Gold(I) catalyzed intermolecular dioxolane addition to alkynes: the role of water

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Abstract

Density Functional Theory (DFT) calculations have been performed on a homogeneous gold catalyzed reaction between acetylene/propyne and the cyclic ketal 2,2-dimethyl-1,3-dioxolane, DMDO, in the presence of water, with the aim of understanding the actual role played by water. After the addition of DMDO to the alkyne, hydrolysis may happen through two possible reaction routes. In the so called H-route (previously proposed for similar intramolecular reactions) a water proton is initially added to the alkyne C atom still linked to gold and, afterwards, an OH group adds to a DMDO C atom to allow the release of acetone, whereas in the newly-proposed OH-route, a water OH group firstly adds to the most substituted DMDO C atom with simultaneous addition of H to the alkyne C atom linked to gold. A 1,3-H transposition from the just added OH group allows the release of acetone. An intramolecular nucleophilic OH addition to the gold activated alkene intermediate formed from both hydrolysis paths drives the system to the corresponding 1,3-dioxolane product. The H-route is unable to explain the formation of the dioxolane addition products (observed in similar intramolecular reactions) instead of those coming from the direct addition of water to the alkyne, since it is energetically more demanding than the direct hydration. However, OH-route goes through structures that are more stable than those in the water addition, so, it is the one actually happening for the reaction under study. The regioselective addition of DMDO to the internal C atom of propyne is predicted on the basis of the large polarity of the structures formed in this approach, which makes them capable of strong interactions with water.

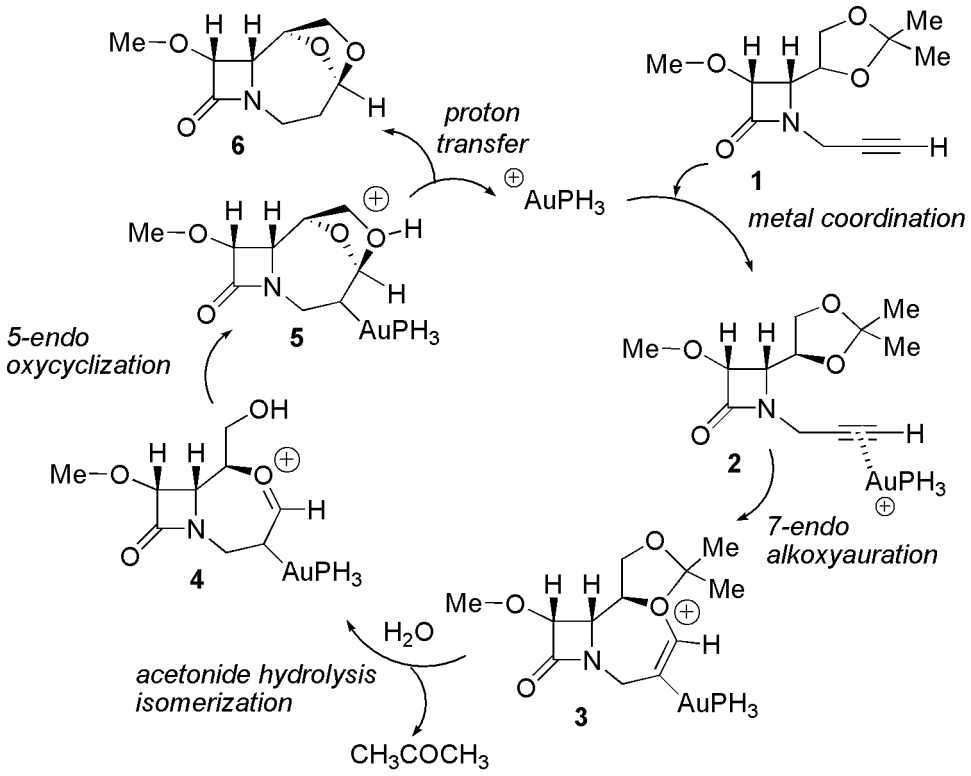
Keywords: homogeneous catalysis, gold (I) catalyst, cyclic ketals, alkynes, computational chemistry.

Introduction

It is well known that the soft Lewis acid character of cationic gold complexes enables them to activate unsaturated C-C bonds under homogeneous catalytic conditions [1, 2]. Reactions involving compounds with a triple C-C bond where new C-O links form, like hydration and alkoxylation of alkynes, have largely benefited from this catalysis since the initial applications of gold in homogeneous catalysis [1–5]. Particularly, gold-catalyzed intramolecular hydroalkoxylation reactions have been often used in the synthesis of several heterocycles [6–8] and natural products [9], mainly starting with free alcoholic groups as O-suppliers; only a few cases have used an ether (linear or cyclic) as a nucleophile, and even less have studied the double addition of two consecutive O atoms belonging to the same molecule.

Alcaide *et al.* have reported some intramolecular bis-cyclizations of acetonides tethered to alkynes where the bridge between these functionalities contains a linear ether/amine [10], a 2-azetidinone ring [11], or a 2-azetidinone ring plus a double bond [12]. When the bridge is a 2-azetidinone ring [11], 1,2 diols and acetonide cycles were independently considered as nucleophiles, and both rendered the same tricyclic product, although under different experimental conditions. The reaction of the acetonide did not need the presence of an acid but it did require the participation of water. Actually, the absence of an acid prevented the hydrolysis of the acetonide to the corresponding diol. Authors claim that, looking for a maximal total efficiency of the organic transformation, the use of 1,3-dioxolanes is preferred over that of free hydroxyl groups from a diol [11]. Theoretical mechanisms where proposed for the reactions starting with the diol and the acetonide and they were different [11]. As seen in Scheme 1, for the acetonide **1**, external water allowed the hydrolysis of the intermediate **3** formed after metal coordination to the triple C-C bond and the first acetonide-O addition leading to the tricyclic product **6** after the second acetonide-O addition and proton transfer. Isotopic labelling confirmed the active role played by water, since it

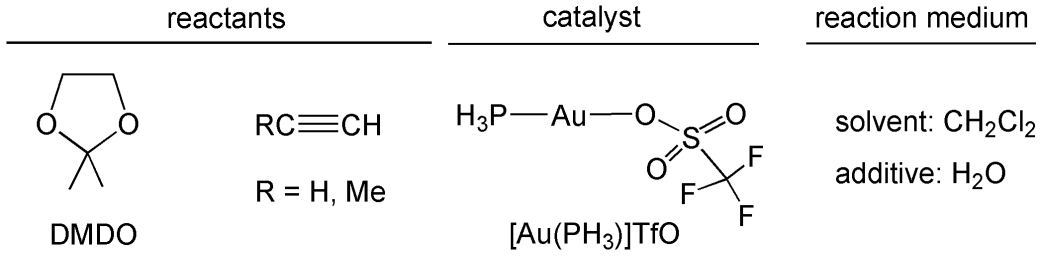
demonstrated that affected H atoms in the product come from external water. However, products coming from the direct hydration of the triple bond were not found.



Scheme 1. Theoretical mechanism found for the gold-catalyzed bis-cycloetherification of alkynic acetonide **1**.

In the present work we wonder whether the mechanism found for the intramolecular cyclization of alkynic acetonides is also operative for an intermolecular process, *i.e.*, the alkyne and acetonide functional groups are not initially bound. This ketalization, with the mandatory presence of water in the reaction media, may render C2 substituted 1,3-dioxolanes, which are relevant to protect carbonyl groups against nucleophiles in the presence of other functional groups when processing multifunctional organic molecules. Besides, many of them have found direct applications as fragrances, in cosmetics, as food and beverage additives, in pharmaceuticals [13], and in detergents, as well as participating in the synthesis of marine alkaloids [13]. In this scenario, to accomplish that task, we selected 2,2-dimethyl-

1,3-dioxolane (DMDO) as the acetonide to be added to simple alkynes such acetylene and propyne in an intermolecular fashion in dichloromethane solution, the solvent experimentally used in the bis-cycloetherification of alkynic acetonides, and using [Au(PH_3)]TfO as catalyst (see Scheme 2). The role of the low coordinating TfO^- anion is carefully analyzed all along the mechanistic study [14, 15]. Besides checking the viability of the intramolecular mechanism, this will be compared to that for the hydration of the alkyne. Experimental data indicate that DMDO addition is preferred over hydration, so, if this cannot be explained with the mechanism suggested for the intramolecular case, a new one has to be operating and we wish to describe it.



