126
C	0.248755817567	-0.400288040804	0.856644144182
C	-1.542606939146	1.308468666792	2.039214849393
C	0.718041957786	0.915165466779	1.238725256785
H	0.971009323079	-1.058793146199	0.364004532081
C	-0.227942228668	1.736824878452	1.857133148952
H	-2.252447496557	1.997782420430	2.491215868498
H	0.034433905300	2.742797010420	2.188003159304
S	-3.742166101858	-0.264347600888	1.788675847741
O	-4.338552798640	-0.324732665042	0.447408746054
O	-4.013010356495	-1.321645107453	2.762529250639
O	-4.333124682932	1.120227691226	2.411595539042
H	-4.365531418014	1.041686906170	3.383851051051
H	-2.072815211924	1.851106586766	-1.414521401444
H	5.864442570782	1.574398147332	3.497520813410
H	4.889108911518	-1.705605318266	0.411750062241
H	-4.993095883376	-4.109660404302	-2.985111189910

DVB_4000-TSB

E_{F4000} = -2312.361877168581 a.u. ($G_{F4000,298K}$ = -2311.755029192329 a.u.)

0 1

C	-5.712213594244	-6.694868543378	0.139257157558
H	-6.529713766087	-7.076617961927	0.755846064738
H	-5.537208952345	-7.174115002567	-0.830001704515
C	-4.957742605206	-5.638645901013	0.597322445276
H	-5.229386196522	-5.246900374899	1.586898807922
C	-3.665589856727	-4.912744742555	0.007015917948
H	-2.814552744685	-5.566561087046	0.252185043634
C	-3.718939444732	-4.892178655188	-1.524784594123
O	-2.852788265861	-5.423534983103	-2.215374876616
N	-4.759844102822	-4.213321735821	-2.063094909348
H	-5.530861806912	-3.883037882889	-1.495235593615
C	-3.286102950596	-3.410652558654	0.594138365452
H	-4.030129727904	-2.708986272584	0.194148476122
H	-3.456067695042	-3.449353134756	1.677007961370
C	-1.824787435419	-2.831293978833	0.357003480631
H	-1.095716117569	-3.250754167704	1.054723618839
C	-1.311781703274	-2.731574266521	-1.050091600644
H	-0.256343247422	-2.422385475799	-1.055877344670
H	-1.333088963762	-3.767592148809	-1.440452985604
C	-2.107611101368	-1.839789791128	-2.030944764801
H	-3.173036879077	-1.860721809036	-1.757235378886
C	-1.589493964397	-0.394344202964	-1.982000315353
O	-0.461967181071	-0.116611303386	-2.384580916151

N	-2.458786395713	0.535919160569	-1.525522840828
H	-3.254357887844	0.257138842102	-0.954252133636
C	-1.972610263323	-2.352461869116	-3.483651279660
H	-2.230933078149	-3.424555830570	-3.488469416459
H	-0.917736222374	-2.259602027711	-3.787842564949
C	-2.864758312550	-1.617213596898	-4.442790774996
H	-3.943022435055	-1.727753064848	-4.262799331196
C	-2.450399306023	-0.846399748983	-5.453341724931
H	-1.383703725792	-0.700727532291	-5.656231444681
H	-3.157218777310	-0.333142080697	-6.112278257106
C	4.062926332729	3.968533894475	1.058014453562
H	4.192492013890	3.991565310376	-0.032935574588
C	5.121018545268	2.987223371308	1.561958942882
O	5.871826800778	2.383012127775	0.788165784642
N	5.180934250878	2.803852310221	2.895978710607
H	4.580667450382	3.300691066210	3.542335156670
C	2.578393874174	3.368303616827	1.354278198903
H	1.862304379447	4.104446585839	0.953754358946
H	2.428745446298	3.353486649922	2.446118726254
C	2.170964724597	1.908102223796	0.768897794967
H	2.907616351194	1.196316254629	1.177963866805
C	3.596157649056	1.328348544535	-1.368888878433
H	4.437296879891	1.964340547312	-1.062158278102
C	3.824494752678	-0.093134910709	-0.830826431363
O	3.067436040932	-1.020156779836	-1.117780468572
N	4.891283191088	-0.233143297475	-0.016117402979
H	5.445815582482	0.572692801965	0.277732786972
C	2.271986661747	1.883424218138	-0.787149380763
H	2.124703826242	2.903035212589	-1.180071608858
H	1.453057567832	1.279723141387	-1.205733446114
C	4.402643530233	5.470464731930	1.583069727503
H	3.632722400222	6.130785624030	1.148018216352
H	4.238686443126	5.514942181145	2.673678037219
C	5.828232419162	6.088104669197	1.251075718148
H	6.415278860592	5.433114228322	0.589978078940
C	6.449268908186	7.266446502080	1.600468080136
H	7.451673489773	7.478555019893	1.219569386882
H	5.983838629808	8.014818107168	2.251640036934
C	3.516375930259	1.287539452022	-2.873717089614
H	2.771051154493	0.591152821350	-3.276720915849
C	4.259363943379	2.031805849166	-3.697926206200
H	5.009988393947	2.732320879822	-3.315423673623
H	4.143947463778	1.970830231738	-4.784200928404
C	-0.965715615308	-0.589528422148	1.066062710271

C	-1.848600363629	0.283123561014	1.712225666013
C	0.334563737354	-0.063214758843	0.806982465049
C	-1.495392136144	1.587514171154	2.084466374442
C	0.748164009904	1.288024257070	1.163517154355
H	1.064516174936	-0.680559858482	0.270718715542
C	-0.211441756669	2.073466345122	1.814520104530
H	-2.224735328293	2.236425165457	2.569749376213
H	0.020684958690	3.098173506129	2.109916125841
S	-3.524502402763	-0.275639833761	1.987238404883
O	-4.218261409555	-0.395801158530	0.697819337957
O	-3.545958237054	-1.400837790502	2.923359624465
O	-4.256968282215	0.989161071703	2.712311348854
H	-4.161945150003	0.900121248986	3.679102597939
H	-2.093249744606	1.470982096229	-1.371514244361
H	5.864334944494	2.158168339177	3.277169742297
H	5.060026093643	-1.138493549434	0.410426265094
H	-4.875560010469	-4.209918779629	-3.070684410587

DVB_4000-TSC

E_{F4000} = -2312.344201391280 a.u. ($G_{F4000,298K}$ = -2311.735721165140 a.u.)

0 1

C	-5.349477515009	-6.706879443401	0.032509196291
H	-6.099367157497	-7.176818962690	0.673669120707
H	-5.246891082372	-7.082176762250	-0.991554300225
C	-4.585087431435	-5.675527238404	0.529072926704
H	-4.782020318027	-5.393100571297	1.572587867406
C	-3.370171223036	-4.835229852749	-0.086126474652
H	-2.474960065584	-5.462893031530	0.050341547986
C	-3.559731597442	-4.745808800978	-1.605375741790
O	-2.800122842099	-5.297468668470	-2.397538178145
N	-4.616920747473	-4.004295101899	-2.017992127650
H	-5.306249271907	-3.646413797216	-1.368281636909
C	-3.059396813560	-3.376740643837	0.582978505514
H	-3.890148908298	-2.733789545447	0.280108789658
H	-3.160979066950	-3.509229706763	1.667447425564
C	-1.642172747776	-2.579638763256	0.332238396777
H	-0.881022951928	-3.220551860418	0.806837233724
C	-1.262617150404	-2.528772050126	-1.169681293906
H	-0.214279472473	-2.211657456101	-1.280656138248
H	-1.306069649140	-3.554231868913	-1.560732120915
C	-2.130339895325	-1.619329133015	-2.065700345483
H	-3.177074721204	-1.673124483444	-1.732586288087
C	-1.652632826092	-0.160061843748	-2.014351158720
O	-0.530786185264	0.160087223245	-2.404971166741

N	-2.557554146239	0.740800156191	-1.571538152242
H	-3.401775646957	0.437102480470	-1.093080349968
C	-2.067751081065	-2.084900077317	-3.540812026725
H	-2.297767821517	-3.163237858984	-3.564193020690
H	-1.034900061530	-1.957269955496	-3.903330641230
C	-3.031601923645	-1.348174510989	-4.426215319919
H	-4.094021784254	-1.483321155369	-4.180724404141
C	-2.697438776623	-0.548192799665	-5.443879946734
H	-1.648880333834	-0.377197538456	-5.711730746990
H	-3.454400642190	-0.035387165852	-6.044963888843
C	4.342976197657	4.101715039270	1.197611436443
H	4.414512977467	4.149757797105	0.100304975326
C	5.390229834250	3.066283404745	1.605282924676
O	5.596604055477	2.072970456722	0.901189476910
N	6.034311014177	3.257413350903	2.771875788091
H	5.894033113526	4.076273193720	3.349276158489
C	2.855646707159	3.433812218618	1.520164409682
H	2.117238865252	4.174500239428	1.172082377452
H	2.766004754284	3.364140070857	2.615563580615
C	2.541671547557	2.032331718437	0.879203528010
H	3.099540760936	1.222509247688	1.346880262746
C	3.461144976627	1.035905991505	-1.347066241432
H	4.457663707108	1.488959319910	-1.248533321168
C	3.499277968172	-0.351580128077	-0.684730245677
O	2.690212903312	-1.238120938319	-0.956233305750
N	4.493341878583	-0.514287325707	0.216707517123
H	5.076367609976	0.272618891917	0.505664685666
C	2.441816296854	1.981576223349	-0.635286892432
H	2.596845499896	2.992468151281	-1.048892532178
H	1.432795811194	1.687849894117	-0.956611395085
C	4.637489272069	5.591493576314	1.752251369354
H	3.834634308847	6.227562838018	1.341287055605
H	4.481125985854	5.619434791953	2.845095696745
C	6.019366553696	6.285896113985	1.386591918443
H	6.532537173518	5.761788385851	0.566707175189
C	6.657115871062	7.419911868124	1.836838293913
H	7.604014575514	7.719965673982	1.380678834678
H	6.260066512270	8.045621704211	2.643882338312
C	3.081901861799	0.908076613991	-2.799225987166
H	2.130139421310	0.394699413549	-2.979428034633
C	3.799870061513	1.391459014714	-3.816990511743
H	4.750393835796	1.911162245465	-3.651814303521
H	3.464669775601	1.287012585324	-4.853360968449
C	-1.308120907397	-1.106175441995	0.965132473809

C	-2.210737538091	-0.171104791599	1.540693143544
C	0.048971432813	-0.593251980721	0.871022986006
C	-1.813260794090	1.105901257873	1.975613619586
C	0.459265870784	0.711042071907	1.288337985612
H	0.797606478598	-1.245956887126	0.409934396848
C	-0.493465733545	1.548706099658	1.856612369147
H	-2.552555284177	1.786945378769	2.392999691437
H	-0.245754591303	2.556162965328	2.200594207407
S	-3.981461607787	-0.490325633648	1.655025871737
O	-4.536505138307	-0.555584054448	0.295018567361
O	-4.275186157426	-1.551106948829	2.618171932887
O	-4.609851120122	0.887565719831	2.257862215016
H	-4.666319117142	0.810865134530	3.229167026806
H	-2.255173926473	1.701493931114	-1.446515495497
H	6.715345892704	2.568825680982	3.074535358095
H	4.527778356365	-1.380141727445	0.744814051377
H	-4.832240611042	-3.965126306429	-3.008087520806

II. PROBE-RADICAL COUPLING REACTIONS

NO_MBAAr1-TS

E = -1988.931159137085 a.u. (G_{298K} = -1988.293982389823 a.u.)

0 1

C	1.683034949372	-2.122493392398	1.498715269000
C	1.059625632435	-2.502122941433	0.156140545169
C	1.845878919310	-1.959679561881	-1.036362747832
C	3.323396058440	-2.412921482468	-1.010041927550
C	3.179040984630	-2.505368311533	1.607865104156
H	1.375121035670	-2.307489133130	-1.969593655175
H	1.591612292980	-1.040070984419	1.629296068452
H	1.124714688881	-2.611263709673	2.312325103891
H	1.819188544729	-0.862795352234	-1.032570877459
N	3.878898509955	-2.082253781595	0.346981763418
O	4.930795393648	-1.362315648052	0.430300148765
C	3.810301705570	-1.766892108168	2.793091176218
H	3.254157535523	-2.024098774305	3.705959025484
H	4.861641686412	-2.055438190667	2.925443925515
H	3.771716461987	-0.681190887291	2.662897049981
C	3.359271390153	-4.020371951182	1.859537669009
H	4.414095560114	-4.305445115723	1.735097218281
H	3.057944741116	-4.247645122110	2.893088724478
H	2.750686790992	-4.649333649560	1.200819236245
C	4.117864761576	-1.658505968611	-2.081092596314
H	5.173503705994	-1.962494119848	-2.071971528319
H	3.691551463281	-1.909094684219	-3.063919203571

H	4.054125883554	-0.574902054192	-1.943567139387
C	3.468734980951	-3.923229554263	-1.308611493484
H	3.239547950644	-4.097339586345	-2.370353269522
H	4.501547351488	-4.250256965206	-1.119102928696
H	2.795117912082	-4.559729106222	-0.725468059389
O	-0.343246679555	-2.143601570655	0.096539576440
C	-0.768463839726	-0.877829276662	0.133884901153
O	-0.028132117311	0.091266986583	0.226986537344
C	-2.243020065821	-0.740086728851	0.049018281125
C	-3.156016712013	-1.878688116987	-0.050910374601
C	-2.756177597336	0.546462033727	0.066088002893
H	-2.050841810545	1.377793628145	0.139904683645
O	-4.513131011258	-1.550158806508	-0.116813081772
C	-6.399667365964	-0.144089907426	-0.178673699957
C	-5.019633432784	-0.287658520859	-0.105321725624
C	-4.135585529749	0.816805555874	-0.010242145964
C	-4.704204166092	2.115921594586	-0.000624167125
C	-6.063373454563	2.316809716488	-0.085061985920
C	-6.945754167143	1.175526825428	-0.158960919089
H	-4.035233853942	2.977906457016	0.069707851937
N	-8.295449836939	1.359760597808	-0.209755836395
C	-7.310141307754	-1.342786574842	-0.286918949358
C	-8.583340750779	-0.959871540011	-1.038253552440
C	-9.232432582318	0.247925204966	-0.379838998785
H	-10.073929092643	0.610782289106	-0.991761670875
H	-8.337644199604	-0.718783822813	-2.086386582594
H	-9.301798563081	-1.793061425222	-1.052461710560
H	-7.571179802256	-1.710840125885	0.722569862104
H	-6.784829876275	-2.167674210871	-0.788562347928
H	-9.651448019387	-0.029289469287	0.606570829469
C	-8.017799406224	3.691377757419	0.603295476580
C	-6.662383821851	3.702499449632	-0.100409419632
C	-8.928489385955	2.672624734609	-0.065450525709
H	-6.801826789608	4.036421746852	-1.145451529365
H	-5.971483314742	4.418726820085	0.369140256868
H	-7.883624115938	3.429144667149	1.666492932943
H	-8.497088097481	4.681154009653	0.566118664386
H	-9.242394368261	3.035130685471	-1.062961256666
H	-9.848423114032	2.536638565997	0.526328788485
H	1.005605928494	-3.596619337538	0.080349335670
O	-2.905523055125	-3.060067846382	-0.082096587448
C	7.000539130653	2.171472946853	-0.178932955284
H	7.310321215890	2.237151671630	0.876280797717
C	6.147110550083	0.894947741507	-0.380418112629

H	6.808528334283	0.032785162459	-0.189708753369
H	5.832917515213	0.814506870550	-1.431966808042
C	4.961654004055	0.762210695721	0.513992696872
H	5.150346217994	0.777557953438	1.589668054331
C	6.308970394819	3.520596695595	-0.464980755092
O	6.772322958293	4.553737543600	0.009295872226
N	5.251237858770	3.513607572048	-1.309834335433
H	4.705006922599	2.673932629606	-1.517935065288
C	3.624310820272	1.120095991312	0.059922202694
O	3.356914514906	1.327325137228	-1.143869221984
N	2.640112904904	1.167916747339	0.997123862368
H	2.834191355167	1.001525907788	1.975505425601
H	1.668979255842	1.132652815141	0.692271562502
H	4.788954045083	4.405072678815	-1.460808508166
C	8.241292349405	2.108820156458	-1.040049502177
H	8.055487697655	2.043011856607	-2.120259455597
C	9.496623087817	2.121814290681	-0.583583513866
H	9.713877307604	2.187017087347	0.488010002855
H	10.352214079377	2.066784277035	-1.263128195132

NO_MBAAr1-R

E = -1988.936066609848 a.u. (G_{298K} = -1988.303800441388 a.u.)