Scheme 2.

Computational Details

All the quantum chemical computations were carried out with the Gaussian 09 series of programs [16]. Full geometry optimizations of local minima (reactants, products, and intermediates) and first-order saddle points (transition states, TSs) were performed in dichloromethane (DCM) solution from the outset at the PCM(UFF)-M06/VDZ level of theory in conjunction with a modified Schlegel algorithm [17, 18]. DCM solvent effects on molecular geometries and energies were taken into account through the Polarizable Continuum Model (PCM) approach of Tomasi and co-workers [19, 20] together with the integral equation formalism model [20, 21], the Universal Force Field (UFF) radii [22], and a relative dielectric constant of 8.93. M06 is a hybrid meta generalized gradient approximation (HM-GGA) functional that is parameterized for both transition metals and nonmetals with a percentage of Hartree-Fock exchange of 27% [23]. VDZ is the correlation consistent double-zeta basis set augmented by diffuse functions aug-cc-pVDZ here used for the non-metal atoms [24, 25] plus aug-cc-pVDZ-PP for Au [26], in which the valence electrons are represented explicitly by aug-cc-pVDZ while the core electrons

are modelled by the corresponding double-zeta Stuttgart-Koln energy-consistent relativistic pseudopotential. Harmonic vibrational frequencies at the same theory level confirmed the nature of minima or TSs of the critical points located on the potential energy surface of the reaction. IRC calculations have been performed to check the connections between each TS and the intermediates it joins [27,28]. At hydration/hydrolysis steps a number, *n*, of explicit water molecules have been considered, as discussed below. Since these water molecules are not present in the remaining reaction steps, the connection between a particular anhydrous and hydrated structure in the corresponding energy profile has been done assuming that the difference in energy between the anhydrous species + a cluster of *n* water molecules and the hydrated one, ΔE, corresponds to a stabilization that all the anhydrous species would undergo if allowed to interact with the water molecules. Thus, ΔE would have to be added to the energy of the structures involved in steps other than the hydration/hydrolysis ones or, equivalently, subtracted to the energy of the structures in the hydration/hydrolysis steps. For comparison purposes, following previous computational strategies used in related gold-catalyzed systems [11, 29], all energies given in the text correspond to the energy including the effect of the bulk solvent CH_2Cl_2, which was obtained by adding the contribution of the Gibbs energy of solvation to the gas phase total energies. Natural bond orbital (NBO) population analysis were also performed to quantify the atomic population at relevant structures [30, 31].

The choice of the computational scheme PCM(UFF)-M06/VDZ is supported by similar theory levels used to investigate related gold-containing systems [32]. The combination of M06 with relatively small split-valence basis set has proven to be one of the best theory levels in investigating the energetics of homogeneous gold-catalyzed reactions of propargyl esters [33]. Besides this, it has been found that the use of larger basis set does not produce appreciable changes in the energies. Relativistic effects other than those incorporated in the aug-cc-pVDZ-PP basis set have not been considered on the basis of previous works on the related gold-catalyzed cyclizations where no significant changes in the rate-determining energy barrier were found [34].

Results and Discussion

A detailed description of all possible routes for the reaction of DMDO with acetylene in the presence of water will be initially provided. Afterwards, the effect of a methyl group linked to the triple bond, as it is in propyne, on the regioselectivity of these mechanisms will be analyzed. Unless otherwise stated, relative energies will be given with respect to isolated reactants in kcal/mol.

Addition of DMDO to acetylene in the presence of water

Figure 1 displays the energy profiles of the accessible routes theoretically obtained for the reaction of DMDO and acetylene in DCM solution with the participation of water. Figures 2-6 collect the optimized geometries of the species involved in them. Atom numbering shown for the reactants in Figure 1 will be followed in the text.

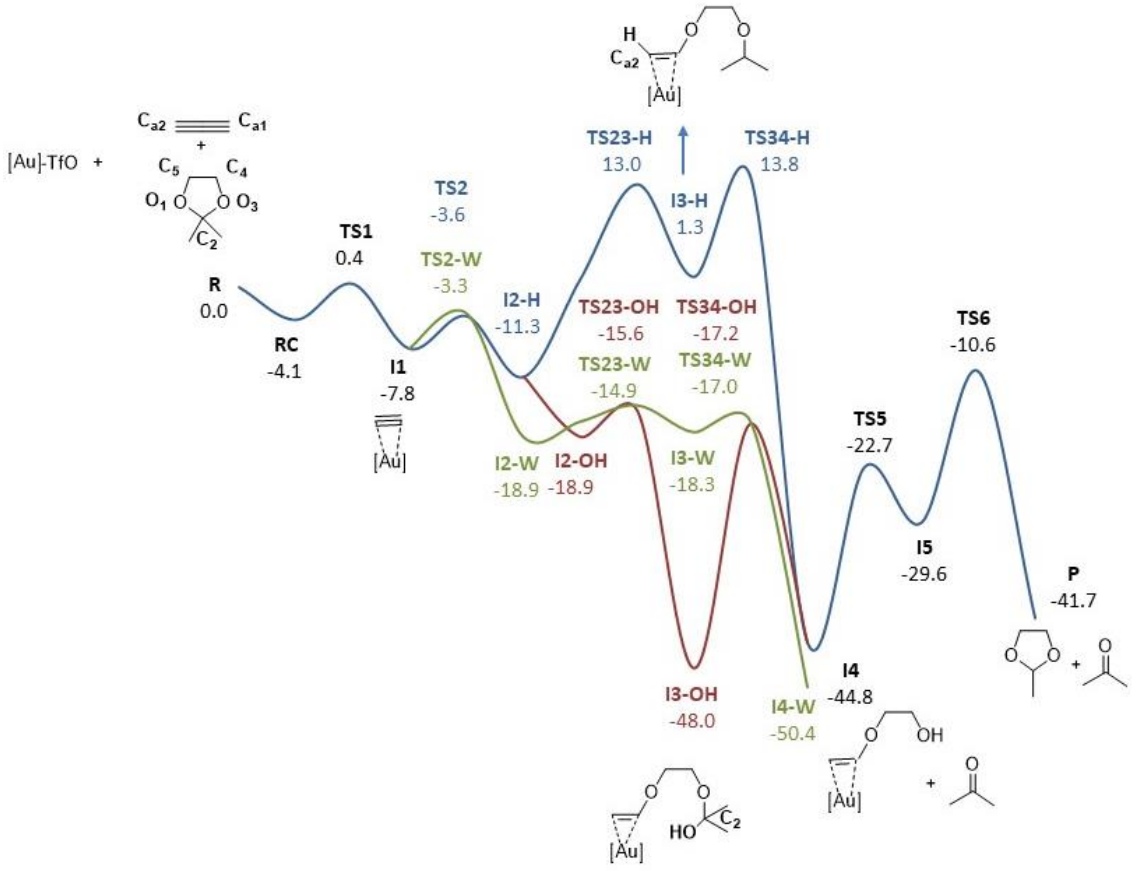
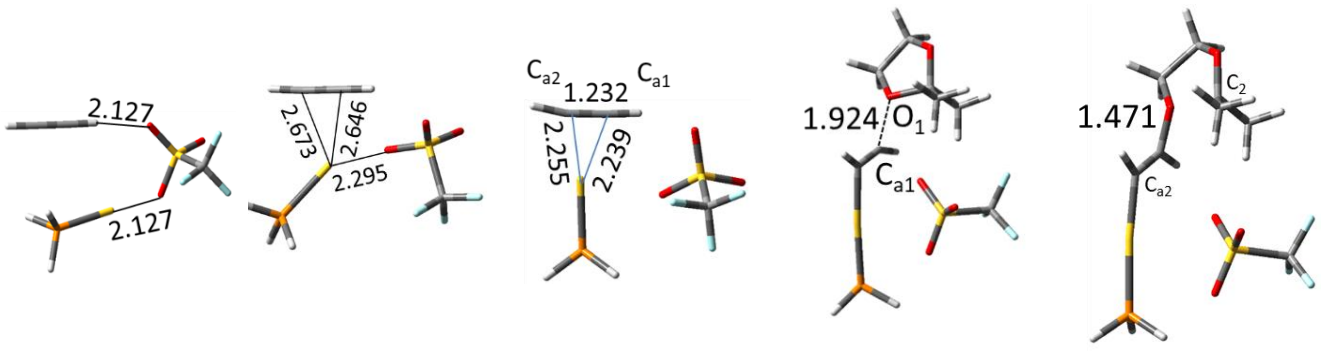


Figure 1. PCM(UFF)-M06/VDZ energy profiles in DCM solution of the possible mechanisms for the addition of DMDO to acetylene in the presence of water (blue and red lines) and for the hydration of acetylene (green line).