0 1

C	1.802381954501	-1.929506598559	1.359192984488
C	1.126717195404	-2.356187566905	0.062770651478
C	1.889418535470	-1.815831899404	-1.139845649721
C	3.337274696821	-2.343958963057	-1.188500864064
C	3.258210971031	-2.428280677576	1.456859651495
H	1.377225168289	-2.108651105448	-2.069647753245
H	1.793833500671	-0.835054858635	1.419262127981
H	1.239661768527	-2.316188159441	2.222875742696
H	1.912244196131	-0.718871730977	-1.093440875172
N	3.976730334367	-2.165934465267	0.161843468883
O	5.248879746607	-2.230347231442	0.201826756349
C	3.980917838660	-1.640190949877	2.557768887545
H	3.430667834686	-1.748373104720	3.504254700287
H	5.005099149054	-2.008853280670	2.696077558459
H	4.028636619481	-0.572004461249	2.303594992627
C	3.335554226366	-3.932848882208	1.787321216018
H	4.378595853244	-4.271508920781	1.704753221166
H	2.990451695791	-4.104258790124	2.818100158829
H	2.717823453653	-4.548536586969	1.120495113051
C	4.138435367116	-1.515043595806	-2.201752945387
H	5.167279114438	-1.888409401241	-2.283367477503

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O	-12.571852669195	6.168166628446	1.096536189004
C	-13.510358831007	3.649804779613	0.396331910402
H	-13.796850076124	2.812927953054	-0.258237696013
H	-12.418953895264	3.753756144335	0.389259983733
H	-13.829991654001	3.414555116944	1.422980525518
C	-13.642376164683	5.300242091321	-1.492161057138
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H	-14.162936695157	6.161429359722	-1.934375228797
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H	-14.499797339777	6.889914156259	3.295353270904
C	-14.297412552939	8.354347635922	0.148754042354
H	-14.794187032254	9.293831700264	0.434688721233
H	-13.209376388691	8.511757657598	0.160382818270
H	-14.598607883793	8.111429912138	-0.879886863961
O	-17.902893330875	5.849025188109	-0.351236513502
C	-18.663711605384	5.205521486828	0.542712454875
O	-18.234118313809	4.721729706684	1.577104113924
C	-20.096806536796	5.124575261820	0.158400756078

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C	-24.184938208987	4.763327949301	-0.761315417408
C	-22.844144879891	4.860799971785	-0.408671009384
C	-22.315420327497	4.280401996663	0.771534510087
C	-23.211819449388	3.582611979409	1.619822739447
C	-24.552177853742	3.467290083498	1.326434175879
C	-25.063937686307	4.048217893469	0.107502133919
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N	-26.383098165987	3.912958060010	-0.211005369792
C	-24.714383994499	5.400380157066	-2.022822727846
C	-26.183170599883	5.775019789738	-1.836660907991
C	-26.976625347790	4.559281584201	-1.382483123175
H	-28.005620809366	4.851590320754	-1.117649720875
H	-26.269510232313	6.573482171871	-1.080291545036
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H	-27.056169261813	3.822036171662	-2.204505106553
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C	-25.507177858271	2.743662603364	2.244930087494
C	-27.310651273189	3.085159672611	0.562907751551
H	-25.979467368287	3.466403593215	2.936102324851
H	-24.958399271608	2.023273505443	2.870020267571
H	-26.144781019383	1.280534908133	0.781977566065
H	-27.332078320656	1.556519760420	2.073819203041
H	-27.942822475375	3.740038202724	1.192643170893
H	-27.985628934957	2.583655529007	-0.149886621692
H	-16.207394622852	6.592723385576	-1.061317095242
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C	-5.691216064824	3.051114241812	-0.976561048522
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H	-5.488515599981	3.878638601580	-0.272317754857

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O	-7.366196125686	1.511485683735	-0.152014103756
N	-8.094416221427	3.433621030775	-1.116998786728
H	-7.839935556950	4.361920153568	-1.438377968915
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H	-10.101599066337	3.677119845732	-1.570076006771
H	-9.679397067030	2.162016413463	-0.711835065850
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H	-10.001361816033	3.246352524412	1.300089457161
C	-9.885030070905	5.197207993399	0.626101718648
O	-9.571044700404	5.932099674660	-0.306163431888
C	-10.356610079413	5.727302145683	1.986223704270
H	-9.835257211897	5.152671265832	2.771772723731
C	-10.031907480658	7.213041918349	2.139726588978
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H	-8.949964723542	7.392753064041	2.055299522518
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C	-15.735400545321	4.773825041773	-0.230747317620
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C	-13.550792951366	3.608147536495	0.013492046935
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O	-18.218457490080	4.602093913598	1.524705470696
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C	-22.874128748615	4.925723500101	-0.327646125285
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C	-25.077164315057	4.044069418749	0.145373919430
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C	-26.251520258528	5.974800223419	-1.559359774515
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H	-26.322611684495	6.679729207494	-0.713706147855
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C	-25.461557384293	2.500195959498	2.129142194246
C	-27.308048980587	3.020072788280	0.541947217306
H	-25.919248056620	3.135393207818	2.910282961620
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H	-26.129903648324	1.210277917386	0.523800823918
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H	-27.998839296299	2.598872873660	-0.206724048817
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C	4.836661068670	-6.301861526211	-0.857102287410
H	3.971811732888	-6.173557802403	-0.190723451680
H	4.577104131536	-7.035621153455	-1.635263742332
H	5.675960876169	-6.698333585618	-0.268312581692
C	4.091001535852	-4.407125897492	-2.346187927848
H	4.124865884990	-3.376432200066	-2.697604737338
C	0.393127922524	-1.137306897882	0.122792952231
C	-0.634515613481	-1.927359885805	0.921674624550
C	-0.727229128230	-3.348080257746	0.380560371432
C	0.605930208106	-4.107148614855	0.515453876737
C	1.804738620293	-1.747593308725	0.216544092788
H	-1.506291636506	-3.908686883592	0.919687036679
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H	0.436707083434	-0.097973410765	0.483034725075
H	-1.021716682404	-3.303539398488	-0.676403873821
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C	2.656866056735	-1.206492545525	-0.940091688416
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H	3.667793163417	-1.626804196230	-0.905204229981
H	2.207482133172	-1.474341187025	-1.908325730309
C	2.486139857369	-1.418802816858	1.559790128772
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H	2.694018887615	-0.340129002783	1.623689393154
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H	1.868751123208	-4.999266705242	2.038858347719
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O	-1.917820289314	-1.266741509562	0.999321099708
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C	-3.944869900246	-0.341550771384	0.205117376729
C	-4.389790967369	0.000533327058	1.555757172727
C	-4.747937035158	-0.026414882942	-0.877461040843
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O	-5.626616252113	0.647957597336	1.629714173152

C	-7.619358518476	1.608385342626	0.825258857578
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H	3.278691382569	-5.058354070872	-2.672530496143
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H	7.312139916175	-2.038523972691	0.389621769431
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H	7.286994021994	-0.655755886872	-1.712853444293
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O	6.993224976417	0.539112441008	-0.027740184943
C	7.186583956578	1.790529571203	-0.642293741977
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H	8.576370636980	2.415241494382	0.900951486117
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H	9.015279716437	6.099795766895	-1.058681672245
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C	4.995357545265	-6.379960340655	-0.678599167011
H	4.041594344109	-6.248174286520	-0.148505550153
H	4.870147450458	-7.160756946752	-1.444138298321
H	5.753597778608	-6.716217208693	0.042705938857
C	4.421596667087	-4.587746000355	-2.362235632066
H	4.471308276368	-3.571106909171	-2.751870032970
C	0.444973180383	-1.274544054727	0.088028118198
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C	1.839515734593	-1.925310153064	0.162187825525
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H	0.515783133506	-0.250463778109	0.485720996946
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O	2.853712300121	-4.024530611930	-0.153891375932
C	2.706460787734	-1.372266045776	-0.977738602064
H	2.802317162809	-0.281040393891	-0.873895182752
H	3.703028930418	-1.826381627662	-0.961476449701
H	2.245567842177	-1.591541874084	-1.952868350709
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H	3.454803450068	-2.248121135982	1.574411350859
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C	0.521024643598	-5.462305287151	-0.574268637224
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H	-0.358190334749	-6.079891239176	-0.336722276104
H	0.436774591666	-5.121668457030	-1.617591190505
C	0.818430695768	-4.758356799087	1.820333679133
H	0.050112488882	-5.496494712570	2.095772626142
H	1.806596296670	-5.235900720795	1.882173243135
H	0.784811984932	-3.942751107665	2.556381047519
O	-1.871226957734	-1.372374379216	0.953431724517
C	-2.600883324881	-1.071577744949	-0.128006675416
O	-2.268594037468	-1.346862527042	-1.269168013289
C	-3.865506306498	-0.357432841985	0.185663103878
C	-4.305214422422	-0.048535300094	1.545932932942
C	-4.652609466378	0.022148098577	-0.887980125112
H	-4.300480610944	-0.227374702838	-1.892027422063
O	-5.518786956871	0.639110296671	1.638322227939
C	-7.472189642449	1.697815818996	0.861181015428
C	-6.293753838764	1.014676995925	0.585228125722
C	-5.872587623269	0.709320780158	-0.733390018018
C	-6.708721442130	1.119784060633	-1.802286417182
C	-7.893536587690	1.787089851713	-1.585888683339
C	-8.291543615183	2.105817877791	-0.234799237388
H	-6.398854884903	0.890923180459	-2.825573455214
N	-9.446560709805	2.794669452252	-0.008601080003
C	-7.892472838326	1.999067182983	2.279015992348
C	-9.415570651346	2.072116848980	2.363361186868
C	-9.946136575750	3.064960334402	1.340387619412
H	-11.046726357699	3.024618914607	1.303696532496
H	-9.846385686163	1.075886008993	2.165828483160
H	-9.743433164338	2.378612220891	3.367952022472
H	-7.455944252505	2.961003413659	2.605785620319
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H	-9.674409038470	4.098489146061	1.629525435914
C	-9.494066977652	3.513724698775	-2.386467537989
C	-8.791970735078	2.200711875383	-2.726549965334
C	-10.266213382652	3.354603960267	-1.085245504724
H	-9.554735826390	1.419437645165	-2.902433117794
H	-8.208844484984	2.285795994130	-3.655850128264
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H	-10.190594893427	3.814199459254	-3.183551668836
H	-11.151342357540	2.708614198997	-1.241093286317
H	-10.643721499321	4.332415514714	-0.743989589483
H	-0.314075199962	-2.137910612249	1.912182394127

H	3.678144912706	-5.279887324599	-2.761404172131
O	-3.771506995407	-0.303072529796	2.599636399336
O	5.963496954329	-2.798468525138	-0.843084069818
C	6.317806240246	-1.727800699532	0.037102493406
H	7.230828117404	-1.981131350079	0.598581488785
H	5.510743480603	-1.549206308741	0.764107223034
C	6.530359652428	-0.500081505769	-0.826676607548
H	7.348585038224	-0.682693866619	-1.551792304921
H	5.612137374108	-0.291337719997	-1.410736465374
O	6.837205517287	0.567326509860	0.038729854680
C	7.034242705415	1.798834552245	-0.613743295360
H	6.135184042919	2.099454995208	-1.188543309756
H	7.880101600658	1.747597712824	-1.328452644620
C	7.327481634185	2.832616735566	0.456201311902
H	6.488082424217	2.911328475724	1.165186030500
H	8.228490163906	2.560035736628	1.028596793434
O	7.526860681768	4.080128089263	-0.216399189748
C	7.782316181969	5.157779115953	0.547509621059
O	7.862712954167	5.100720339415	1.753921776297
C	7.935947416514	6.412497462274	-0.297605442173
H	8.698588023616	6.168650182012	-1.058320364842
C	6.618960823269	6.718781937243	-1.034174009228
H	5.812340772783	6.936071690931	-0.314805455215
H	6.744085732727	7.600942551632	-1.680538315057
H	6.305310855449	5.870731123537	-1.659469469041
C	8.415427161935	7.589193878696	0.550741590885
H	9.364499795651	7.359388492399	1.057731366407
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C	4.777496242415	-4.624582030681	-1.213714980890
H	5.317574376328	-4.656868546484	-2.175589254830
C	4.631463566048	-6.034420423018	-0.642110502732
H	4.084378004220	-6.007234425017	0.310926731831
H	4.074686448631	-6.671759539524	-1.345279200825
H	5.613985530294	-6.492699213510	-0.458575896001
C	3.427246186240	-3.953113026617	-1.491547582124
H	3.570662590303	-3.014497765785	-2.047482713614
C	0.258244528832	-1.086804114285	0.214998377176

C	-0.780227357500	-1.978905654281	0.882237738270
C	-0.810548684162	-3.349056881782	0.217213150623
C	0.566329237021	-4.044129894056	0.269562825997
C	1.671737825401	-1.706572555133	0.255518820001
H	-1.554671645287	-3.992385563570	0.712375472049
H	-0.034581489210	-0.928099348069	-0.831330707030
H	0.285803773301	-0.103949670797	0.710981240822
H	-1.113533786611	-3.226822542488	-0.830963679359
N	1.565811338811	-3.090365773224	-0.295845891712
O	2.848437743878	-3.703050455764	-0.216770817689
C	2.567551317715	-0.893624389911	-0.696070213695
H	2.556836067696	0.168353846673	-0.406329459658
H	3.606047485979	-1.246676008328	-0.654946653299
H	2.207983193265	-0.976656994817	-1.732474997236
C	2.291815762675	-1.626581762040	1.669005481167
H	3.216940538134	-2.218601260767	1.705050806098
H	2.542256000207	-0.580566324970	1.903074193972
H	1.622852769540	-1.987597320263	2.459528599954
C	0.515915581797	-5.267222728196	-0.663592101053
H	1.444484833117	-5.852005185259	-0.598953774548
H	-0.318185166870	-5.925045395056	-0.374750330215
H	0.366781323143	-4.951859315429	-1.706969596763
C	0.893293112181	-4.548705666310	1.693286966016
H	0.248420874972	-5.406806558133	1.937285918489
H	1.939988504102	-4.878787529686	1.741714118884
H	0.736400837477	-3.791062025301	2.470582946626
O	-2.086638121641	-1.358620616463	0.963547681299
C	-2.787921251293	-1.029607702391	-0.126270984109
O	-2.405781250583	-1.226099696755	-1.268334156419
C	-4.098876084960	-0.396126049989	0.176994945451
C	-4.569705980889	-0.117842263755	1.533466617523
C	-4.895997343046	-0.059765365260	-0.903127643845
H	-4.516513842487	-0.278503052971	-1.904332093777
O	-5.828735471820	0.484860408575	1.615730390996
C	-7.843255968816	1.408534342578	0.822215693183
C	-6.616899438723	0.810962239208	0.556000521259
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C	-7.012051328106	0.901286974589	-1.835141939460
C	-8.242854864138	1.483386109352	-1.628676078284
C	-8.676792432867	1.765609776646	-0.280697742869
H	-6.675937164748	0.700195503212	-2.856009154590
N	-9.879315548714	2.371770929223	-0.063920508197
C	-8.298691083236	1.670695330962	2.236983675726
C	-9.824047510329	1.639754764171	2.304561530559

C	-10.409889669523	2.600308188930	1.280835528233
H	-11.504789999227	2.485811130264	1.232394025580
H	-10.184077759960	0.617791618612	2.097016242715
H	-10.182781411205	1.917256916790	3.307036808164
H	-7.932044929001	2.657624370630	2.574954043193
H	-7.855232422059	0.929163331382	2.916427248537
H	-10.211754837048	3.648225851588	1.578030080446
C	-9.950396547556	3.099741341387	-2.438508523368
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H	-8.569593535384	1.971088757407	-3.699610484656
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H	-11.560574611375	2.175520658057	-1.316175703448
H	-11.171817291441	3.827485518937	-0.805028114817
H	-0.531038689577	-2.095844085446	1.945329225929
H	2.790544009147	-4.619875056665	-2.095725274264
O	-4.026627550529	-0.330491839626	2.591697895426
O	5.795857960361	-2.516826095041	-0.816298117951
C	6.481571779761	-1.558433108029	-0.002610914524
H	7.474439597047	-1.940337990267	0.281742031672
H	5.910517494331	-1.373272962910	0.921237312693
C	6.606137921070	-0.288134150129	-0.821517080051
H	7.160062816470	-0.497812176712	-1.758493146523
H	5.600159276620	0.078165445586	-1.107631783109
O	7.282924961940	0.651990187776	-0.021715525131
C	7.476460029456	1.903082986447	-0.637363543760
H	6.511249856316	2.364204193310	-0.928326080781
H	8.088439374379	1.811236324787	-1.557127267136
C	8.187075261745	2.789502712569	0.367070825422
H	7.581487367677	2.911009488320	1.279164307814
H	9.154272932205	2.350937383749	0.660198639589
O	8.389930832231	4.057154524012	-0.265596147466
C	8.993940489667	5.015987223232	0.459830672491
O	9.374061631524	4.836056723355	1.594822730899
C	9.110330280183	6.314218898146	-0.322864937491
H	9.594856516336	6.045809244645	-1.278287534898
C	7.708371426180	6.863477858569	-0.644949199180
H	7.167459530987	7.116383302362	0.281733187877
H	7.791293324787	7.779024356939	-1.250365385459
H	7.111384275024	6.129078322705	-1.204343414609
C	9.975030096066	7.328036025340	0.424765611167
H	10.978201896426	6.926216765947	0.631926207810

H	10.085018857116	8.246977894022	-0.170832532381
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E = -2184.133498651629 a.u. (G_{298K} = -2183.388535679966 a.u.)