At the beginning of the reaction the triflate counterion of the gold catalyst plays a significant role by simultaneously interacting with the active $[Au(PH_3)]^+$ moiety and one H atom of the alkyne in a stable pre-reactive complex, **RC** (-4.1 kcal/mol), where the alkyne is well orientated for the subsequent approach of the gold moiety (see Figure 2). Then, $[Au(PH_3)]^+$ coordinates to the acetylene triple bond in a η^2 fashion via **TS1** (0.4 kcal/mol) to give the activated alkyne **I1** (-7.8 kcal/mol), after surmounting a small barrier of 4.5 kcal/mol from **RC**. The σ and π coordination of up to four gold fragments to acetylene has been previously reported [35, 36]. However, our results suggest that triflate anion tends to block one of the σ coordination positions while favoring the η^2 gold coordination, so this seems to be the preferred coordination in the reaction route. Previous theoretical calculations on gold catalysis also support the η^2 gold coordination as the most reactive one [37]. At **TS2** (-3.6 kcal/mol) DMDO approaches one acetylene carbon, C_{a1}, in *trans* disposition to the catalyst to render the vinyl ether intermediate **I2** (-11.3 kcal/mol), where gold moiety is interacting in σ fashion with the other acetylene carbon, C_{a2}, (see Figure 2).

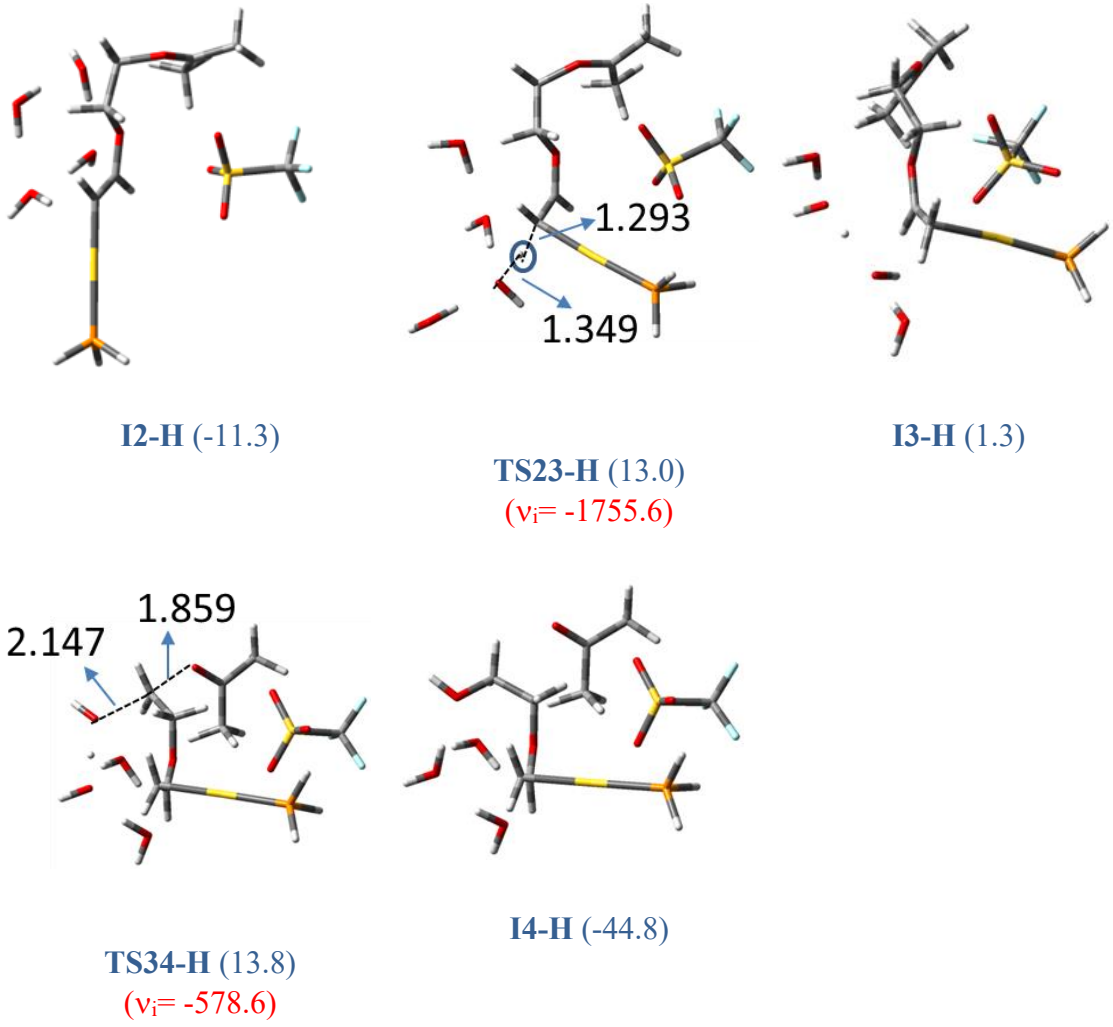


RC (-4.1) **TS1** (0.4) (ν_i= -78.1) **I1** (-7.8) **TS2** (-3.6) (ν_i= -300.8) **I2** (-11.3)

Figure 2. PCM(UFF)-M06/VDZ optimized structures in DCM solution of the species involved in the initial steps of the gold catalyzed reaction of DMDO with acetylene. Some relevant distances are given in angstroms. Relative energies in kcal/mol are also included in parenthesis.

After the addition of the dioxolane moiety to the alkyne water comes into stage. Firstly, for the hydrolysis steps, we consider the mechanism already proposed for the intramolecular DMDO addition to a terminal alkyne when both units are linked by a 2-azetidinone moiety [11]. A cluster made of four water molecules is used at this point. Since the Au-linked acetylene carbon atom, C_{a2}, is the most nucleophilic center at **I2** (NBO charge = -0.565 *e*) a water molecule can orientate one of its H atoms towards this C atom, as it is in intermediate **I2-H** (see Figure 3). We call this hydrolysis approach H-route (see blue line in Figure 1). The difference between anhydrous **I2** and **I2-H** energies amounts to 17.7 kcal/mol. This value was subtracted from the energy of the structures involved in the H-route hydrolysis, as previously explained. The water disposition in the H-route supports the addition of a proton to C_{a2}, through **TS23-H** (13.0 kcal/mol), releasing a hydroxyl anion that is stabilized by the remaining water molecules in the environment, as it is in **I3-H** (1.3 kcal/mol). Then, this OH^- performs a S_{N2} nucleophilic substitution through its attachment to the methylene C of the DMDO moiety furthest from Ca1, C_4, with simultaneous elimination of acetone, as represented by **TS34-H** (13.8 kcal/mol), yielding the very stable alcohol **I4-H** (-44.8 kcal/mol). The difference between **I4** and **I4-H** energies is now 8 kcal/mol. To connect both structures this value was added to **I4-H** energy, assuming that this is the solvation energy for the structures in the latest steps. Analogous steps have been found with a model made of three water molecules for acetylene (see Figure EMS1). Both water models predict a H-route for the hydrolysis in two steps, one for the addition of H^+ to C_{a2}, to which gold is still bonded, and the other for the addition of OH^- to C_4, with simultaneous elimination of acetone. The main difference between them concerns the hydration intermediate formed between the two TSs, **I3-H**. With three explicit water molecules **I3-H** is a stable alcohol resulting from the 1,2 addition of a water molecule to

the C_{a1}-C_{a2} bond, whereas the four-water model allows the formation of a new intermediate where a free OH^- ion is stabilized by its neighbor water molecules. This last possibility is in agreement with recent accurate observations [38], which indicates that the four-water molecules model is more reliable than the smallest one.



I2-H (-11.3)

TS23-H (13.0)
(ν_i= -1755.6)

I3-H (1.3)

TS34-H (13.8)
(ν_i= -578.6)

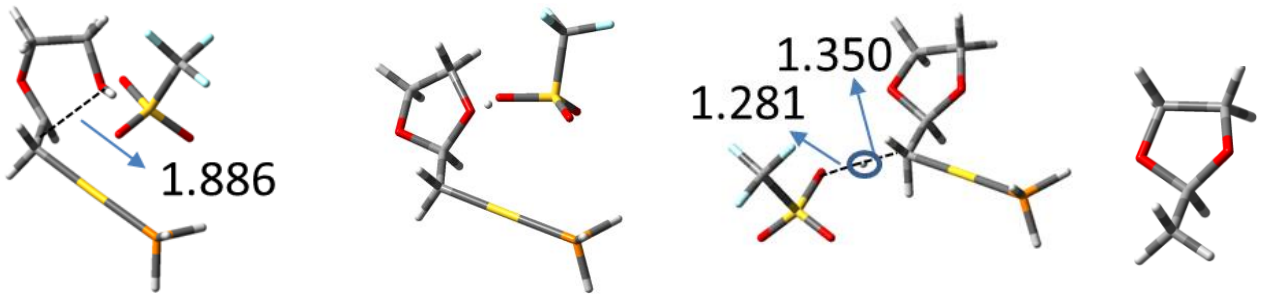
I4-H (-44.8)

Figure 3. PCM(UFF)-M06/VDZ optimized structures in DCM solution of the species involved in hydrolysis steps (H-route, blue line in Figure 1) of the gold catalysed reaction of DMDO with acetylene. Some relevant distances are given in angstroms. Relative energies in kcal/mol are also included in parenthesis.

Finally, after some conformational rearrangements, the hydroxyl group just added at C_4, as it is in **I4**, performs a nucleophilic addition to C_{a1} through **TS5** (-22.7 kcal/mol) and releases a proton to the triflate

anion which, in turn, donates it to C_{a2} at **TS6** (-10.6 kcal/mol) in a step known as protodeauretion, since the gold catalyst is recovered after its separation from the C atom where it stood linked all along the reaction (see Figure 4). A new acetal, 2-methyl-1,3-dioxolane forms (**I6**, -41.7 kcal/mol), whose C_2 carbon atom (the DMDO C initially bearing the dimethyl group) comes from the acetylene reactant.

The theoretical characterization of the previous structures ensures that the mechanism described for the intramolecular addition of DMDO to an alkyne group [11] also exits for an analogous intermolecular process in the case of DMDO and acetylene. Along this reaction path the hydrolysis steps are clearly the rate-limiting ones with a barrier of 25.1 kcal/mol for **TS34-H** measured from its most stable previous intermediate, **I2-H** (see blue line in Figure 1).

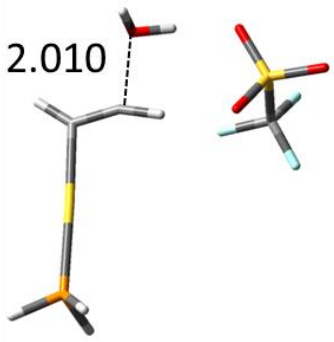


TS5 (-22.7) (ν_i= -326.1) **I5 (-29.6)** **TS6 (-10.6)** (ν_i= -1177.83) **P (-41.7)**

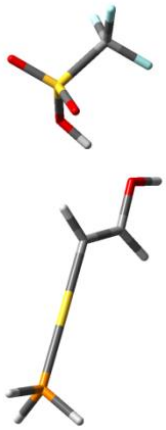
Figure 4. PCM(UFF)-M06/VDZ optimized structures in DCM solution of the species implied in final cyclization of the gold catalysed reaction of DMDO with acetylene. Relevant distances are given in angstroms and relative energies in kcal/mol are also included in parenthesis.

To have a comprehensive view of the reactivity of our system it is interesting to consider that water could produce the direct hydration of the alkyne in competition with the addition of DMDO. Among other relevant reports on hydration or hydroalcoxylation of alkynes [39, 40], Krauter *et al.* have theoretically studied the hydration of propyne to render 2-propanol, assisted by five explicit water molecules or, alternatively, by the triflate anion [41]. The anion assistance rendered the most accessible

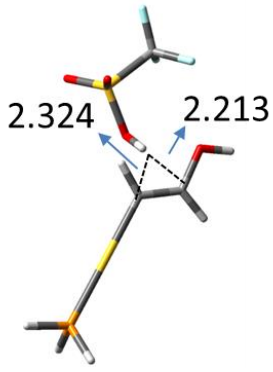
route with a barrier of 5.8 kcal/mol, which corresponds to the initial water addition. This barrier is much lower than that for the addition of DMDO to acetylene following the H-route above described, which suggests that acetylene hydration could happen instead of DMDO addition. For a proper comparison with the chemical system here considered, we have analyzed the addition of water to acetylene, instead of propyne, using the best model proposed by Krauter *et al.*, that with triflate assistance. The green line in Figure 1 represents the energy profile for the addition of water to the activated acetylene, **I1**, and Figure 5 collects the geometry of the involved structures denoted with the **W** label. The green profile shows that the barrier for the initial water linkage to acetylene, controlled by **TS2-W** (-3.3 kcal/mol), has nearly the same value as that for the addition of DMDO (**TS2**, -3.6 kcal/mol), since the attacking O atoms of both molecules have similar nucleophilic character. Afterwards, in the water addition, the triflate anion carries, in two smooth steps, a proton from the added water molecule to C_{a2} to yield ethenol. The comparison of blue and green lines in Figure 1 clearly shows that the direct acetylene hydration is preferred over the DMDO addition following the H-route for the hydrolysis step. However, in the intramolecular addition of DMDO to an alkyne group, products coming from the DMDO addition have been observed [11]. This fact suggests that a different more accessible route for the DMDO addition might exist.



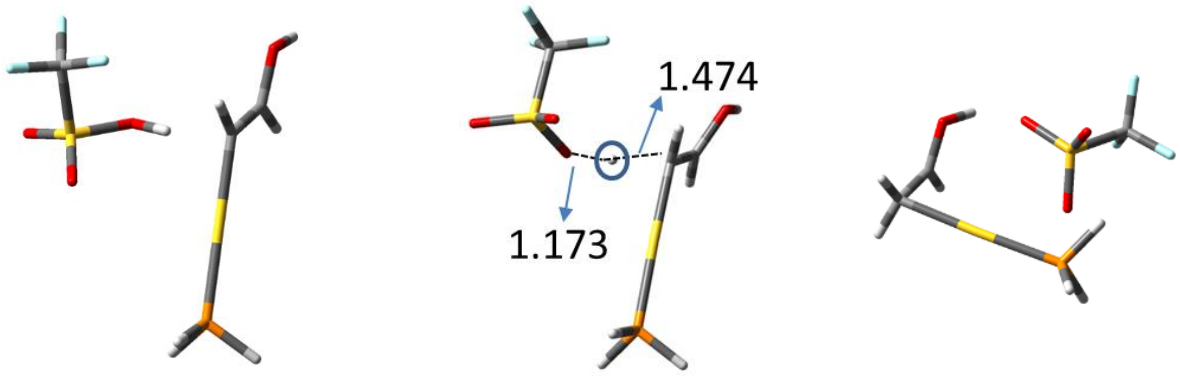
TS2-W (-3.3)
(ν_i= -267.5)



I2-W (-18.9)



TS23-W (-14.9)
(ν_i= -154.5)



I3-W (-18.3)

TS34-W (-17.0)
(ν_i= -427.7)

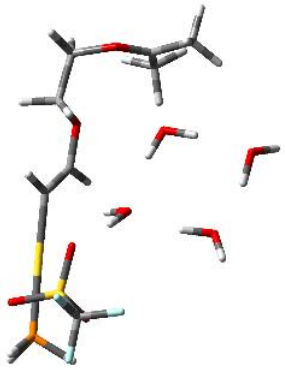
I4-W (-50.4)

Figure 5. PCM(UFF)-M06/VDZ optimized structures in DCM solution of the species involved in the gold catalysed addition of H_2O to acetylene assisted by the triflate anion. Relevant distances are given in angstroms and relative energies in kcal/mol are also included in parenthesis.