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C	1.091464147181	-0.993648660260	1.421838770659
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C	1.116537725208	-1.244209780723	-1.068667592452
C	2.640590511112	-1.470007533827	-1.101093809487
C	2.618075888324	-1.176857310349	1.519247975667
H	0.662033705774	-1.770124223765	-1.922407841286
H	0.866454220003	0.076196449995	1.329700093391
H	0.631505741654	-1.351336020595	2.355908101044
H	0.913240692122	-0.172244581161	-1.190955624447
N	3.238088581548	-0.941813530415	0.171600603174
O	4.525227536699	-0.814817098116	0.179793996217
C	3.162539827537	-0.126735485233	2.497344192636
H	2.724675145542	-0.299474227386	3.491559692051
H	4.255283978590	-0.190725214553	2.575553818606
H	2.885548833910	0.886492044393	2.177288160638
C	3.006232559898	-2.577888843153	2.038345230887
H	4.096076151588	-2.706507723996	1.965869893011
H	2.710723615013	-2.680460457641	3.093307051274
H	2.525250927851	-3.389657513754	1.478086566204
C	3.208759378780	-0.677381760617	-2.287253027036
H	4.295937132233	-0.787411608332	-2.368213071255
H	2.758251209168	-1.060544093164	-3.215135585357
H	2.966177690925	0.389303784051	-2.215382471798
C	3.002836973272	-2.959857798821	-1.284311866914
H	2.697905560174	-3.293864492646	-2.287391990300
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H	2.513563398812	-3.614523196289	-0.552526646314
O	-0.962046994015	-1.635259431653	0.212984063015
C	-1.603829187582	-0.467818678365	0.088370005078
O	-1.041668620178	0.608708053062	-0.035257107376
C	-3.083701470635	-0.594323782955	0.109370970981
C	-3.785216952626	-1.865143364401	0.288765587638
C	-3.814184392719	0.571216759717	-0.048240231406
H	-3.262778079145	1.505508831440	-0.179627211018
O	-5.180725175774	-1.781432669360	0.285108854017
C	-7.286867748322	-0.739051175039	0.150176530316
C	-5.901036955837	-0.638561188941	0.125113035991
C	-5.222483780544	0.594054833018	-0.047487144431

C	-6.010534919655	1.761862854143	-0.207585649156
C	-7.386690863675	1.718313401105	-0.204317413149
C	-8.055817187278	0.453881761111	-0.006724109927
H	-5.502366661517	2.720478035159	-0.343142816779
N	-9.417951611806	0.401570115884	0.029809438962
C	-7.975794533923	-2.069745733311	0.328959250511
C	-9.335799283357	-2.045628453377	-0.365450618559
C	-10.151762752831	-0.861054499657	0.129394519194
H	-11.075156720389	-0.758820185784	-0.463429986941
H	-9.193859969585	-1.963930251236	-1.456452054723
H	-9.895281567392	-2.973830307225	-0.175539786397
H	-8.112351940738	-2.282605224846	1.405407877177
H	-7.341514909343	-2.875879657506	-0.065854884005
H	-10.463146933942	-1.019497779081	1.179830047291
C	-9.509568707651	2.854685807629	0.415256269992
C	-8.221604668631	2.961073058867	-0.398593468821
C	-10.263918179758	1.596847350327	0.010709822290
H	-8.479229909481	3.073881848875	-1.468183261444
H	-7.642066536870	3.853695189010	-0.118954996045
H	-9.267994595903	2.813693743005	1.490976715989
H	-10.157918605001	3.729462068999	0.256424443534
H	-10.697833103520	1.718065997175	-1.000269684004
H	-11.107323666860	1.420351570201	0.698279319005
H	0.637838691315	-2.803005458923	0.340777651766
O	-3.332530187064	-2.974725525728	0.442574626413
C	1.129142899375	3.208864309378	0.873337503535
H	0.537694727085	3.934834929446	1.439812957262
H	0.616861704633	2.298125930951	0.546385439157
C	2.415121733506	3.442040283643	0.590871531020
H	2.886022822305	4.376472244366	0.923511795138
C	3.307964861882	2.509533017746	-0.197279102413
H	2.817829448695	1.529329355971	-0.264015823199
C	3.360057409222	3.018783903206	-1.649394333613
O	2.516647446387	2.662735508840	-2.467635206348
N	4.342933218387	3.894045509828	-1.958292550724
H	5.030940413135	4.207579449255	-1.286292169360
C	4.675242616483	2.335654929694	0.484358562989
H	5.200373218777	3.316716421158	0.536530749659
H	4.507756141579	2.088369291979	1.545775474890
C	5.578204869533	1.311643965718	-0.116467423586
H	5.492696497694	1.107896178398	-1.186196240689
C	6.898442003663	1.080950455705	0.547449343180
H	7.635198551925	1.807417999714	0.140093366405
H	6.809048294662	1.320428864170	1.621128892959

C	7.513323501898	-0.333077876476	0.429679587325
H	6.799879904052	-1.039929691605	0.876974216896
C	7.715270243899	-0.702923274981	-1.044688400888
O	8.712335772427	-0.360026677467	-1.674197845465
N	6.705595871914	-1.427056289178	-1.584327430051
H	5.815719093405	-1.472755078513	-1.082341119290
C	8.852803658709	-0.419633721513	1.183967722236
H	8.712078298936	0.023509081810	2.185744233901
H	9.597737451238	0.191222439095	0.650482242212
C	9.342767236609	-1.833084195940	1.333924158220
H	8.717129780560	-2.487170773413	1.956748535478
C	10.437346068374	-2.340257267529	0.757875899176
H	11.078738814112	-1.725794841509	0.116992742973
H	10.730073749929	-3.384879637357	0.900990714103
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H	4.374774184979	4.284200505139	-2.893926518848

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E = -2184.136756510969 a.u. (G_{298K} = -2183.396886951897 a.u.)

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C	1.075015552499	-1.411821831137	-1.031025523391
C	2.587830234123	-1.699131598067	-1.066549495861
C	2.560592683960	-1.391649225087	1.573117082517
H	0.603058311289	-1.918026867581	-1.886887776873
H	0.863804107100	-0.068400824619	1.347768069864
H	0.563940261394	-1.471122812155	2.389197745650
H	0.911250011464	-0.333182722232	-1.152069789674
N	3.213835992035	-1.244504199200	0.224379646236
O	4.486508010010	-1.153365857438	0.241913862190
C	3.159029260442	-0.330466318946	2.506603465392
H	2.670188596110	-0.401966427908	3.489507771434
H	4.238176603733	-0.480525332711	2.636477095009
H	2.984101723739	0.679433352671	2.111207496163
C	2.880632042369	-2.794435039420	2.127784934118
H	3.964952164778	-2.969861238972	2.078439338332
H	2.560825222633	-2.856984239216	3.178541111645
H	2.374205619105	-3.596040131051	1.574031736979
C	3.205413935371	-0.895084744639	-2.219166262907
H	4.281589399492	-1.081463174558	-2.311179349623
H	2.722909549530	-1.204082589234	-3.158720643919
H	3.048029725383	0.185584462072	-2.097616097298
C	2.893468009569	-3.197043698615	-1.270147404938

H	2.564280819010	-3.505720716850	-2.273437301527
H	3.976314542917	-3.372014980388	-1.190425806250
H	2.387922369204	-3.839403952955	-0.537376210728
O	-1.018980447824	-1.744920037400	0.243130313455
C	-1.630719606098	-0.562360709628	0.103801808707
O	-1.039518979721	0.496703884427	-0.032661714499
C	-3.112637210000	-0.650595383007	0.122928868171
C	-3.846224869098	-1.898345570602	0.332605705328
C	-3.812884947809	0.528864230436	-0.066189688232
H	-3.237682279953	1.445538182297	-0.217998305899
O	-5.239072477616	-1.780433661245	0.318552286830
C	-7.317802052756	-0.690047644839	0.144629241732
C	-5.929870518009	-0.624393236335	0.125895566125
C	-5.219976295283	0.586547258900	-0.072893907916
C	-5.977914565910	1.769157655638	-0.266510797865
C	-7.354640266166	1.759651729367	-0.270729075573
C	-8.056041414278	0.517342579935	-0.046100646819
H	-5.445268889334	2.711201693696	-0.422594230997
N	-9.419092414051	0.499620570342	-0.016527525814
C	-8.040328378734	-1.998710549306	0.351051043069
C	-9.395957039761	-1.957782345768	-0.351049261556
C	-10.184468838775	-0.741659381016	0.110587411344
H	-11.102510707218	-0.631226879455	-0.488986206114
H	-9.246899201843	-1.906139257760	-1.442922232855
H	-9.979254938953	-2.866949436115	-0.141756279172
H	-8.187203343335	-2.182631266137	1.431441604059
H	-7.424258541256	-2.829301606663	-0.021231834378
H	-10.504015981189	-0.866287339267	1.163106198748
C	-9.452259833924	2.963293231655	0.306372158866
C	-8.157276615843	3.017262227199	-0.501510934541
C	-10.235094108704	1.714505331178	-0.071117009683
H	-8.405705483518	3.109197960083	-1.575253236142
H	-7.557429826366	3.902127239560	-0.240679260565
H	-9.218089415581	2.943744968132	1.384307317684
H	-10.077830944726	3.849388509504	0.121253026478
H	-10.659996862916	1.820559216206	-1.087587874367
H	-11.086534933196	1.576273547049	0.615260632044
H	0.550128644492	-2.950374237912	0.384994973942
O	-3.421422655774	-3.013715251854	0.520081103294
C	1.185295411328	2.918005306205	1.033933138293
H	0.555383761569	3.509020275692	1.705828463406
H	0.717240545472	2.052381180225	0.554898847998
C	2.460085077345	3.256716799335	0.813540337093
H	2.872743693249	4.143836184689	1.312156265088

C	3.403015982856	2.520654213445	-0.111692371400
H	3.031962580199	1.498619066569	-0.267364230002
C	3.389170225154	3.158847866540	-1.511572845550
O	2.998025254346	2.542041953870	-2.497995649290
N	3.828815165390	4.436851107133	-1.584886756444
H	4.143564817956	4.952332876855	-0.772682229056
C	4.831358028753	2.444915010434	0.460941673643
H	5.192364393432	3.469200170782	0.694633868260
H	4.781751297205	1.948607151280	1.450940753839
C	5.818307475416	1.741946032049	-0.408796600488
H	5.486897322442	1.289280214090	-1.347510819839
C	7.224084160362	1.534065653186	0.048514358968
H	7.946894737417	1.971431780995	-0.668321644194
H	7.380514262803	2.057806067574	1.006828357408
C	7.616833792822	0.042819620393	0.239172434595
H	6.817015456687	-0.451043392286	0.812178198581
C	7.746363648754	-0.620844089743	-1.137458558152
O	8.701751944887	-0.378518856434	-1.872484162221
N	6.752112541432	-1.472120504620	-1.473817491880
H	5.894305699707	-1.522903487442	-0.918503678857
C	8.950243531598	-0.098774536908	1.000505464066
H	8.880565501759	0.501719554639	1.924930613361
H	9.755545123245	0.330032670613	0.383411011682
C	9.264231901207	-1.524535969151	1.358636420399
H	8.557678118588	-2.005369937572	2.049011176680
C	10.295279370032	-2.234034127111	0.888322240672
H	11.014680327460	-1.796119958530	0.187790745924
H	10.457903968459	-3.275352438046	1.182491579182
H	6.762845273981	-1.875992337792	-2.404749336685
H	3.835176027923	4.907185003718	-2.483255497403

NO_DVBr1-P

E = -2184.190156187528 a.u. (G_{298K} = -2183.440531115384 a.u.)