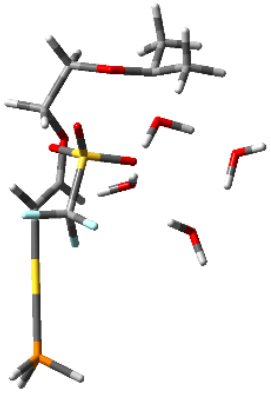
Coming back to the NBO charges of the backbone atoms of the vinyl ether intermediate where DMDO has just linked, **I2**, an alternative approach of water can be envisaged. Since C_2 is the most electrophilic centre at **I2** (NBO charge = +0.650 *e*) a water molecule can orientate its O atom towards this area, as it is in intermediate **I2-OH** (see Figure 6). This is the starting species of the hydrolysis path we call OH-route (see red line in Figure 1), as it begins with the addition of OH^- to C_2 with the concomitant bonding of H^+ to C_{a2}, where gold is still bonded, through **TS23-OH** (-15.6 kcal/mol). The difference between anhydrous **I2** and **I2-OH** energies amounts to 17.2 kcal/mol. This value was subtracted from the energy of the structures involved in the OH-route hydrolysis. The barrier of **TS23-OH** amounts to only 3.3 kcal/mol from its previous intermediate, **I2'-OH** (-18.9 kcal/mol), an isomer of **I2-OH**, and yields the very stable alcohol, **I3-OH** (-48.0 kcal/mol). Afterwards, an adequately oriented cluster of four water molecules is able to perform a 1,3 H-transfer from the just added OH in C_2 to the O atom of the DMDO moiety furthest from Ca1, O_3, with the simultaneous elimination of acetone. **TS34-OH** (with a barrier of 30.8 kcal/mol from **I3-OH** but 17.2 kcal/mol under the energy of the separate reactants) describes the molecular movements involved in this transposition-elimination process, which eventually renders an

alcohol plus free acetone (see **I4-OH** at Figure 6). A value of 17.1 kcal/mol was added to the energy of **I4-OH** to connect this species with **I4**.

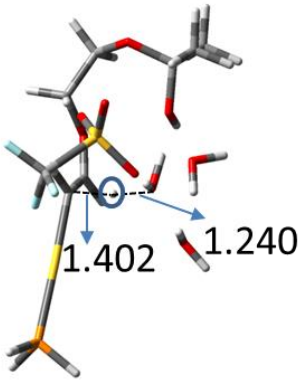
The comparison of the red and green energy profiles in Figure 1 indicates that the OH-route now found justifies the formation of the products coming from the DMDO addition to acetylene instead of those coming from the direct hydration, as observed in the similar intramolecular reaction [11]. Alcoholic intermediate **I3-OH** is the most stable structure along the OH-route and acts as a sink of DMDO-linked acetylene. Once **I3-OH** is formed its evolution towards the products is energy demanding but preferred over the backward motion towards reactants. OH-hydrolysis route render alcohol **I4**, whose H atom comes from an external water molecule, in good agreement with experimental labelling results obtained for the similar intramolecular process [11]. **I4** is essentially the same intermediate obtained along the H-route, so it evolves to the final product following the transformations above described (**TS5 → I5 → TS6 → P**).



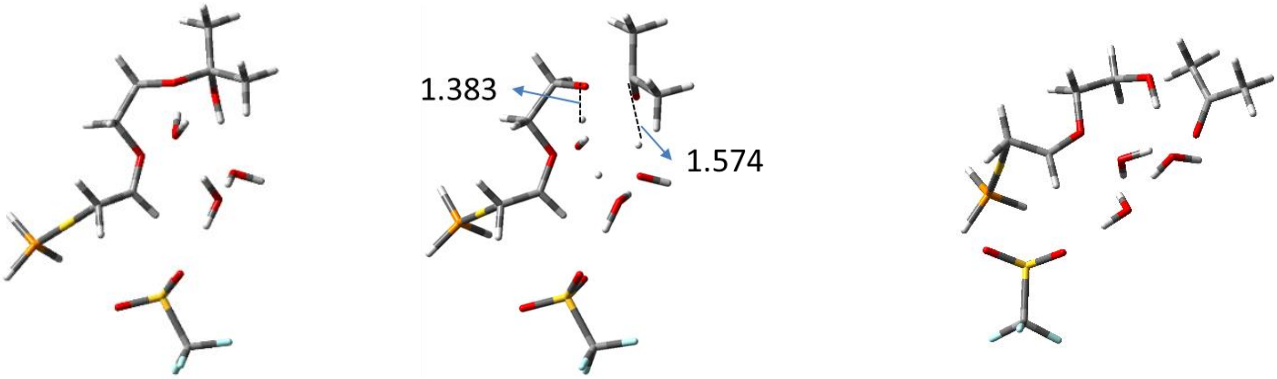
I2-OH (-11.3)



I2'-OH (-18.9)



TS23-OH (-15.6)
(ν_i= -623.3)



I3-OH (-48.0)

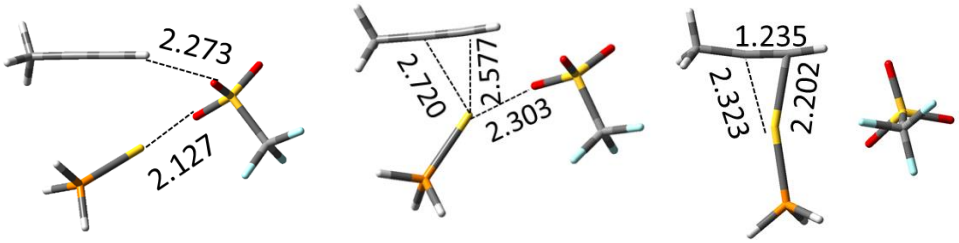
TS34-OH (-17.2)
(ν_i= -597.3)

I4-OH (-44.8)

Figure 6. PCM(UFF)-M06/VDZ optimized structures in DCM solution of the species involved in hydrolysis steps (route OH) of the gold catalysed reaction of DMDO with acetylene. Relevant distances are given in angstroms and relative energies in kcal/mol are also included in parenthesis.

Addition of DMDO to propyne in the presence of water

The study of the addition of DMDO to propyne raises the point of the regioselectivity of the process. The linking of DMDO to the terminal alkyne C atom leads to the formation of 2-ethyl-1,3-dioxolane, whereas that to its internal C atom gives 2,2-dimethyl-1,3-dioxolane, the same compound as one of the initial reactants, although with the brunched C_2 moiety coming from propyne. Based on the results found for acetylene, we assume that the OH hydration route is preferred over the H-one for both DMDO additions to propyne, so it will be the only one considered in the comparison between terminal and internal DMDO approaches.