0 1

C	1.005768097103	-0.523477619452	1.737507193504
C	0.490374916583	-1.412264034987	0.615491127641
C	1.170663385081	-1.061693348787	-0.699391677282
C	2.709717775150	-1.158777806251	-0.613112866515
C	2.539238548180	-0.604596669732	1.892830122052
H	0.816583646660	-1.735161835892	-1.495739711585
H	0.726366797521	0.516172921870	1.521906955733
H	0.534549272087	-0.810617211715	2.690607119766
H	0.898013186298	-0.035237064781	-0.978326091058
N	3.133978534790	-0.310477838177	0.548611586755

O	4.554059906036	-0.370107143554	0.692432961855
C	2.951920341335	0.501578083732	2.877553586807
H	2.420840940892	0.355736248511	3.830343345642
H	4.029953489794	0.463465114875	3.081839649381
H	2.692458594663	1.497981482135	2.496862585909
C	2.983038914350	-1.951833559212	2.511182451183
H	4.073179873605	-2.059374923549	2.428211018356
H	2.715910995813	-1.971583420463	3.578675641398
H	2.514908446806	-2.825851924531	2.044843601504
C	3.265157377632	-0.543340427009	-1.909715945210
H	4.347876451236	-0.698161017254	-1.995563410268
H	2.797200118708	-1.042000418376	-2.772843149102
H	3.038965942709	0.528572479063	-1.969646836163
C	3.194174022858	-2.626306301792	-0.553279364543
H	3.131489877956	-3.077477938719	-1.555086635498
H	4.242318562925	-2.657832945509	-0.226016906643
H	2.608195684077	-3.258406996819	0.123950134107
O	-0.955651878420	-1.414207680010	0.517664066535
C	-1.650225928975	-0.308527095180	0.228996646709
O	-1.143644358374	0.783657038044	0.029653766209
C	-3.120704143076	-0.524863487259	0.174800841993
C	-3.755915658523	-1.825530866466	0.383251791695
C	-3.906941928563	0.582191040143	-0.092260861291
H	-3.403439932871	1.539507313557	-0.248404902247
O	-5.151861198546	-1.827453085563	0.303838185394
C	-7.304472783579	-0.923960544686	0.001679582063
C	-5.927182813188	-0.740895517843	0.041345170052
C	-5.312650281858	0.518871869339	-0.168547427275
C	-6.156813502738	1.625308892775	-0.438356489197
C	-7.526512905117	1.498287475273	-0.503478260467
C	-8.131300068158	0.209017253417	-0.265106379297
H	-5.698231756125	2.603976858059	-0.604126997595
N	-9.488532418240	0.076000438418	-0.295114880891
C	-7.923545081345	-2.282438401094	0.223074962675
C	-9.244355169379	-2.379801901034	-0.537362829733
C	-10.151904697071	-1.220925546214	-0.153696574819
H	-11.048616716652	-1.209724972294	-0.794157790759
H	-9.050544871464	-2.350628829656	-1.623039503092
H	-9.758400406329	-3.328199738210	-0.320679755991
H	-8.103785275300	-2.443892385776	1.302043175618
H	-7.223480063610	-3.068836935861	-0.092526335334
H	-10.506063908686	-1.337857794173	0.888672179523
C	-9.742993870125	2.536875811847	-0.065196051402
C	-8.419536747186	2.675200594386	-0.814849986710

C	-10.399379342070	1.214276559142	-0.432286025579
H	-8.622954500380	2.712051927938	-1.901306491315
H	-7.909011823306	3.615717118859	-0.558592526788
H	-9.560343919895	2.572033555820	1.022287579739
H	-10.430801559855	3.360045215565	-0.310394022981
H	-10.781388425071	1.250786055159	-1.470497938518
H	-11.269090518452	1.027079246721	0.218695942351
H	0.691688684164	-2.463502143700	0.861614464312
O	-3.248088835683	-2.897466125108	0.613619057688
C	2.119902478478	4.298074128495	1.491623204321
H	1.920617765204	5.238770438355	2.013169900021
H	1.301200218957	3.572417416506	1.438662664470
C	3.310554896243	4.042057789346	0.940192164089
H	4.111850955058	4.790036078815	1.005744299089
C	3.653423446916	2.767677985027	0.205299286856
H	2.826828303170	2.055544209270	0.306837151022
C	3.696407903996	3.073759856215	-1.301829041698
O	2.698706753056	2.923263413808	-2.001294670893
N	4.864644218183	3.538450198048	-1.803608093032
H	5.686940116888	3.689550189433	-1.234387145932
C	4.932162966400	2.123583295538	0.773459359854
H	5.788669775119	2.799485436642	0.608099948041
H	4.844129559241	2.047834868151	1.864795999022
C	5.312427524533	0.751383266583	0.200967874192
H	5.224496875796	0.801415324921	-0.896488916349
C	6.759037007524	0.402549124071	0.561300636128
H	7.410775022081	1.206556416271	0.186257035238
H	6.850822576031	0.384440006882	1.660128993860
C	7.264148995399	-0.929079237967	-0.009664834814
H	6.585124831362	-1.732515097628	0.313143609559
C	7.295395955064	-0.858847979115	-1.538833877811
O	7.861913695812	0.059219068666	-2.124084033557
N	6.680802886590	-1.871539195582	-2.194377408572
H	6.206479776761	-2.620510435477	-1.706842139277
C	8.689864902110	-1.243041308696	0.502242381462
H	8.664762192988	-1.201151109713	1.605824402513
H	9.372182478988	-0.447524294055	0.160024500483
C	9.195831627616	-2.589163126997	0.065984627032
H	8.612670075336	-3.451857304851	0.415640839758
C	10.262022037378	-2.797192896407	-0.713045665832
H	10.863219196564	-1.962532638108	-1.090503361064
H	10.574277010711	-3.805201086861	-1.001837241767
H	6.683088097858	-1.881109382596	-3.208889079012
H	4.911083125002	3.788618537115	-2.785432504907

NO_DVBr2-P

E = -2389.572828130172 a.u. (G_{298K} = -2388.954768005742 a.u.)

0 1

C	2.173137141339	-0.613013950067	-1.104452098584
C	1.680555472577	0.234537866340	0.057260061293
C	2.190503861760	-0.347459752341	1.365903064842
C	3.733455987070	-0.420498989106	1.428167541669
C	3.713423883330	-0.699367513131	-1.146612061741
H	1.840455255124	0.263683630361	2.211808584020
H	1.757108807081	-1.623235940281	-1.000623754935
H	1.819835081444	-0.196353058452	-2.060105205104
H	1.782332939556	-1.359054247560	1.486796239345
N	4.178808255748	-1.168735896087	0.198645988003
O	5.628144913690	-1.148627085730	0.104766489254
C	4.070501266901	-1.786299753614	-2.172246718230
H	3.722754459459	-1.499388617615	-3.174712915614
H	5.160453428543	-1.925797384887	-2.234866003830
H	3.551143477554	-2.723238485161	-1.917066874317
C	4.340083578535	0.630503108915	-1.625004511544
H	5.434557794042	0.591652746574	-1.547515124530
H	4.075017750787	0.797087158682	-2.679681284233
H	3.989024232428	1.501010023317	-1.059794269626
C	4.069575481999	-1.256361067805	2.681440983392
H	5.131515608516	-1.199011263602	2.951356706249
H	3.497706925892	-0.860761552143	3.534773749581
H	3.795166551455	-2.306885976444	2.525642823547
C	4.364520109548	0.976376482802	1.601242104974
H	4.152931327216	1.342923602365	2.616917533602
H	5.454752948574	0.923916235796	1.479966568396
H	3.979872260106	1.723016311010	0.896858404646
O	0.248067778851	0.434081612707	0.047861689878
C	-0.613564597902	-0.583397709588	0.167044597196
O	-0.276203683168	-1.750828911758	0.275678272502
C	-2.039220784599	-0.163412972330	0.150175436759
C	-2.472459267931	1.230603312334	0.061407399257
C	-2.988143824066	-1.168046276903	0.230423534012
H	-2.633953259799	-2.199454503131	0.300702921977
O	-3.856823542516	1.425417206291	0.054809704461
C	-6.129504896456	0.815672037498	0.110471259113
C	-4.791558510698	0.440282592357	0.133745272384
C	-4.373312435701	-0.910960054008	0.225169057297
C	-5.379532469548	-1.906710391363	0.304283925853
C	-6.719652093044	-1.590331923557	0.299586935817

C	-7.121871427073	-0.208265157488	0.183851464595
H	-5.073872518576	-2.954044666067	0.376933629261
N	-8.446060762040	0.115750845682	0.144943815777
C	-6.537618248963	2.265776138831	0.020084099232
C	-7.888882545333	2.466903945677	0.702695314390
C	-8.912951054702	1.502784830981	0.123421484536
H	-9.850553917504	1.549063660189	0.700581387634
H	-7.787538936809	2.287352449539	1.786482161350
H	-8.249848331252	3.498152194904	0.572861256110
H	-6.607804720855	2.572902561158	-1.039831717275
H	-5.764078474419	2.901396860629	0.473663014476
H	-9.164368990989	1.786863817860	-0.916637969836
C	-9.015133796765	-2.240664845023	-0.400707491372
C	-7.787275300792	-2.652155335523	0.409055495411
C	-9.511962352238	-0.886576759966	0.083389095923
H	-8.080168787444	-2.778505919315	1.468019332703
H	-7.391479630013	-3.622738777105	0.074157470671
H	-8.752538850517	-2.179834572916	-1.470529091349
H	-9.826282219019	-2.977607126897	-0.301938779053
H	-9.976875811728	-0.983804988913	1.083120334377
H	-10.293123686045	-0.502869093587	-0.593156747613
H	2.044428594811	1.264312966835	-0.055910533614
O	-1.806934379322	2.236831141711	-0.005524790033
C	9.627772903709	-1.188399384978	2.798049911832
H	9.895168162326	-1.561945537635	3.799885308955
C	10.828724037633	-1.352701598572	1.852751631178
H	10.595933596195	-0.962057733836	0.849188127908
H	11.103452207522	-2.414207598726	1.745145780383
C	6.369473862152	-1.952334490248	0.921289206708
C	6.176421185087	-3.316867735828	1.246700221071
C	7.496517305677	-1.300133267153	1.444886360290
C	7.080014226695	-3.943528612869	2.121951467776
C	8.407489353877	-1.925203292247	2.300197492781
H	7.626757567504	-0.250764029052	1.172295806960
C	8.169579002981	-3.262730722277	2.653150416515
H	6.920863699079	-4.992605896777	2.369871413722
H	8.847435213271	-3.780301681604	3.335805848091
S	4.943612015557	-4.425670331296	0.550307762588
O	5.303594259011	-5.789518943398	0.930139629993
O	3.565172295172	-3.986727259213	0.757660823997
O	5.299676103870	-4.350824505308	-1.034807743517
H	4.912881044483	-3.539290452780	-1.421384362739
H	9.391296284274	-0.117585688658	2.907926548176
H	11.706008863035	-0.808938786775	2.237036651182

III. FORMATION OF HYDROXYL RADICAL VIA REACTION WITH O_2

R1

E = -781.340903775825 a.u. (G_{298K} = -781.101411543927 a.u.)

0 2

O	2.294636663091	0.547759033356	1.132818557617
C	2.534171070051	-0.134958817800	0.120748942222
N	3.715556378444	-0.041205512947	-0.539982319578
H	4.425445223025	0.591473362074	-0.188804592760
H	3.937304127891	-0.618900655195	-1.341230438380
C	1.547362307831	-1.068049719096	-0.428831773263
H	1.738107606583	-1.555945069604	-1.389470644451
C	0.282957796655	-1.350418627451	0.297889668631
H	0.367758738435	-0.978777177734	1.331003291589
H	0.141648678669	-2.444154825635	0.359724931923
C	-0.946039967814	0.723090768399	-0.675617188845
N	-0.300880877571	1.522017873366	0.212682902706
H	-0.243804961739	2.505696688868	-0.034357276433
H	0.440258007986	1.168999728951	0.823262831421
O	-1.543226882752	1.168329636408	-1.651439803939
H	-1.153968976418	-1.258497300848	-1.332546821178
C	-1.002707002287	-0.774367925180	-0.355420690190
C	-2.215707193032	-1.115400738341	0.540107048241
H	-2.088969439873	-0.635715768642	1.527117905348
C	-3.619749440765	-0.833390857527	-0.021931024230
H	-3.682560467827	-1.245131812730	-1.042134124183
H	-2.162012254061	-2.197181424475	0.743820568841
C	-4.027562717589	0.636612055833	-0.175374984454
O	-4.792509725882	0.988745045523	-1.066898485966
N	-3.613271214947	1.493472048480	0.796052019724
H	-3.825492284696	2.477548015160	0.668783782457
H	-2.832825779126	1.275275099918	1.402745378359
C	-4.684299021857	-1.547237240270	0.851738270040
H	-4.374051910826	-2.600713136047	0.957991914690
H	-4.650586143968	-1.113219072439	1.866762896091
C	-6.113458634912	-1.500107163380	0.310882412944
H	-6.168188122901	-1.940844391591	-0.698232419253
H	-6.492646329247	-0.470144706300	0.238714968203
H	-6.792383155113	-2.069252027042	0.965677474377

O_2

E = -150.205000430466 a.u. (G_{298K} = -150.221086639456 a.u.)

0 3

O	5.567240158851	-5.122735922147	5.881475426665

O	5.567240158851	-5.122735922147	7.081019157377

R2

E = -931.586412975247 a.u. (G_{298K} = -931.342650301184 a.u.)

0 2

O	-0.582677589726	-0.936035148711	0.942698944457
C	0.422151610743	-1.545702876412	0.602351142329
N	0.633910029384	-2.855658466811	0.821372368132
H	-0.077665410463	-3.393306327262	1.304951293482
H	1.479129038880	-3.321533690992	0.514303959480
C	1.544289835147	-0.775666889180	-0.111315524780
H	2.003475431294	-0.102802930884	0.629557752594
C	1.012472164240	-0.003674220815	-1.314330323704
H	0.109796303612	0.527099539724	-0.973840615932
H	0.670696859642	-0.733789368042	-2.065843745056
C	2.625516212916	1.974342210526	-0.996648815120
N	1.760899637210	2.584758289318	-0.146564960079
H	2.113373528864	3.308136030025	0.470746691002
H	0.763103770391	2.415790571773	-0.155774145544
O	3.822839793098	2.229836548843	-1.007115296973
H	2.876649894658	0.382780136763	-2.338176730716
C	2.014866098496	0.959591934957	-1.971789484064
C	1.346868720220	1.650127113322	-3.181713698413
H	0.532489590908	2.308335107071	-2.829879890021
C	2.274520997910	2.400382033276	-4.152955479636
H	3.094074520783	1.724268913963	-4.445056886653
H	0.842066407630	0.862897135671	-3.764894417388
C	2.985895284344	3.642333743801	-3.603408125510
O	4.148141800599	3.893660198195	-3.901897988706
N	2.228990736830	4.496567582058	-2.868164264381
H	2.678935738999	5.309409919097	-2.461439314131
H	1.311198197261	4.250118542263	-2.521763435350
C	1.496427638998	2.795620190281	-5.432365017866
H	1.019464001578	1.882916012418	-5.828433838544
H	0.672932833557	3.474663210414	-5.148999807379
C	2.346247011371	3.437586819604	-6.529030875906
H	3.176248903793	2.775189751383	-6.825037371689
H	2.788470788153	4.390839617838	-6.201366103702
H	1.736956150038	3.638055852648	-7.424379122447
O	2.581728987425	-1.704678365740	-0.539699231936
O	3.783943336248	-1.188391306785	-0.489785498128

TS_CH_gamma

E = -931.549707568989 a.u. (G_{298K} = -931.311404158435 a.u.)

0 2

O	-0.477916030679	-1.099926562152	1.239530402818
C	0.450171917879	-1.639921245575	0.651994736860
N	0.663869227821	-2.967943476415	0.612437271793
H	0.021125782077	-3.587310136842	1.094283844525
H	1.447234072868	-3.363041110776	0.105628587755
C	1.485593213677	-0.777255203181	-0.079118455408
H	2.156142426380	-0.341319067216	0.684431956126
C	0.826595434359	0.346609131081	-0.903162318268
H	0.217761052500	0.952266492690	-0.212652496862
H	0.127080554694	-0.120429369703	-1.612181919442
C	2.728357085120	2.130448686010	-0.882769883409
N	2.206773300383	2.656084223687	0.251072614007
H	2.762601849974	3.334006408766	0.762458738380
H	1.230934110052	2.564796028394	0.501484575251
O	3.868166713036	2.383441056003	-1.262771991656
H	2.798265385843	0.200389074218	-1.764657717948
C	1.866669566935	1.151845612483	-1.660552789348
C	1.466430301908	1.521197457189	-3.082850023433
H	0.499569487920	2.062158659800	-3.039542586244
C	2.461463936046	2.285194318195	-3.971454566656
H	3.432802428780	1.768930424762	-3.941714208483
H	1.215217593075	0.578080659345	-3.596036246951
C	2.780406178022	3.725625536946	-3.554763941178
O	3.845823299193	4.251200341764	-3.858466157440
N	1.800986397892	4.412132319454	-2.913040730843
H	1.975576354931	5.376221581465	-2.652139071185
H	0.914037850606	4.004282266907	-2.651310305270
C	1.948232999736	2.287481797468	-5.434538683711
H	1.677023476407	1.249799629908	-5.693425960527
H	1.008963691947	2.867774505132	-5.476556493038
C	2.937434324874	2.816510893735	-6.473064026190
H	3.872396311886	2.232250398502	-6.458494838589
H	3.204860902532	3.866583380470	-6.287035621914
H	2.508861819076	2.743593590697	-7.485321460746
O	2.254129136052	-1.578225469108	-0.970595775035
O	3.354724370622	-0.828042817490	-1.391674137796

R4

E = -931.578591934406 a.u. (G_{298K} = -931.336473640924 a.u.)

0 2

O	-0.346893319731	-0.796205353776	1.383397938353
C	0.386687402409	-1.343157279599	0.568115858961
N	0.336545833124	-2.646997582727	0.240811380592

H	-0.345288430586	-3.249846544707	0.687438666171
H	0.971473740659	-3.023711172904	-0.453077016549
C	1.467748467369	-0.523753406937	-0.153032052583
H	2.236110530520	-0.292182025212	0.602148937039
C	0.879991435639	0.797276182251	-0.713081792167
H	0.571999996670	1.402506474178	0.154897376056
H	-0.028464943743	0.574190216008	-1.292825345993
C	3.195551882208	1.829039415253	-0.972434006462
N	3.185714732745	2.570934985616	0.153077233827
H	4.070221032363	2.803731522680	0.592804296204
H	2.363108602635	3.094305130829	0.427659021862
O	4.244940081633	1.347833975329	-1.438358712034
H	3.816186465873	-0.455470568619	-1.379246571561
C	1.887811155152	1.489535989224	-1.581486693121
C	1.815772284158	1.311150586520	-3.067790142571
H	0.754401674494	1.263177846829	-3.364710278687
C	2.539873549548	2.378332031836	-3.918340603398
H	3.603037860026	2.367289912363	-3.639649727329
H	2.236608334122	0.317749399304	-3.324055525016
C	2.043748770792	3.764613827592	-3.496321525368
O	2.633055383155	4.415440239297	-2.637111328392
N	0.896124723092	4.200060549961	-4.069449577202
H	0.510410327482	5.092807385082	-3.782116947633
H	0.403358177989	3.671923085834	-4.777904248744
C	2.424743539788	2.067425558645	-5.418498017411
H	2.815259596163	1.047957000909	-5.578297568842
H	1.361689515935	2.017961165265	-5.718181451685
C	3.178156978525	3.052799767867	-6.312667429152
H	4.246684913347	3.090473180751	-6.043841821243
H	2.772390272421	4.072713906649	-6.216556626992
H	3.106814488503	2.763177647098	-7.372675025169
O	2.089886150197	-1.280581044547	-1.194777072707
O	3.517124338208	-1.321364351026	-1.004857168133

TS_CH_delta

E = -931.550262178253 a.u. (G_{298K} = -931.309021092690 a.u.)

0 2

O	1.804877792454	0.817312426716	1.208357228430
C	2.376909640209	-0.046162303150	0.540740996260
N	3.700174203450	-0.079659972060	0.340571833437
H	4.289528354854	0.629708210612	0.762837510815
H	4.116873841432	-0.823329826650	-0.208303558175
C	1.563987188264	-1.143989627002	-0.177545981277
H	1.219400055772	-0.672163424580	-1.114660813231

C	0.320296641093	-1.593509565526	0.597072582013
H	-0.189357636684	-2.336205519157	-0.031172829705
H	-0.339883491826	-0.716416339838	0.633992358847
C	-0.284026728723	-1.407327907149	3.120594586783
N	-0.021144796849	-0.085938441427	3.193910755976
H	-0.514440228861	0.462691542156	3.889940918712
H	0.584471653807	0.383451128980	2.513592531342
O	-1.051026231389	-1.992086548782	3.876832676676
H	0.021144118013	-3.181009943543	2.041014059444
C	0.496203470617	-2.191405107184	2.034700436432
C	1.940600047203	-2.391750148107	2.472257469758
H	2.530183523423	-1.469748107872	2.571593380250
C	2.266705807223	-3.435740021218	3.514822415881
H	1.757799140253	-4.376764522133	3.252881685604
H	2.394849445263	-2.927877095825	1.327126162799
C	1.742799621458	-3.111550905682	4.935349219800
O	1.276642033250	-3.992163996989	5.644308730674
N	1.926616987777	-1.840887398669	5.366487729347
H	1.555305158882	-1.584820534992	6.275352198453
H	2.170247966843	-1.086492231050	4.736464292226
C	3.792447720628	-3.695431396702	3.583151999030
H	4.135324594065	-3.922486184708	2.559823437970
H	4.295940250263	-2.758163566927	3.876861735483
C	4.200885938244	-4.828526356166	4.523214356206
H	3.707764673936	-5.773339445041	4.241819599407
H	3.928877534505	-4.613547814263	5.567882610054
H	5.289445094061	-4.989644669403	4.483314088938
O	2.433594521063	-2.196634000364	-0.624291944815
O	2.366272054262	-3.335698139638	0.195410537444

R5

E = -931.564722247344 a.u. (G_{298K} = -931.320852350102 a.u.)

0 2

O	2.043361994313	0.636889958167	1.135769398395
C	2.456418599043	-0.291035394671	0.441237895518
N	3.746750024788	-0.441090700446	0.088697250957
H	4.418673870353	0.268387742039	0.362491429517
H	4.013526153016	-1.120240779375	-0.615274464658
C	1.491712553892	-1.344248180661	-0.127107600863
H	1.101997137089	-0.896017670550	-1.059365788698
C	0.285453791719	-1.636370772298	0.767404634222
H	-0.252703417239	-2.467658752183	0.290110543840
H	-0.373532539037	-0.761696306874	0.680617926151
C	-0.374471121379	-1.054287978685	3.188770812772

N	-0.152321863295	0.269468115388	3.023720612242
H	-0.645336610988	0.925909196482	3.618408365801
H	0.552993900879	0.605526382531	2.363894880017
O	-1.165700023007	-1.514035250380	4.005927978624
H	0.073914981336	-2.979291219565	2.459278202294
C	0.485495668042	-1.975451480621	2.290444424708
C	1.879229458884	-1.958939550795	2.849662400136
H	2.373524655219	-0.997265198855	3.005073539371
C	2.465894183650	-3.172370466816	3.498596698413
H	2.306583800519	-4.041709377951	2.838946365936
H	3.379037693802	-3.059855890942	0.711368186564
C	1.655051106460	-3.534069237269	4.766223411971
O	0.963425124775	-4.543241742582	4.822056610437
N	1.756132798676	-2.656694841115	5.794360663414
H	1.177816001327	-2.795343965359	6.615767313014
H	2.238642756201	-1.771962885661	5.696432251540
C	3.972148723545	-3.019108398883	3.778878225038
H	4.470493582999	-2.773355164175	2.824888042932
H	4.139746349690	-2.142242197190	4.428686485066
C	4.613708037144	-4.259704748592	4.397699833465
H	4.465258907649	-5.144345413840	3.756863970336
H	4.178624666472	-4.484826941137	5.385046406514
H	5.697110373837	-4.119467856865	4.535082896604
O	2.165077421037	-2.489704944922	-0.645364698304
O	2.512898644128	-3.395498563066	0.415505790908

TS_CH_eps

E = -931.563139237890 a.u. (G_{298K} = -931.320403262430 a.u.)

0 2

O	0.866489020478	0.970883993995	-0.004191552604
C	1.842993852664	0.224033802461	0.060693715458
N	3.100592194488	0.649096854174	0.248280284247
H	3.279831146960	1.644928560201	0.325557623257
H	3.877614359643	-0.001729238032	0.262521731549
C	1.631753017936	-1.286460032309	-0.082814028516
H	1.257804112193	-1.430698816877	-1.113171552674
C	0.569900879409	-1.865903913380	0.863924737155
H	0.413025619830	-2.905347188380	0.549440252356
H	-0.371597229208	-1.340857368469	0.645232773582
C	0.490233440504	-0.663185929064	3.236357635840
N	-0.107040416896	0.390844601636	2.636649374735
H	-0.288827359442	1.199624867986	3.222760924076
H	-0.078453553617	0.547994687225	1.629988684341
O	0.704795382288	-0.686532397542	4.447120869777

H	0.077282056352	-2.635333402094	2.762228421925
C	0.818721028029	-1.909285027076	2.387197860226
C	2.208211562719	-2.428176191679	2.808862214358
H	2.233033438242	-2.429968026821	3.914210995875
C	2.629943453330	-3.812342353036	2.341809537721
H	2.655803397536	-3.666911257513	1.001132253647
H	2.978963228041	-1.706799136936	2.493884989184
C	1.579715340640	-4.891787484483	2.530848637460
O	0.561765458432	-4.927432363098	1.840611474451
N	1.812315206153	-5.793711146583	3.513500533263
H	1.115103957673	-6.508958678964	3.692420652020
H	2.612423958756	-5.742094867219	4.130684568753
C	4.081612219796	-4.152954966677	2.645447009032
H	4.688798463004	-3.260129331732	2.423517239769
H	4.194826691566	-4.308355955557	3.737684313595
C	4.641131092575	-5.352781724133	1.875440185689
H	4.587434764568	-5.167872660361	0.791317113444
H	4.080712262315	-6.274716205806	2.092555632315
H	5.694934826900	-5.527315624712	2.140551314806
O	2.916943073760	-1.916888124010	0.018542177629
O	2.808186783948	-3.295057034413	-0.124271602157

R3

E = -931.588378222689 a.u. (G_{298K} = -931.339672687645 a.u.)

0 2

O	2.178607967311	0.623057556833	0.766270315399
C	2.498875992448	-0.434417329679	0.224031703691
N	3.722329839191	-0.662074766599	-0.281198384039
H	4.435514182485	0.055422152956	-0.206971785844
H	3.943478680797	-1.551820558637	-0.713192848086
C	1.478600435185	-1.562799497453	0.015726222442
H	1.039906521441	-1.359533343574	-0.981123544162
C	0.313524323927	-1.604535582484	1.007483564865
H	-0.327971924590	-2.422835061652	0.656404180492
H	-0.262846154988	-0.682725474483	0.840920919441
C	0.061749265558	-0.630221546442	3.395254925788
N	0.418481121704	0.607345717192	2.991620042454
H	0.150278497574	1.396336192589	3.569514086456
H	1.005464365886	0.756586006810	2.165678631824
O	-0.585814796229	-0.839092838639	4.420179917494
H	-0.066931063369	-2.643018525513	2.855940706142
C	0.557871122855	-1.805164906700	2.531675647500
C	1.997616287462	-2.115228341542	2.999768718668
H	2.019231866304	-1.940402126879	4.095061938967

C	2.627627729515	-3.464122772767	2.813706776236
H	1.014686562451	-4.207241515593	0.153909375550
H	2.694779272419	-1.352475940188	2.609076859362
C	1.930197877137	-4.638252038930	2.291505156838
O	0.791777693723	-4.585353709068	1.768025385193
N	2.577784713970	-5.830931669324	2.347035391108
H	2.098083746853	-6.646893800925	1.984619917612
H	3.470555912437	-5.965714471860	2.801213437689
C	4.086759281591	-3.538225798370	3.176900634910
H	4.331916709040	-2.701668609855	3.850753259755
H	4.306675355817	-4.452375665365	3.756257489170
C	5.007346596789	-3.475980185906	1.941932044770
H	4.844952908290	-2.540182282481	1.387899949003
H	4.804005088154	-4.312366887473	1.255940234754
H	6.065064794808	-3.523419509651	2.244289910817
O	2.214470920517	-2.779049716270	-0.078939751432
O	1.373750817134	-3.779065904532	-0.671626342966

TS-3_6

E = -931.559475032513 a.u. (G_{298K} = -931.313589780447 a.u.)

0 2

O	2.102731820267	0.355254702566	0.965051358619
C	2.438316885051	-0.692804846552	0.408320937403
N	3.646774781703	-0.886246200357	-0.144497981395
H	4.340065053280	-0.147176580002	-0.106289254792
H	3.861801647047	-1.767212956259	-0.606561185887
C	1.478992676343	-1.887466923446	0.254942319331
H	1.109784365816	-1.846570718234	-0.784432819322
C	0.242859524997	-1.854702915653	1.157100809715
H	-0.415206579733	-2.654015577217	0.788373002675
H	-0.276249189176	-0.908867797867	0.946576242614
C	-0.125054289835	-0.885207917830	3.535929213814
N	0.246117624083	0.355152843927	3.152349233560
H	-0.057703991013	1.144245504714	3.712088073665
H	0.870188927758	0.505983821258	2.353428631204
O	-0.823869524336	-1.108133309237	4.521819397277
H	-0.169815650253	-2.903792503822	2.995526744001
C	0.431886135416	-2.041314871531	2.688202405176
C	1.889349305722	-2.292717987482	3.153846438707
H	1.868431827798	-2.446822334270	4.252246862305
C	2.633764028177	-3.433318745614	2.513715527471
H	2.882760233651	-4.434694730148	-0.869838731776
H	2.475182950207	-1.372932130743	3.011424713945
C	2.060598951895	-4.814992510643	2.474920276133

O	2.426222674253	-5.652075984553	1.649882315520
N	1.092055756657	-5.100302690226	3.392807201452
H	0.741371240509	-6.052011823063	3.422471395477
H	0.911352846273	-4.515806637938	4.199255741726
C	4.127068408166	-3.258390292602	2.436114313557
H	4.321238613135	-2.219678477635	2.123796350425
H	4.495511259611	-3.315341422834	3.483032532295
C	4.950844034648	-4.203198741779	1.560840365009
H	4.623830425713	-4.142471853581	0.514572205861
H	4.860687258356	-5.249523794851	1.879875336991
H	6.012184198991	-3.911753427156	1.610250428054
O	2.162979958505	-3.121823242866	0.402853550631
O	2.729922541888	-3.501446005735	-1.103466955866

R6

E = -931.644920497343 a.u. (G_{298K} = -931.396632190614 a.u.)

0 2

O	1.438931741035	0.497016815099	0.409647600697
C	2.227930493518	-0.448417734458	0.475266817796
N	3.560568772454	-0.305912670441	0.521426383903
H	3.970892194111	0.620992353310	0.493873358011
H	4.156444128084	-1.124710898050	0.562413769707
C	1.721303216325	-1.903290130937	0.455230910571
H	1.572372367990	-2.142269950644	-0.611293841457
C	0.388583460769	-2.083677873650	1.182913204071
H	-0.014553508437	-3.055113958790	0.869422724933
H	-0.310461930533	-1.319220607489	0.819649911182
C	-0.032443365039	-0.867438213984	3.497882394259
N	-0.086716941722	0.318405403818	2.854672555271
H	-0.377028478161	1.128637200300	3.391928823444
H	0.306802065732	0.466916980685	1.922697462185
O	-0.370436246580	-1.008128728265	4.671399889648
H	-0.063590227364	-2.917926074513	3.125395697481
C	0.517742816978	-2.074520117264	2.726500331112
C	1.989015122339	-2.296143801425	3.144575503542
H	2.040094293156	-2.606468758089	4.197443799093
C	2.682058698545	-3.313073410131	2.225015647620
H	2.340177550128	-4.621472244816	-0.392514929656
H	2.559313626605	-1.356300900223	3.071372795101
C	1.919685255459	-4.668471555620	2.181921229264
O	1.588243233816	-5.187103194694	1.115940580767
N	1.676553950171	-5.251688214537	3.368817952233
H	1.217033154757	-6.156457443366	3.386576006814
H	1.942498733195	-4.836275924609	4.252473580135

C	4.144357870031	-3.569723717340	2.639007302972
H	4.659325214317	-2.597237802821	2.577560918863
H	4.170059005497	-3.872065063243	3.698098785465
C	4.853482484550	-4.608881059054	1.767851852244
H	4.696808832148	-4.398834758305	0.699610943648
H	4.471965485173	-5.623465232053	1.965741450866
H	5.934557012164	-4.614651038266	1.972665790451
O	2.740057143503	-2.800683637400	0.893492283385
O	2.793446265612	-4.344132780256	-1.234484393078

TS-3_7

E = -931.551823803930 a.u. (G_{298K} = -931.310840930762 a.u.)