RC-p (-3.7)

TS1-p (-1.0)
(ν_i= -70.0)

I1-p (-9.4)

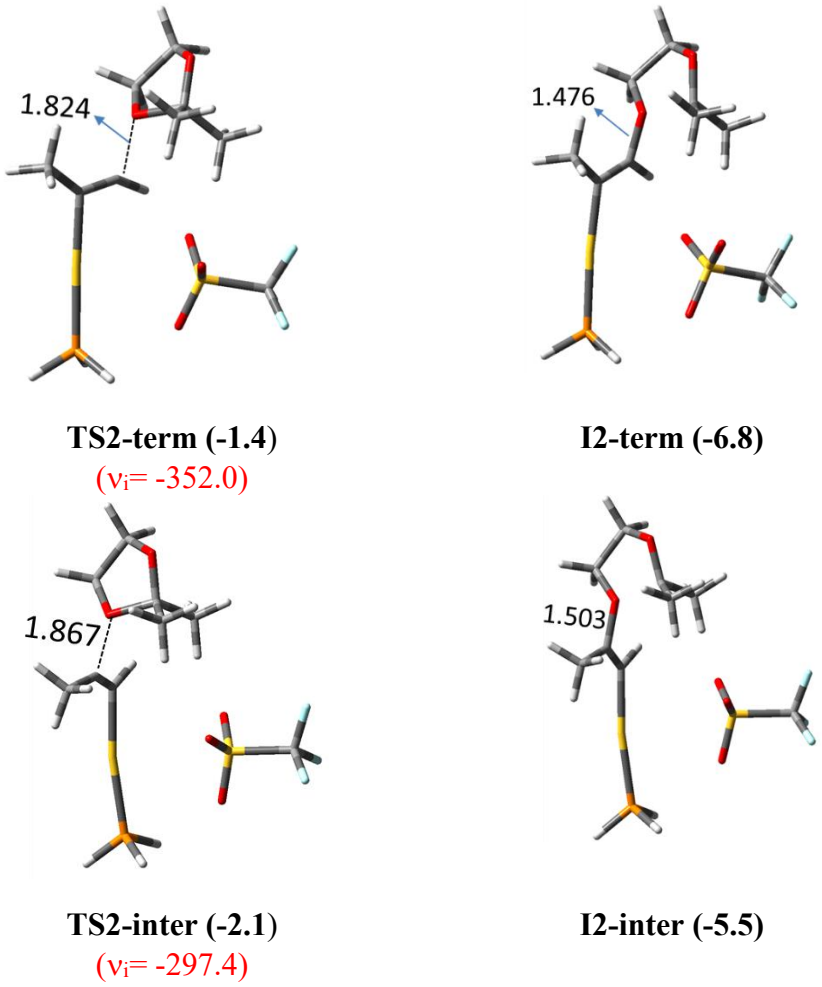


Figure 7. PCM(UFF)-M06/VDZ optimized structures in DCM solution of the species implied in the initial addition of DMDO to the terminal/internal C atom of propyne. Relevant distances are given in angstroms and relative energies in kcal/mol are also included in parenthesis.

Both isomeric additions start with the activation of propyne (see Figure 7), which leads to **I1**, a more asymmetric intermediate than that formed in the activation of acetylene. Actually, gold interacts more strongly with the terminal C atom, provoking a concentration of electron density in it (NBO charge = -0.315 *e*) with a partial de-concentration in C2 (NBO charge = -0.009 *e*). As a consequence, the nucleophilic addition of DMDO on the intermediate propyne C atom through **TS2-inter** (-2.1 kcal/mol) is slightly preferred over that on the terminal propyne C atom through **TS2-term** (-1.4 kcal/mol).

The small difference in the barriers for the two possible orientations in the addition of DMDO to propyne could not be enough to determine a regioselective route. However, we have observed that the dipole moment of **I2-inter** (14.7 D) is considerably larger than that of **I2-term** (12.9 D), and this feature highly affects the interaction of these intermediates with the polar water molecules in the hydrolysis steps. As a matter of fact, structures involved in the hydrolysis of **I2-inter** (see Figure EMS2) present absolute energies around 10 kcal/mol lower than the corresponding ones in the terminal DMDO addition. Likewise, all of the structures in the final cyclization and protodeaureation have lower energy for the internal addition and this seems to be the preferred reaction route.

In summary, this study has proved that the addition of DMDO to acetylene goes by a mechanism where, after activation of the triple bond and the initial addition of the di-ether, a hydrolysis step takes place with the concomitant elimination of an acetone molecule. Last stages of the reaction correspond to the cyclization of the product and the protodeaureation, which is the recovery of the gold catalyst. Two alternative routes have been described for the hydrolysis steps. In the so-called H-route a proton from water is firstly added to the triple bond C-atom linked to gold; in the OH-route a OH water group adds to the branched C atom coming from DMDO. Only the OH-route is able to explain the formation of products other than those coming from the direct hydration of the triple bond, as experimentally found in similar reactions, so it seems to be the actual operating mechanism. On the other hand, although the initial addition of DMDO to the terminal or the internal C atoms of propyne have similar barriers, the internal approach renders much polar structures capable of stronger interactions with water, which makes the process regioselective.

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ELECTRONIC SUPPLEMENTARY MATERIAL

Gold(I) catalyzed intermolecular dioxolane addition to alkynes: the role of water

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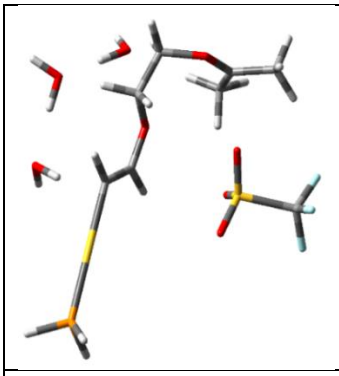
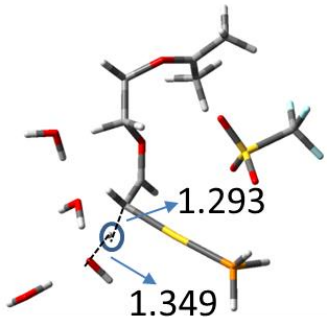
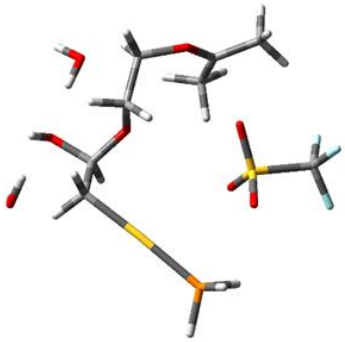
Figure EMS1. PCM(UFF)-M06/VDZ optimized structures involved in the H-hydrolysis route of the intermediate formed after gold catalysed addition of DMDO to acetylene assisted by three water molecules. Relevant distances are given in angstroms.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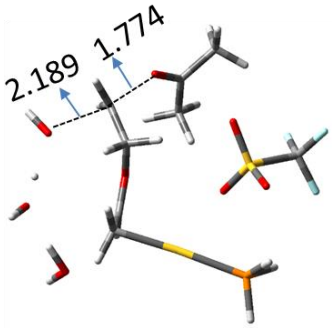	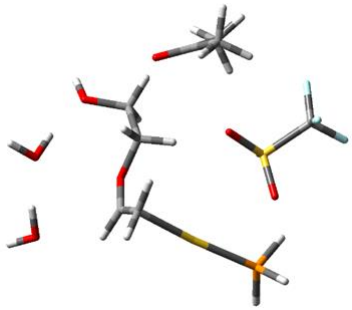	
TS34-H-3w	I4-H-3w	

Figure EMS2. PCM(UFF)-M06/VDZ geometries of the structures involved in the hydrolysis, cyclization, and protodeauration steps for the terminal and internal additions of DMDO to propyne. Relevant distances, in Å, are given as well.