0 2

O	0.956931982966	-2.827501855032	-1.378846064830
C	1.674877888550	-1.938265868132	-0.926692720051
N	2.629017583165	-1.307833327788	-1.650255029634
H	2.796816911901	-1.618573576081	-2.600614038125
H	3.285940266942	-0.672667106264	-1.210599457278
C	1.553177095383	-1.522433078546	0.523013486543
H	2.175209613426	-2.496944249726	1.201924959371
C	0.195298321988	-1.654049823436	1.173715445799
H	-0.248329887679	-2.554887780850	0.736014767850
H	-0.441361683893	-0.797149867181	0.895184867483
C	-0.209943635731	-0.595794137991	3.509427221790
N	0.359758157255	0.581473587001	3.153768743424
H	0.119652955507	1.420501727955	3.669602755076
H	1.054428208210	0.635301668132	2.415697222687
O	-1.021223746088	-0.688155492174	4.425970755293
H	-0.469968465693	-2.610336471259	2.981284515464
C	0.249559010083	-1.827450726345	2.721007946086
C	1.647868916689	-2.257701035274	3.255076358372
H	1.517137871734	-2.698934591349	4.258886429594
C	2.431833128825	-3.203856743274	2.350620213918
H	3.809652697732	0.502873799949	1.115092494837
H	2.265870736678	-1.357679939884	3.389138808333
C	1.757345365347	-4.534112531701	2.125776233403
O	0.548202136112	-4.615454051795	1.896065701467
N	2.532411795051	-5.649809273479	2.181443313406
H	2.074646817548	-6.548757283196	2.077202891677
H	3.492027824855	-5.644433089146	2.499145084157
C	3.948943528834	-3.155142916930	2.482894468572
H	4.227713855860	-2.135944210593	2.787851736409
H	4.268353515489	-3.813479756210	3.315360045013
C	4.722310266191	-3.500520479075	1.201583923164

H	4.476516888042	-2.782287982197	0.405428835071
H	4.487741747506	-4.508175169255	0.827722546854
H	5.807910772988	-3.450819493136	1.379313046179
O	2.118227645247	-0.306683806710	0.890490203794
O	3.581507954353	-0.408776004316	0.859193155562

R7

E = -931.638016596001 a.u. (G_{298K} = -931.398575017010 a.u.)

0 2

O	0.511155250882	-2.153862383565	-1.703950796821
C	1.391890617091	-1.557272118749	-1.096973894944
N	2.626089228752	-1.287047194230	-1.545289786263
H	2.897885510419	-1.613833809350	-2.466743533902
H	3.312249892217	-0.818505303658	-0.948692894073
C	1.098242720037	-1.021954797281	0.324619653770
H	2.563853881096	-2.977919371890	1.058121985469
C	0.094471054536	-1.800416725595	1.132995911426
H	0.013019385245	-2.801568701164	0.691301648934
H	-0.889774578931	-1.318577231918	0.993355657125
C	-0.139740719537	-0.819147792139	3.535393466441
N	0.173545713261	0.443957111696	3.171617744034
H	-0.145483113512	1.213778967712	3.749186399942
H	0.760106462982	0.626928235155	2.360483431724
O	-0.805087874213	-1.084244160256	4.532872598120
H	-0.117277188857	-2.831423706930	2.985399718149
C	0.421434167902	-1.936629166690	2.643298567710
C	1.923315120261	-2.134815145022	2.949959598120
H	2.023034325067	-2.362669324266	4.024095415625
C	2.621328929811	-3.236242151031	2.127238312249
H	3.960546449975	0.676521969250	0.820005568569
H	2.468881612717	-1.194935770759	2.777413910980
C	1.847894876705	-4.553952132912	2.232954212182
O	1.094668553029	-4.930404903179	1.337887377150
N	2.003053057726	-5.247502238494	3.385066213179
H	1.485267275329	-6.109684543842	3.515619160996
H	2.628062806758	-4.948005437711	4.122519940549
C	4.114036530900	-3.336401019443	2.485149233881
H	4.551380323560	-2.338261695055	2.321440180869
H	4.231665615922	-3.546327651550	3.563587953497
C	4.874013372685	-4.374259237428	1.659111307710
H	4.784836275231	-4.160382764467	0.581058211673
H	4.486777382843	-5.391359150954	1.833012493908
H	5.945200170900	-4.377112505712	1.914229788499
O	1.651364303450	-0.011165723137	0.727187868297

O	4.138195732842	-0.282213687827	0.715657775965

TS-3_8

E = -1081.797975437299 a.u. (G_{298K} = -1081.549258293884 a.u.)

0 2

O	1.635966736024	0.832680264281	0.198598817794
C	2.024408421803	-0.244873429335	-0.255141316506
N	3.237394484699	-0.426357606387	-0.799184742064
H	3.888058863104	0.351101985009	-0.836117806215
H	3.511380214032	-1.335839085640	-1.154967784974
C	1.088856103813	-1.460232703703	-0.264715165726
H	0.383572710560	-1.263913576065	-1.095635341057
C	0.248446377425	-1.652253499857	1.003425126646
H	-0.378227956461	-2.527351797979	0.793026794768
H	-0.441175770421	-0.798384130262	1.070044200778
C	0.830419825185	-0.706485240101	3.374720672698
N	0.788893374263	0.548500226892	2.882397620175
H	0.788275407289	1.310997758516	3.551690781110
H	0.955945901678	0.760154314395	1.894634164242
O	0.807602914810	-0.946451884414	4.581700610386
H	0.365803781092	-2.662563421619	2.887670522996
C	0.937460512579	-1.878271929209	2.375937145054
C	2.426772010911	-2.336193173788	2.389268359275
H	2.889585960632	-1.878779497064	3.278826177264
C	2.764784838004	-3.794502991123	2.486272620625
H	0.900408971745	-4.132176581384	-0.123311672777
H	2.987051402258	-1.900208768303	1.543511136252
C	1.803856177085	-4.855193822586	2.151096016259
O	0.808132834875	-4.664157955639	1.419306214470
N	2.033338963564	-6.093107710057	2.654170931157
H	1.367970785976	-6.825018261240	2.431100070375
H	2.737519896679	-6.291445161510	3.352622322755
C	4.100730647641	-4.166561127483	3.080065692760
H	3.953412021445	-4.355002848164	4.165470781744
H	4.430076874711	-5.128546679776	2.654695162768
C	5.231453921667	-3.143936710474	2.914788046643
H	5.024064144002	-2.201563192253	3.442379203836
H	5.405873996958	-2.906912486344	1.855145432502
H	6.165489243847	-3.553504581432	3.327827163545
O	1.870114837329	-2.597110078700	-0.601394235227
O	1.004209720364	-3.665858678501	-0.999398405082
O	3.975547542542	-4.463555844092	0.046442139476
O	4.582488080758	-3.559965820501	-0.464808526410

R8

E = -1081.833643051469 a.u. (G_{298K} = -1081.580335237127 a.u.)

0 2

O	2.040648927946	-2.577867520533	-1.493869700963
C	1.650515069702	-1.413368057878	-1.407315867658
N	1.235295189618	-0.682837996650	-2.451862353549
H	1.256460059031	-1.086801814137	-3.381982770831
H	0.928907537244	0.275292524198	-2.334734860154
C	1.610014706986	-0.724105856811	-0.031095442083
H	2.644129083479	-0.719072012579	0.336389698848
C	0.673013561117	-1.487707375228	0.913040542279
H	0.658206713498	-2.523962486775	0.561422845923
H	-0.350775080197	-1.113547181963	0.747971793040
C	0.488341690644	-0.326746053506	3.272867272254
N	0.227336579593	0.835962708406	2.639336161430
H	-0.062562407546	1.628442771406	3.202497516594
H	0.409980796188	0.979106334782	1.649189714120
O	0.366767129431	-0.462629008605	4.487756528015
H	0.383896236578	-2.356293392335	2.826161153994
C	0.976685746468	-1.518742571446	2.425863881393
C	2.438719695966	-1.781188836653	2.857587041633
H	2.417445846895	-1.866477422601	3.952093261012
C	3.184705496671	-3.018896550560	2.318830541415
H	2.554152752769	1.863626125436	0.213252597089
H	3.080003701257	-0.914201308759	2.632674217611
C	2.240680892831	-4.205610556108	2.039995455764
O	1.723558868588	-4.771993627448	2.995623634656
N	2.050198447834	-4.554249821558	0.752256683411
H	1.368240059363	-5.284271262654	0.569425176269
H	2.317875010513	-3.945320968888	-0.026044872246
C	4.294879695053	-3.450646822879	3.289937212644
H	4.884643983217	-2.553406210294	3.533681067249
H	3.785617238992	-3.773507825055	4.209490575319
C	5.200798199002	-4.561544652194	2.761798564208
H	5.719129130768	-4.253497399063	1.841443028165
H	4.631012077670	-5.478203934892	2.541866932479
H	5.965870095825	-4.815446947109	3.510846871331
O	1.151580407011	0.628731684667	-0.097976614983
O	2.211827683718	1.459875971373	-0.605453226704
O	3.816307709617	-2.691222947716	1.014258792127
O	4.693691874106	-1.728378848998	1.079850848618

TS-8_9

E = -1081.803341891916 a.u. (G_{298K} = -1081.557245516122 a.u.)

0 2

O	1.669030904589	-2.589833145927	-1.567827400104
C	1.730456359630	-1.367344725124	-1.450917771923
N	1.909230932144	-0.526085579499	-2.485123678219
H	2.041908967262	-0.921910417183	-3.409686934016
H	2.051591016989	0.467841584906	-2.352266122096
C	1.626714317764	-0.746279704903	-0.054593682967
H	2.896648736459	-0.995280602520	0.323831413548
C	0.686043449719	-1.489053643547	0.871993472172
H	0.659175491177	-2.513796095897	0.489297390377
H	-0.330433438209	-1.088084989250	0.703949770190
C	0.384137533735	-0.426849480753	3.268432804620
N	0.237533562582	0.790490974244	2.703267675440
H	-0.086953407895	1.552764897413	3.288728040871
H	0.544047182072	0.998901153134	1.758770252486
O	0.115116723121	-0.647857893864	4.446081724382
H	0.349695695784	-2.431334133348	2.734997628586
C	0.941582603154	-1.566773887275	2.396125755625
C	2.390979026862	-1.810280368578	2.875557950837
H	2.329852813508	-1.980328945757	3.958680001168
C	3.178013399049	-2.998687575156	2.292779827007
H	2.922763009866	1.741376787414	0.276277421040
H	2.999052254585	-0.906522503123	2.730842349983
C	2.283295115815	-4.259672668876	2.275695636212
O	1.969663418046	-4.786385726093	3.336269258770
N	1.877118375831	-4.691042713598	1.064569297587
H	1.249508734002	-5.486778261086	1.018737374814
H	2.111935887627	-4.187917623595	0.212060693833
C	4.446644504904	-3.253520224195	3.126126957305
H	5.003954905384	-2.303005278606	3.165144685081
H	4.126361386139	-3.489128713893	4.151856500441
C	5.335805347986	-4.368127420309	2.578016308178
H	5.641961914976	-4.156740775526	1.542677853196
H	4.813695259407	-5.338537053647	2.586772680691
H	6.244935251205	-4.473216529215	3.189592198502
O	1.413652315769	0.623297135094	0.042011695386
O	2.512151401677	1.366522034183	-0.524940163455
O	3.567102458448	-2.784772655328	0.908495013510
O	3.939815516970	-1.479572918863	0.648875743552

R9

E = -1081.890729599315 a.u. (G_{298K} = -1081.639513054590 a.u.)

0 2

O	1.112189760416	-2.753124854089	-1.463591516952

C	1.488216491734	-1.601135139785	-1.278833033153
N	2.080068858112	-0.815302118480	-2.184312135967
H	2.316282027147	-1.215871304778	-3.086419502036
H	2.507983477855	0.069700370306	-1.905564743721
C	1.251728184378	-0.920490947036	0.103004409427
H	4.011172503501	-0.564994190372	0.313219068115
C	0.382807959053	-1.671780767313	1.069126444665
H	0.336324702759	-2.710014901695	0.723368538316
H	-0.637699587894	-1.269937635695	0.928791234799
C	0.148183622021	-0.449810918927	3.356015870876
N	0.326796170105	0.785448453384	2.837681381792
H	-0.034808788589	1.585582843380	3.344932177861
H	0.857706583477	0.931828055467	1.983614836312
O	-0.442218018680	-0.653081537481	4.412528524423
H	0.310861149250	-2.503063241033	3.024080147519
C	0.768909453972	-1.615184697568	2.569603903278
C	2.280979251693	-1.672628801258	2.881791536186
H	2.384317771579	-1.819817131442	3.966114574321
C	3.099415679014	-2.753081618713	2.149149998231
H	3.448624229929	1.682008063170	-0.103227530890
H	2.766709233720	-0.715130846046	2.642078285446
C	2.309831756100	-4.079810661257	2.049628387684
O	1.891446574934	-4.591615529638	3.081590917026
N	2.154693780960	-4.620348959324	0.825640726699
H	1.581214899232	-5.453585697486	0.741986218225
H	2.372956414210	-4.098965176285	-0.017340026713
C	4.411117335374	-3.054029975248	2.902931611179
H	4.894217132616	-2.094719394768	3.137852437737
H	4.115497322202	-3.514900794600	3.857560194825
C	5.376306711042	-3.961657066097	2.142331392637
H	5.691985573093	-3.492589293702	1.199411453470
H	4.918424930128	-4.934292816011	1.901423087622
H	6.275762780647	-4.155786276689	2.746733288224
O	1.701267536097	0.188670101126	0.351185158023
O	3.641424875356	0.888434566869	-0.641479294911
O	3.364436303932	-2.319538715731	0.795482778033
O	4.401541668122	-1.321128198369	0.818103458306

IV. ADDITIONAL CALCULATIONS

PAMPS-TS

E = -686.205825170364 a.u. (G_{298K} = -686.015811108889 a.u.)

0 1

C	-1.878525215357	-1.674766281447	-0.364181947516
H	-1.214450511556	-1.754576585223	0.515964512080

H	-2.888884090246	-1.466048864387	0.019076050455
H	-1.883381419386	-2.652846655827	-0.866767851553
C	-1.422686479868	-0.571962851449	-1.290640181562
H	-1.971102496945	-0.081052774350	-3.745750368773
C	-1.593129267937	0.861819749715	-0.807562350032
H	-1.190277076043	1.540441459333	-1.574048603563
H	-2.669205429965	1.077937302884	-0.708735134515
C	-0.923015560977	1.180253558070	0.550343405784
H	-1.385355837557	0.552955274943	1.328734843531
C	-1.130534500740	2.655944850549	0.915900458547
H	-0.640990985633	3.301533987850	0.170818078171
H	-2.203278026995	2.901770772432	0.941701300977
C	-0.166014017247	-0.799788693583	-2.120377561381
O	-0.027682888970	-0.241669354681	-3.211018684298
C	0.576466984310	0.882338583029	0.471862910070
O	1.289778160669	1.429767370119	-0.360887642541
H	-0.701553609440	2.882939861560	1.904333735268
N	1.047721572284	-0.045465261717	1.343160106558
H	2.046246840845	-0.228530079688	1.365241386637
H	0.485865901038	-0.395805631867	2.109607294131
N	0.754630285714	-1.649420556657	-1.618729481174
H	1.631801035049	-1.752405134359	-2.119383654334
H	0.728622657467	-1.961744151136	-0.655441107837
O	-2.809815019247	-0.339936366080	-3.311496827864
H	-2.329564135282	-0.591346838711	-2.280719499598
O	-3.751038642060	0.074559655958	-4.989578178090
H	-4.239353197823	0.765165273576	-4.506572329136

PAMPS-P

E = -686.278958967214 a.u. (G_{298K} = -686.078196533836 a.u.)

0 1

C	-1.620820455751	-1.981396187967	-0.086803699847
H	-0.840936285603	-1.832116693746	0.676521126597
H	-2.591480536879	-1.892665128068	0.424770345538
H	-1.530084565316	-3.010520499314	-0.466075998831
C	-1.535011320241	-0.958403645161	-1.223004330795
H	-1.517800502996	0.384847909247	-3.768355860210
C	-1.814393624124	0.497211399300	-0.769590677747
H	-1.624458286802	1.168201619165	-1.619848934307
H	-2.891789446874	0.573307468617	-0.550804410753
C	-1.052137958849	1.011216417420	0.464888952411
H	-1.310663974280	0.386344479026	1.334621556544
C	-1.453351637420	2.461664878814	0.775013093910
H	-1.172858469678	3.117493217621	-0.063594489270

H	-2.541030091493	2.538394360095	0.928339888650
C	-0.267345883563	-1.036040514658	-2.076576839691
O	-0.237015948169	-0.523747370825	-3.204687940268
C	0.459661916570	0.959864035929	0.233877810078
O	0.979085297846	1.530143382201	-0.719549815147
H	-0.951592603338	2.830212823128	1.683555162499
N	1.177284778169	0.238643945079	1.131267005508
H	2.188420737506	0.216860833849	1.046102754556
H	0.760409198849	-0.149631199613	1.968220294733
N	0.797892859275	-1.695231732608	-1.588907187201
H	1.659538948967	-1.687778371385	-2.124710293708
H	0.843105127111	-2.008604678378	-0.627987004923
O	-2.280094530887	0.938571220223	-4.098797585831
H	-2.327497290594	-1.179858516646	-1.955189697098
O	-3.413083813224	0.147015024021	-3.692983259640
H	-3.609298672620	-0.358340649040	-4.499988826859

PAMPS-R

E = -686.243107587729 a.u. (G_{298K} = -686.054976630529 a.u.)

0 1

C	-0.871617423002	-2.305268402903	0.767273786680
H	0.206267904429	-2.490687331363	0.933925175245
H	-1.299803033064	-1.954604350201	1.716648597944
H	-1.324747853361	-3.288326329487	0.539663686656
C	-1.107523224660	-1.320711079900	-0.334693155434
H	-1.727779377658	0.636343939189	-2.946713669425
C	-1.803818940960	-0.031358564345	-0.048323826556
H	-2.205954636164	0.404161756279	-0.971890811933
H	-2.648331023263	-0.221475230489	0.636015350228
C	-0.902422352705	1.046045394406	0.635900629889
H	-0.525521528119	0.623299527428	1.582939605499
C	-1.710739069830	2.309650827716	0.927069459650
H	-2.054960347668	2.757711385473	-0.016614066200
H	-2.588242489499	2.075901158441	1.549081204315
C	-0.581235672934	-1.550523036343	-1.686546395000
O	-0.719721562731	-0.723865511318	-2.609415914377
C	0.295071486722	1.367810261890	-0.266457551665
O	0.254984941902	2.246208314784	-1.119946610822
H	-1.101660196012	3.059005608265	1.455949176188
N	1.390599816702	0.590578726414	-0.076185224077
H	2.193700791306	0.712214558473	-0.683576246836
H	1.441446872714	-0.111112499792	0.650839831890
N	0.088971822199	-2.710171483465	-1.911984425054
H	0.458737301012	-2.878010090443	-2.840394225041

H	0.237588491803	-3.417930694583	-1.205888136284
O	-2.416928529448	1.319228323843	-3.137288691794
H	-3.173356834963	0.782114897956	-3.414790069779
O	-2.167852447072	0.940582521921	-5.472239276847
H	-2.061355442849	1.902139503436	-5.341556321572

PVC-TS

E = -1267.957807084255 a.u. (G_{298K} = -1267.838961400541 a.u.)

0 1

C	2.054317139179	0.899379826579	1.635125417024
H	1.820486958879	1.961263384763	1.455832580335
H	1.372085988266	0.517776120269	2.409942662234
H	3.086169647174	0.828369388757	2.006706387536
C	1.892731827101	0.118482594975	0.341293326367
H	2.612196870091	0.474048257669	-0.408569737211
C	0.471420864588	0.190536377320	-0.208561711961
H	-0.247111879325	-0.138668526255	0.558999574484
H	0.258843314328	1.259682315941	-0.398241101918
C	0.203370806951	-0.562692775063	-1.499042435366
H	0.126081976575	-1.849216917910	-1.151208101313
C	1.231691547150	-0.547525309326	-2.597610595555
H	1.412946448526	0.486225615489	-2.941661628130
H	2.178567803665	-0.968343729457	-2.228270536876
H	0.893239276800	-1.147346412707	-3.453387876114
Cl	2.375593178111	-1.634220018022	0.633763704067
Cl	-1.444511050619	-0.196182319735	-2.101464045077
O	-0.147454194730	-2.987541669027	-1.065102390274
H	-0.956353436509	-2.997924705610	-1.604266863592
O	-0.422394514711	-4.925698582315	-0.824020434427
H	0.499588193440	-5.058744781552	-1.108978584795

PVC-R

E = -1267.990352013546 a.u. (G_{298K} = -1267.869079480422 a.u.)

0 1

C	1.426821571294	-0.218358180530	2.039048469693
H	0.903790924933	0.692501510654	2.372096868525
H	0.837278807093	-1.092746854530	2.353458081926
H	2.410767741098	-0.253536090592	2.526792232238
C	1.564529561613	-0.190542295938	0.527388535481
H	2.193160759860	0.650526683610	0.205525801474
C	0.215712991013	-0.185754026785	-0.185505305373
H	-0.372852835961	-1.041516577423	0.179993254995
H	-0.313291906375	0.729828926358	0.155995769660
C	0.264897600569	-0.207746524902	-1.680680594681

H	0.809580025707	-2.840856718118	-1.405991271008
C	1.249745541709	0.538626975822	-2.509793338851
H	1.052122197012	1.630181698891	-2.498159919333
H	2.269677856979	0.379448026139	-2.126879535991
H	1.219550963603	0.205963094625	-3.557738868483
Cl	2.542930384680	-1.680593736814	-0.001696201864
Cl	-1.285899361500	-0.548297510855	-2.437058826426
O	0.078502587388	-3.480752063391	-1.403150090687
H	-0.696810931054	-2.923316303013	-1.570014469671
O	-0.379100357822	-3.259180583024	0.971763027676
H	0.595548511904	-3.203526614026	0.906115223671

PVC-P

E = -1268.035101672049 a.u. (G_{298K} = -1267.903369143881 a.u.)

0 1

C	1.675560927566	0.432721075575	1.825316127942
H	1.264814785396	1.455277182772	1.838528840931
H	1.004613081110	-0.219599451433	2.404563948258
H	2.662141030322	0.448223146810	2.309301363994
C	1.781208953385	-0.042045512592	0.387275438900
H	2.492260265525	0.579345230890	-0.173047397615
C	0.429146742150	-0.112181486621	-0.315040181427
H	-0.230151650624	-0.780889069608	0.258198264713
H	-0.012731045450	0.897999693981	-0.272924459003
C	0.472396424960	-0.573915614317	-1.771429284949
H	0.849422771443	-1.601524699235	-1.832553128070
C	1.224310040949	0.338433592501	-2.721247518840
H	0.834826129008	1.367053066293	-2.676264994627
H	2.291408978709	0.354492978002	-2.447258836030
H	1.149428678125	-0.025933295657	-3.755428387610
Cl	2.579186146205	-1.719105614322	0.375748418763
Cl	-1.279891525644	-0.733959469661	-2.350622737942
O	-1.146348551885	-3.078668245741	-0.074066165570
H	-1.434517299386	-2.512799082301	-0.817833949510
O	0.064291130556	-3.653043684448	-0.604699159360
H	0.752750796092	-3.172545304959	-0.103772195690

PDMS-TS

E = -1489.379103851769 a.u. (G_{298K} = -1489.111226361319 a.u.)

0 1

O	1.134294302259	-0.889687637590	1.295995547172
Si	0.236793031982	-1.417807902921	0.015356411624
O	-0.196549465564	-0.079713018716	-0.879479464358
Si	-0.822461619196	0.477397055239	-2.349724182085

Si	1.146095698869	0.301781861249	2.494866688616
C	0.796117203184	1.979958258296	1.720947759890
H	-0.264636794634	2.075570401837	1.440869743081
H	1.030472038860	2.783696117086	2.439452611529
H	1.408992131663	2.136420962791	0.818667598722
C	-0.184798017938	-0.120980232093	3.752977149143
H	-1.170787845948	-0.099695108008	3.261526370279
H	-0.028196551124	-1.124104791132	4.182533368280
H	-0.193782358859	0.609835080010	4.578887449799
C	2.861180447767	0.248123272506	3.256488725570
H	2.947032924857	0.980490863759	4.076420895962
H	3.077729709090	-0.751829137149	3.667317984670
H	3.632830489462	0.484553716630	2.505245443838
C	-1.381445887553	-2.128827944800	0.663741357683
H	-1.689384903813	0.467118107666	0.371600948217
H	-2.066132294476	-2.601855928836	-0.054482496040
H	-1.388551438985	-2.631977055840	1.641033827259
C	1.220770340212	-2.628912269059	-1.001397050409
H	1.528632975010	-3.495927144348	-0.395810961467
H	0.624538632172	-2.993532166994	-1.853074409781
H	2.126228200914	-2.138919588684	-1.395168684771
C	-1.159471786105	2.301718857551	-2.073839930059
H	-1.637165024998	2.758221667401	-2.956368802381
H	-1.823686583750	2.438378947388	-1.204235007030
H	-0.220118010275	2.842746178283	-1.872187491457
C	-2.416959916665	-0.466998829657	-2.667264987836
H	-3.078315495410	-0.376166070206	-1.789949523747
H	-2.951534602762	-0.075099728712	-3.548084436143
H	-2.216870164892	-1.538141773429	-2.836265089085
C	0.451450042844	0.178643318266	-3.694788498991
H	0.668097511231	-0.897283770086	-3.797575144256
H	0.088030545053	0.548492290979	-4.668030899074
H	1.395006234011	0.698464765232	-3.460896809557
O	-2.376836089067	0.134881507723	0.980624646330
H	-2.057399937404	-0.989398064676	0.959220667375
O	-2.800678738498	2.104327076005	1.160924159200
H	-2.562441913732	2.038951570367	2.103586621332

PDMS-R

E = -1489.407936671132 a.u. (G_{298K} = -1489.137481101512 a.u.)

0 1

O	1.173494829891	-0.419802792809	0.994307530289
Si	0.421560515958	-1.493012192360	-0.023388614163
O	-0.791011648462	-0.665239960202	-0.847351958482

Si	-0.939351272041	0.398553497851	-2.168894804553
Si	1.026579164416	0.395318751101	2.464447814759
C	0.589945424997	2.185888889342	2.105290981696
H	-0.419167963409	2.273934742061	1.672196748830
H	0.616789202878	2.778929293187	3.035370546592
H	1.308314354928	2.630967098366	1.397258660785
C	-0.318284630890	-0.417632323069	3.496177551836
H	-1.280558078157	-0.375141436484	2.960736169744
H	-0.079556894538	-1.475099554787	3.696522203302
H	-0.431754423000	0.099947515338	4.463778218389
C	2.701698772939	0.274682273300	3.309231691268
H	2.692485444037	0.804734889823	4.276364932416
H	2.971448534360	-0.777525252350	3.498924940795
H	3.491117845425	0.722617109643	2.683024500317
C	-0.451312719120	-2.822924081643	0.921442408179
H	-2.103727571545	-0.402943152518	0.310099156495
H	-1.476030239686	-2.692497386831	1.288126014054
H	0.029252385898	-3.764797014559	1.210365161052
C	1.710076279898	-2.157987357234	-1.196879062847
H	2.426015775299	-2.790573189810	-0.647034772892
H	1.252280165173	-2.765004180623	-1.993492894012
H	2.273758122153	-1.335039036273	-1.664413801829
C	-0.064066699353	1.998313191914	-1.724508154771
H	-0.074897404386	2.703013763706	-2.572541330376
H	-0.564855799254	2.481983826752	-0.869312846669
H	0.984765034276	1.808053442749	-1.444467662050
C	-2.782030420816	0.674501116388	-2.394092837926
H	-3.203640309587	1.211592523896	-1.530203559318
H	-2.970076138997	1.280012626084	-3.296196639656
H	-3.314411594303	-0.284109789856	-2.507102093839
C	-0.185366950118	-0.407171094023	-3.688683216120
H	-0.633914784654	-1.397458920824	-3.871132544112
H	-0.368311478490	0.219806743028	-4.577311075486
H	0.902885795712	-0.536789277840	-3.582679745645
O	-2.744787279735	-0.097668964685	0.992868396184
H	-3.585371597028	-0.511679266913	0.748692602822
O	-2.584670011138	2.563047076981	0.490520704819
H	-2.692305147334	1.602134175784	0.759448148289

PDMS-P

E = -1489.454071034124 a.u. (G_{298K} = -1489.176874636785 a.u.)

0 1

O	1.203021347228	-0.749165174725	1.169230437764
Si	0.264400080138	-1.516623102582	0.035862173532

O	-0.653207845811	-0.348201754129	-0.753979017396
Si	-0.898812285682	0.480823442552	-2.218090275374
Si	1.130206838734	0.400910022801	2.396066712200
C	0.981123359519	2.102361580314	1.613581917992
H	0.023515662878	2.193758756122	1.078813397537
H	1.026504578495	2.894113139920	2.380035062712
H	1.796200511165	2.275498290895	0.891839467525
C	-0.370331549217	0.040403735235	3.476289364671
H	-1.293285426989	0.024891899288	2.873585367953
H	-0.276751360139	-0.944590145186	3.962525768911
H	-0.481592947993	0.801836115685	4.266193257035
C	2.721475541394	0.239491257893	3.378454968357
H	2.744585688697	0.966347077138	4.207447000685
H	2.818339019693	-0.771534865320	3.807405370061
H	3.598953668542	0.425600638137	2.737319756159
C	-0.954619566243	-2.662595267605	0.872410739970
H	-1.993393389920	0.137171727529	0.291500541296
H	-1.546201440049	-3.211505006420	0.121500202268
H	-0.433533588288	-3.397756956884	1.506673292469
C	1.403626119941	-2.406276136634	-1.144523474198
H	1.976635519048	-3.172324786701	-0.596710427640
H	0.836561858851	-2.909303817317	-1.943577097473
H	2.118914059215	-1.710999382238	-1.610152919080
C	-0.713910063451	2.309427079918	-1.847021153269
H	-0.922724386881	2.914251964674	-2.745014865600
H	-1.414525777095	2.602526701590	-1.049641925492
H	0.308418337450	2.537497431205	-1.504947639484
C	-2.657125803220	0.069580266726	-2.734436921563
H	-3.346058368377	0.286844008388	-1.901800609547
H	-2.970665836826	0.660693806758	-3.610474715029
H	-2.752090507740	-0.999510558224	-2.986565794213
C	0.350192548148	-0.082341157076	-3.501569453654
H	0.267835391255	-1.161650483493	-3.703992527681
H	0.172250267346	0.456672849680	-4.447348945894
H	1.381456208692	0.132488134084	-3.178445135142
O	-2.760865590860	0.397824895413	0.858063197932
H	-1.652001056291	-2.092917520569	1.506874657593
O	-2.511839495462	1.801905545037	1.063707265250
H	-2.194627260751	1.819935417079	1.983060236946

NOOH

E = -1531.673403761575 a.u. (G_{298K} = -1531.191044246722 a.u.)