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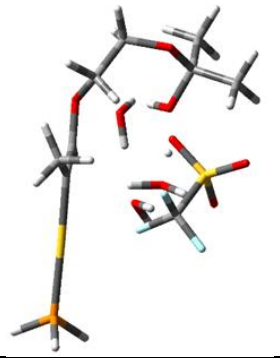
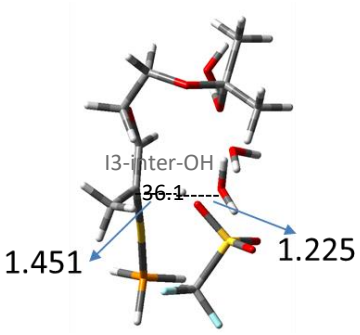
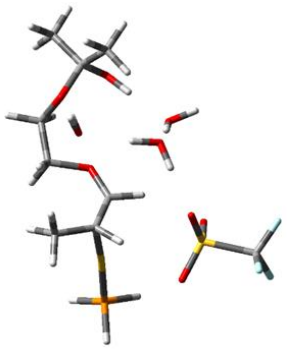
<tr><td>  </td><td> 
</td><td>  </td></tr>
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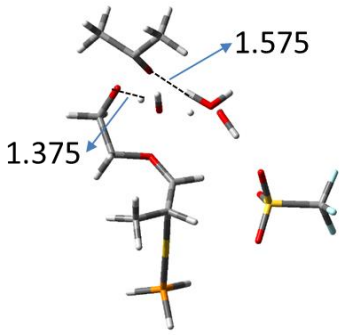
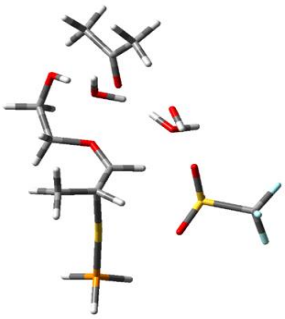
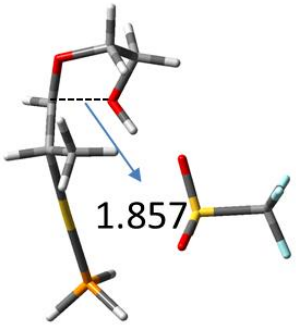
<tr><td> 
</td><td>  </td><td> 
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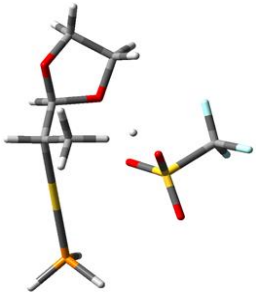
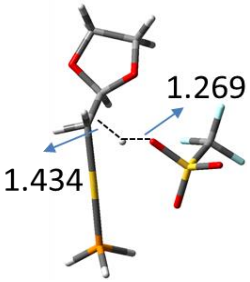
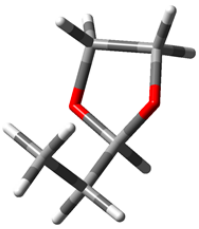
<tr><td>  </td><td> 
</td><td>  </td></tr>
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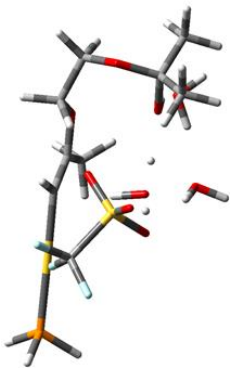	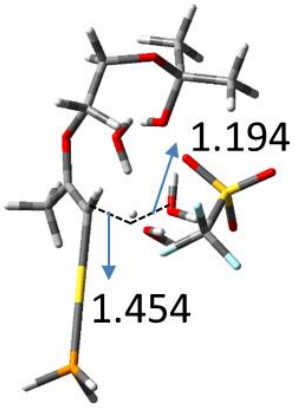	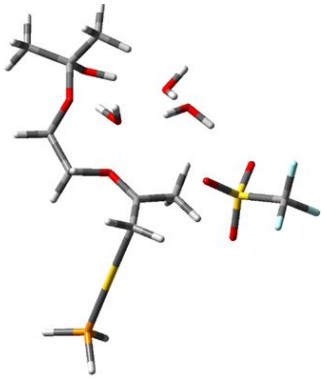
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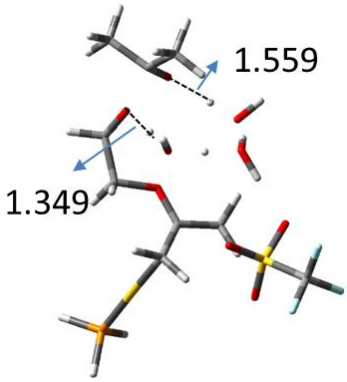	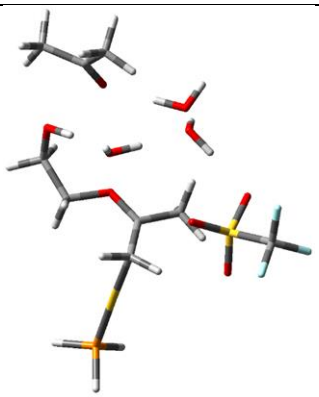	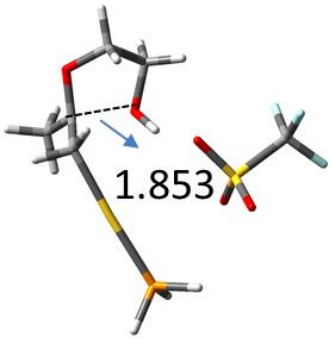
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	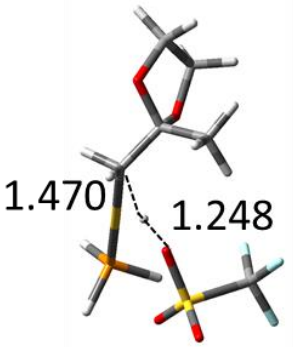	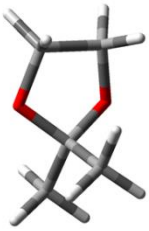
I5-inter	TS6-inter	P-inter

Table EMS1. PCM(UFF)-M06/VDZ optimized cartesian coordinates, in Å, of all the species located in the reaction between DMDO and acetylene in DCM solution catalyzed by [Au(PH_3)]TfO. Energies in solution are also given in hartree.

Acetylene (C_2H_2) E = -77.271445
C,0.2153283636,0.0000986609,-0.0004377462
C,1.4255659479,-0.0000231696,0.000074984
H,2.4983242292,-0.0001311606,0.0005294697
H,-0.857429949,0.0002066519,-0.0008922318

2,2-dimethyl-1,3-dioxolane (DMDO) E = -346.804911
C,0.4894753285,-0.4534453354,-0.0103746568
C,1.0829040798,-1.8705237625,0.0576752235
H,0.9601858845,-2.31653022,1.0584752865
H,0.6485833588,-2.5546273732,-0.6830456956
O,2.4557404165,-1.6943771159,-0.2541703294
O,1.5807125772,0.365845678,-0.3952773418
H,0.0807348876,-0.1359839261,0.963477668
C,2.7627254831,-0.3268095419,-0.0201478187
C,3.0824719752,-0.0912987499,1.4448583136
H,3.2798142009,0.9754880544,1.6180348099
H,2.2501277657,-0.3999811892,2.0918285049
H,3.9740829081,-0.6661388359,1.7299590277
C,3.8825557057,0.0861517019,-0.9361955037
H,3.5981478791,-0.1026995717,-1.9787987041
H,4.0983842349,1.1553105703,-0.8079726274
H,4.7900120375,-0.485014125,-0.6994130754
H,-0.299110283,-0.3515511779,-0.7667732312

[Au(PH_3)]TfO E = -1440.240931
P,0.6505333572,3.2765666027,-0.0698824201
Au,-0.2088768513,1.1892594201,-0.3313635079
H,-0.1355240349,4.3564378656,-0.5393340881
H,0.9160060833,3.6747376243,1.2624581731
H,1.8937562983,3.5348563906,-0.6963069798
O,-1.0028916915,-0.763081263,-0.635495877
S,-1.0010495814,-1.7525134517,0.5407766189
O,-0.8923510611,-1.0946752698,1.8598069199
O,-2.006011258,-2.8138839891,0.3553998867
C,0.6400324561,-2.6053301481,0.2992169921
F,0.804458503,-3.5178248555,1.2502355319
F,0.6780554856,-3.1995645194,-0.8869392805
F,1.6279652945,-1.7175724067,0.3724660308