0 1

C	1.001677352613	-0.519954858230	1.721857294753

C	0.492867675543	-1.416339578789	0.600885374768
C	1.178513863951	-1.050430288000	-0.708935304512
C	2.706110745074	-1.248496625413	-0.647926063161
C	2.517191856027	-0.674086779490	1.958778378245
H	0.778871890973	-1.667121130629	-1.528395690400
H	0.776755852957	0.523616080140	1.465440569944
H	0.475692800890	-0.754316430543	2.659894688658
H	0.955187889891	-0.000930968497	-0.942038283424
N	3.244610215659	-0.706409425931	0.645160411760
O	4.454213419405	-0.356836534996	0.659947591568
C	3.013890143812	0.539435340136	2.757473833496
H	2.420241272322	0.624406770805	3.679758173437
H	4.072663508058	0.432235899598	3.026448771049
H	2.905944827144	1.458266849827	2.166393991917
C	2.846819844613	-1.969857974803	2.725852047515
H	3.937799526529	-2.084976291141	2.807836245613
H	2.422136465778	-1.923412418849	3.740259894184
H	2.444230492053	-2.864309789441	2.230007237868
C	3.347116530239	-0.473336071918	-1.808585361638
H	4.421954168954	-0.688142047244	-1.884759066789
H	2.865738092189	-0.779026767162	-2.749177983248
H	3.218290395733	0.606950371208	-1.663226829292
C	3.093349583678	-2.737429932448	-0.746150316188
H	2.815215312253	-3.132049208657	-1.735330191764
H	4.180464538862	-2.847176019684	-0.618193950820
H	2.595037989616	-3.351823549427	0.016768501618
O	-0.948396976510	-1.425018661427	0.499000425846
C	-1.645016703019	-0.319142843083	0.205562723143
O	-1.134402514619	0.769911113553	0.002000037035
C	-3.113753139636	-0.535309590587	0.154750473009
C	-3.748025752078	-1.836124158735	0.365115571827
C	-3.900926157098	0.572381352852	-0.109751872646
H	-3.398309229352	1.529797981776	-0.268033755527
O	-5.143996296794	-1.837599423807	0.292381075455
C	-7.297673377657	-0.933203127650	0.002369665154
C	-5.920344684905	-0.750725410358	0.034067222237
C	-5.306396714445	0.509026581254	-0.179561004544
C	-6.151732412528	1.615901203561	-0.445044944551
C	-7.521610178766	1.489464686324	-0.502229293840
C	-8.125613519203	0.200330973560	-0.259691319836
H	-5.693625542495	2.594288271866	-0.613652072393
N	-9.482687586696	0.068098460790	-0.281178473934
C	-7.916151290056	-2.291235791315	0.228032382989
C	-9.241721298379	-2.388028150086	-0.524104828275

C	-10.146069105146	-1.228460351692	-0.135189353482
H	-11.046730467716	-1.216674356467	-0.770018028344
H	-9.054748238800	-2.359441170892	-1.610985779701
H	-9.755024054042	-3.335969064009	-0.303770941885
H	-8.089694405868	-2.452095140817	1.308170526623
H	-7.218538081914	-3.078144548144	-0.091660988575
H	-10.493675775533	-1.344481058482	0.909429650490
C	-9.734729559804	2.529291393935	-0.050733505577
C	-8.416004329967	2.666536790880	-0.808826411901
C	-10.393994998798	1.206821183271	-0.412933632180
H	-8.626176921783	2.702578228301	-1.894009951231
H	-7.903421373837	3.606971546109	-0.556483672212
H	-9.545234721091	2.565035884153	1.035547366672
H	-10.423700134190	3.352594980777	-0.292119546213
H	-10.782573106804	1.242724623886	-1.448674835343
H	-11.259460205949	1.020062064394	0.243754167440
H	0.702152302178	-2.467054766002	0.845085734403
O	-3.238641214339	-2.908058861666	0.591656128216
O	4.620362404869	1.373496068955	0.316884674798
H	5.176563942463	1.251296864266	-0.469360437899

NO_Probe-radical

E = -1455.979811685703 a.u. (G_{298K} = -1455.509255516015 a.u.)

0 2

C	1.013534694732	-0.511445519285	1.734727072455
C	0.488111035457	-1.406442443808	0.619787791209
C	1.160449540495	-1.045039999518	-0.698293939512
C	2.688155682129	-1.236962577068	-0.647695362828
C	2.531941803692	-0.668298244370	1.943892127427
H	0.755468470318	-1.666561986644	-1.511750734427
H	0.782981592805	0.532483843824	1.484396769933
H	0.502723881740	-0.747227056245	2.681054562267
H	0.929695819311	0.002254528893	-0.934342717491
N	3.243445621339	-0.651982537760	0.620311153652
O	4.510870096011	-0.526356192352	0.669228649211
C	3.048902708950	0.527243478154	2.756848294783
H	2.508527976426	0.580763749937	3.713887136456
H	4.122772916547	0.425732635476	2.959375834584
H	2.882798334710	1.467588509064	2.209380022762
C	2.880628254546	-1.977269891666	2.679873883520
H	3.972781300370	-2.102253989141	2.703151790700
H	2.506797080905	-1.936252074925	3.714084114160
H	2.442761491006	-2.861804605580	2.197062193971
C	3.324301070826	-0.476730278094	-1.820226589399

H	4.411224467777	-0.627149922472	-1.838581228251
H	2.897482597243	-0.840167123174	-2.767068104998
H	3.121049225292	0.601846417531	-1.737130503856
C	3.085784070134	-2.724390379950	-0.725777634383
H	2.834046135200	-3.127223980423	-1.718425053120
H	4.169936345433	-2.820335128209	-0.569674605773
H	2.573257432956	-3.338145583971	0.027846362438
O	-0.954807609014	-1.411453709312	0.532560191944
C	-1.651980036100	-0.305895700689	0.241598373965
O	-1.142877672749	0.784321801925	0.039856517492
C	-3.120741271165	-0.523612164263	0.188302921031
C	-3.754014489501	-1.825091284292	0.397766073270
C	-3.908456508677	0.582393002489	-0.081155777788
H	-3.406601122530	1.540461631334	-0.237921112710
O	-5.149517935788	-1.829427416381	0.315695998415
C	-7.302832487134	-0.930354359760	0.006956819623
C	-5.926215770407	-0.744589140500	0.050068955463
C	-5.313447796893	0.516344417633	-0.159679941514
C	-6.159157343955	1.621051410581	-0.432730404557
C	-7.528253545145	1.491345523310	-0.501269338628
C	-8.131207944798	0.200911747536	-0.263239150366
H	-5.701982645766	2.600388199147	-0.598392382495
N	-9.487758555550	0.065225374789	-0.296830522206
C	-7.919926332360	-2.289763720712	0.228091719803
C	-9.238362022344	-2.390443691851	-0.536000409368
C	-10.149153545182	-1.232928024194	-0.156061514544
H	-11.044027464045	-1.223848616196	-0.799078456390
H	-9.041574747414	-2.362054844107	-1.621164653111
H	-9.751227348879	-3.339567521021	-0.319731602449
H	-8.102907165256	-2.450261530339	1.306733167071
H	-7.217472322418	-3.075162026887	-0.084644537238
H	-10.505980118197	-1.349246722498	0.885427987928
C	-9.748092047606	2.525867993254	-0.070467056761
C	-8.422732102192	2.666141069944	-0.816363859932
C	-10.400589510940	1.201544609287	-0.438125121473
H	-8.622976608836	2.701419527405	-1.903459361298
H	-7.914823654890	3.607914470613	-0.559551806859
H	-9.568810074548	2.562575731474	1.017524044658
H	-10.436865801414	3.347319084927	-0.318652605087
H	-10.779274631198	1.235881746069	-1.477595297788
H	-11.271882360326	1.013086610644	0.210327398806
H	0.696366282903	-2.457365418096	0.862822440009
O	-3.244326848980	-2.895502242977	0.630753920801

OH-radical

E = -75.671926959465 a.u. (G_{298K} = -75.679849721070 a.u.)

0 2

O	-0.493997295303	0.000000000000	-4.685654603360
H	-0.493997295303	0.000000000000	-5.667251715788

PAMPS-radical

E = -534.176131728159 a.u. (G_{298K} = -534.016146558969 a.u.)

0 2

C	-1.561171807390	-1.698661831737	-0.176975989253
H	-0.969535583293	-2.323137638060	0.518133300131
H	-2.396855624563	-1.264581933757	0.390185880911
H	-1.993576247115	-2.391061323171	-0.924203120134
C	-0.727498277012	-0.639327764542	-0.826667244709
C	-1.091704863646	0.800303574029	-0.666470735766
H	-0.557199137409	1.405428597850	-1.412706158579
H	-2.176763991189	0.920868038686	-0.834305745461
C	-0.784218885373	1.381832592247	0.748585553805
H	-1.261883344868	0.727918113355	1.498198867681
C	-1.339873999010	2.798274004181	0.890887803577
H	-0.850782539847	3.470896844282	0.170767133812
H	-2.424788769796	2.810530587799	0.705289302381
C	0.498854795534	-0.968973426684	-1.570932374908
O	1.226767779088	-0.091086397481	-2.054623666281
C	0.731314970594	1.369944946519	0.976678845295
O	1.447927658920	2.306672023838	0.641591450534
H	-1.157969281783	3.196808767373	1.901120449100
N	1.226326838578	0.241625154203	1.542803335675
H	2.230226984271	0.139274591194	1.644958687743
H	0.635329390048	-0.532088415082	1.817886852779
N	0.817177364044	-2.291899905042	-1.691540722447
H	1.634443150161	-2.536314029397	-2.238029470734
H	0.211957712761	-3.042270313053	-1.387508254217

H_2O

E = -76.364904117308 a.u. (G_{298K} = -76.361409472596 a.u.)

0 1

O	-0.062619375456	0.000000000001	-2.136157141895
H	-0.062619375464	0.755177151951	-1.530625510682
H	-0.062619375464	-0.755177151951	-1.530625510685

$OH(H_2O)_4$-TS

E = -381.203636469288 a.u. (G_{298K} = -381.131984246587 a.u.)

0 2

O	-0.692093262482	-3.043504454374	2.155451350612
H	0.068366061770	-2.656061214551	2.668132725102
H	-0.961605096049	-3.852123833795	2.613065433452
O	1.549521154001	-1.803449535589	2.912391096039
H	2.128741120033	-2.426871122118	2.445370236089
H	1.371922331117	-1.142901710419	2.203669640384
O	1.140284713781	-2.719881390260	0.112153876289
H	0.382104444812	-3.017195553191	0.670769669216
O	-1.817269786288	-0.913774205741	0.952818617153
H	-2.216768834437	-1.245238742432	0.134654111093
H	-1.643720598892	-1.727570805582	1.481126418441
O	0.811823119405	-0.550648847550	0.548769371358
H	-0.186989542687	-0.583353215257	0.653644453704
H	1.024399749743	-1.579001485997	-0.003340396545

$OH(H_2O)_4$-R

E = -381.214219516575 a.u. (G_{298K} = -381.139246048517 a.u.)

0 2

O	-0.747915298634	-3.009494516998	2.125465330076
H	0.024061649527	-2.605470667352	2.600662701595
H	-1.088589823807	-3.711969073535	2.697052758953
O	1.607024864696	-1.860924167328	2.730044283708
H	1.839298121382	-2.316386083427	1.888285129348
H	1.501967164408	-0.937506592600	2.436957758182
O	1.331579083411	-2.969651989903	0.213850901044
H	0.493792827948	-3.250708753095	0.632677407631
O	-1.878596498613	-0.870527067673	0.963291230433
H	-2.206653543894	-1.189196955413	0.108944341491
H	-1.665064659356	-1.698135831187	1.460744411971
O	0.695945281636	-0.326089656950	0.671539449012
H	-0.315342316388	-0.388779752834	0.739565554885
H	1.136253613639	-2.051641983587	-0.059776803935

$OH(H_2O)_4$-P

E = -381.218197598756 a.u. (G_{298K} = -381.142363920564 a.u.)

0 2

O	-0.469888733783	-3.102196929509	2.063687257297
H	0.200382880068	-2.595779106911	2.615184659422
H	-0.776173753444	-3.849563249600	2.596871130346
O	1.325946264697	-1.499801968779	3.104217216738
H	2.201229626138	-1.914637925200	3.086679814703
H	1.283552452131	-0.982448207043	2.251969634339
O	0.914818866600	-3.138467712810	-0.237655094533
H	0.368532178950	-3.286571535162	0.593535304503

O	-1.753120884579	-0.918466965261	1.019788549187
H	-2.111045820101	-1.202426589121	0.165620098456
H	-1.500296771766	-1.761650990857	1.459002416646
O	0.928691271353	-0.432009881371	0.678693524899
H	-0.056998697255	-0.422423307868	0.742875296430
H	1.088383247042	-1.268388992507	0.195140620111

$OH(H_2O)_4$-INT1

E = -381.211229652783 a.u. (G_{298K} = -381.139504426298 a.u.)

0 2

O	-2.585821404130	-0.462285758281	-0.984857849848
H	-1.687542014399	-0.100387038081	-1.022308628377
H	-3.158829122538	0.324277608269	-1.126012067488
O	-3.614051159434	-0.098424622204	1.516832341159
H	-3.630581106839	0.871038625481	1.460818066055
H	-3.132421693275	-0.362781870602	0.693930800204
O	-6.138957418717	-1.061186296059	1.359773408622
H	-6.567816510604	-0.798131457884	2.187411892784
H	-5.201636514488	-0.753700445122	1.467207351609
O	-6.726970348262	0.746279599066	-0.512108278292
H	-7.296776280510	1.386777824687	-0.060724892934
H	-6.616126558068	0.012120808058	0.154493132908
O	-4.240270844894	1.629784822219	-0.439008136706
H	-5.216212954806	1.348162242878	-0.516434001915

$OH(H_2O)_4$-TS1

E = -381.208910812200 a.u. (G_{298K} = -381.137043258699 a.u.)

0 2

O	-3.101293929356	-0.371196708610	-1.082836567096
H	-2.191220517131	-0.090494620730	-1.265058360226
H	-3.618537015383	0.439601196579	-1.232016249192
O	-3.542649328055	-0.274979067746	1.646593451073
H	-3.616441661846	0.696766228281	1.661347951547
H	-3.274206592024	-0.445254974396	0.712800618032
O	-6.134590303160	-1.025619325936	1.511956077719
H	-6.586639493219	-0.531166776396	2.211557098046
H	-5.172984371055	-0.826151737939	1.662370995231
O	-6.173806225483	0.535827144300	-0.654229471382
H	-7.030830840213	0.981194292172	-0.719403699954
H	-6.272104485963	-0.102850449138	0.104912417499
O	-4.096358897020	1.939592414355	0.158256412055
H	-4.990058515426	1.536136917399	-0.099224973798

$OH(H_2O)_4$-INT2

E = -381.218200758417 a.u. (G_{298K} = -381.142502072309 a.u.)

0 2

O	-3.368700415819	-0.787998428459	-1.165561314126
H	-2.787409724323	-0.132321220480	-1.578484364925
H	-4.263173442896	-0.384709115608	-1.236117787385
O	-3.466771521636	-0.238408048087	1.524218359257
H	-3.625761642450	0.719146958154	1.395035584657
H	-3.272958838025	-0.536598722490	0.602641362024
O	-6.062640305902	-0.902790874285	1.459727193184
H	-6.505223978237	-0.367055694307	2.134714343398
H	-5.090572063703	-0.749079314468	1.624066315340
O	-5.767593289197	0.471367182042	-0.754296455613
H	-6.545181388784	0.599697929083	-1.316048194221
H	-6.056753895968	-0.078743832455	0.035408869000
O	-4.360908945619	2.313959019343	0.601338189252
H	-4.952868690280	1.753902297626	0.011948476156

$OH(H_2O)_4$-TS2

E = -381.212071955526 a.u. (G_{298K} = -381.136736648181 a.u.)

0 2

O	-3.331237418113	-0.216318834903	-0.998887398337
H	-2.895009913938	0.525896450594	-1.440161666620
H	-4.284478404852	-0.149907549084	-1.250996284520
O	-3.287804459623	-0.510048125405	1.713088570490
H	-3.355970940095	0.438757329060	1.914572057836
H	-3.167527793015	-0.487583140401	0.732167127954
O	-5.974039989951	-0.477791560177	1.508812993956
H	-6.251705669403	0.193777803625	2.148981027898
H	-5.005865288630	-0.620223073273	1.692178916839
O	-6.008729368537	-0.003341561875	-1.150178904810
H	-6.494515109397	0.810399042100	-1.345555225457
H	-6.181464026150	-0.187514828123	-0.193793928861
O	-4.852815729095	1.777671501938	1.084028439167
H	-4.710346060856	1.368659474821	0.203268132006

$OH(H_2O)_4$-INT3

E = -381.218179398042 a.u. (G_{298K} = -381.142746610741 a.u.)

0 2

O	-3.564408077228	0.409670493950	-0.681563243865
H	-2.974777592754	0.548390406981	-1.436383418870
H	-4.420314640198	0.021238953434	-1.037486978359
O	-3.390923347676	-1.180502446658	1.543131049313
H	-2.891413576857	-0.674376634325	2.200852724642

H	-3.243581435516	-0.686223071627	0.705450417644
O	-5.968886615178	-0.234216163179	1.511536905281
H	-5.698966658091	0.706214255831	1.471909837111
H	-5.104196757479	-0.685254525656	1.668900564160
O	-5.947694950686	-0.578284672065	-1.145632651019
H	-6.529745109795	0.099911997027	-1.519497077313
H	-6.107006684159	-0.522087800261	-0.162100236012
O	-4.659660437266	2.241948890992	0.947395644671
H	-4.148085105316	1.679473622129	0.289134083885