$(H_2O)_4$ E = -305.672354
H,3.3194139472,1.9490372388,1.0256998215
O,1.249069011,1.7326313647,3.5955768954
H,1.0383342719,0.813628462,3.7851560415
H,-0.0523902364,2.7052321772,2.8532331225
O,-0.7263189534,3.2463219494,2.3902680516
H,-1.1340218106,3.7864550775,3.0727663384
H,0.4931808587,5.3157153032,0.2396035794

O,0.2100020882,4.4228524242,0.0254729952
H,-0.1189642029,4.0578775707,0.8704324811
O,3.4937913265,1.6892531023,1.9369991195
H,4.2543534614,2.2175128276,2.2023114234
H,2.0462755985,1.7013829324,3.0299868005

$(H_2O)_3$ E = -229.251504
H,1.45115,2.69322,1.35256
O,1.51374,3.57787,1.75692
H,1.36794,3.43044,2.69681
H,0.25439,4.5787,0.90189
O,-0.42432,5.10217,0.42726
H,-0.13775,6.01666,0.50636
H,-3.29752,5.09669,1.88114
O,-2.92678,4.36315,1.38354
H,-2.03617,4.66263,1.10625

RC E = -1517.518909
C,-3.0272677138,2.0496869305,1.1078825274
C,-1.8477552772,1.9905012506,0.8369552682
H,-0.7951288171,1.9524532443,0.6004394133
Au,-0.6074675334,-0.8993264881,-0.5358990681
P,-2.6816734789,-1.4234845668,0.2371377665
O,1.3222505037,-0.419321561,-1.2901311926
H,-2.9008395856,-1.1884746911,1.6160439197
H,-3.7580106702,-0.7193926299,-0.3552785203
H,-3.1081391633,-2.7680041008,0.1026358221
S,2.1053395415,0.7444347321,-0.6662830278
O,1.2536141291,1.6847730161,0.0968842009
O,3.1000279681,1.2957646189,-1.601122488
C,3.1084290037,-0.1351471252,0.6380525171
F,2.2994462765,-0.7536415729,1.4929210404
F,3.8433250361,0.7528454698,1.2968895595
F,3.9075787295,-1.0291725293,0.0693405735
H,-4.0713822587,2.1101328827,1.3464432183

TS1 E = -1517.5116862
C,-2.308405668845,2.046886967954,0.452803731081
C,-1.150979005488,2.245134026800,0.772431692574
H,-0.122355514938,2.416911521562,1.054387575017
Au,-1.056913164815,-0.245606775069,-0.115306036557
P,-2.344783883102,-2.141873643291,0.086355741185
O,0.872085659494,0.647968430158,-0.979713910405
H,-3.688970087689,-1.982583327478,0.507457999513
H,-2.526507327570,-2.934035292707,-1.074644026772
H,-1.895197159203,-3.118894170222,1.009020414275
S,2.120039735625,0.998318623596,-0.190637865055
O,1.840906410344,1.593564586844,1.141640066662
O,3.155083695798,1.647150387922,-1.020176116443
C,2.845231920880,-0.673496030140,0.210896702518
F,2.006172134648,-1.380638083036,0.966169429209
F,3.985648618869,-0.511820279126,0.873808856539
F,3.084937608877,-1.347123986016,-0.909853250952

H,-3.346263692950,1.937778562297,0.200516647658

I1 E = -1517.524732
C,2.3263521546,-1.8464033779,0.1031751426
Au,1.4336780254,0.2221591981,0.0021469936
O,-1.2214412374,0.5437713744,-1.2230443757
S,-2.2697066222,-0.4621013437,-0.871545752
C,-2.6422399514,-0.0631922459,0.9129870455
F,-3.0574248505,1.1987674177,1.025291544
C,1.1374863908,-1.9895275634,-0.1875478293
P,0.891108621,2.4972649355,0.0100287642
O,-1.7747252106,-1.8718153565,-0.8006667018
O,-3.5754722126,-0.2833153701,-1.5490709699
F,-1.5472365637,-0.2141352792,1.6636731072
F,-3.590599776,-0.8696612429,1.3830004118
H,0.0884638875,-2.1672359225,-0.4459290562
H,0.5666107314,3.0403322298,-1.255666575
H,-0.2647574249,2.815701399,0.7642383695
H,1.8259884427,3.4407954159,0.5019895152
H,3.3707039559,-1.9366919482,0.3484599762

TS2 E = -1864.323076
C,-0.72111,-2.22589,0.17115
C,-1.2215,-1.15593,-0.3061
H,-1.07454,-0.16853,-0.74209
C,-3.77577,-0.86274,-1.49455
C,-5.0511,-0.09284,-1.12853
H,-5.04556,0.92634,-1.54402
H,-5.96435,-0.60233,-1.45503
O,-5.05209,-0.06695,0.29214
O,-3.14276,-1.08514,-0.2242
H,-3.10749,-0.28783,-2.15355
Au,1.34149,-1.81969,0.05446
P,3.59974,-1.21044,-0.04912
O,2.39879,1.58561,-0.39563
H,4.02193,-0.5722,-1.23962
H,4.04356,-0.2941,0.93419
H,4.57792,-2.23188,0.07139
S,0.9394,1.77768,-0.1677
O,0.43623,1.33643,1.16249
O,0.06966,1.40218,-1.32455
C,0.7449,3.63021,-0.10259
F,1.47717,4.14177,0.88631
F,-0.53334,3.94865,0.10687
F,1.13778,4.18108,-1.25044
C,-3.71392,-0.10848,0.71104
C,-3.03232,1.23578,0.56912
H,-1.99003,1.19828,0.91383
H,-3.0429,1.59578,-0.46842
H,-3.57511,1.96173,1.18841
C,-3.6271,-0.68606,2.09338
H,-4.12603,-1.66207,2.12475
H,-2.57543,-0.79841,2.38756
H,-4.11557,-0.00551,2.80236

H,-3.96682,-1.84427,-1.94188
H,-1.17652,-3.11628,0.59648

I2-H E = -2170.035795
C,1.4310443294,0.7481410331,-0.8278771329
C,0.3564287259,0.8934487047,-0.0323432874
H,0.2702020112,0.4470845224,0.9614241825
C,-0.9306526779,2.1478343464,-1.5696516265
C,-2.2886323336,2.7715849218,-1.6416289296
H,-2.4999200075,3.3873708361,-0.7607407869
H,-2.397684476,3.3636606102,-2.5547991919
O,-3.3223995633,1.7407213721,-1.7871077187
O,-0.7820369264,1.6012968726,-0.2799216048
H,-0.1845015058,2.9409138687,-1.7453562014
Au,3.0241687915,-0.4470670569,-0.3295735161
P,4.8440766573,-1.849889433,0.217173677
O,-2.4604393131,-1.047566284,-0.9912909452
H,4.8385724336,-3.1811423867,-0.2779589518
H,6.1479225572,-1.4577602492,-0.1874801252
H,5.0969809881,-2.1141158142,1.5893894551
S,-1.898327703,-1.7847001691,0.1803135444
O,-1.8535232762,-0.994703384,1.4446757199
O,-0.7016984241,-2.614264563,-0.1026974792
C,-3.2285461182,-3.0436025327,0.5369381742
F,-4.3804591074,-2.4262981379,0.8264256213
F,-2.8915430315,-3.8071086207,1.5755193011
F,-3.4304500488,-3.8312075181,-0.5196575963
C,-3.9396416673,1.1907337848,-0.8168214186
C,-3.707881197,1.4790184992,0.5944098958
H,-2.9697661123,0.7250611844,0.9405611469
H,-3.2876597045,2.4697860875,0.7975755901
H,-4.6340359484,1.3051538694,1.1542316434
C,-5.0258475619,0.2874839332,-1.2255670709
H,-4.8551220759,-0.1178542735,-2.2265874068
H,-5.1734136757,-0.5047428106,-0.4850325475
H,-5.9424757901,0.9027079596,-1.2393507547
H,2.1912503503,2.1608101836,0.6806392392
O,2.1728262056,2.9170994025,1.3001314244
H,3.0775604692,3.0452837908,1.6025116248
H,0.6821546463,2.6481687267,2.3589208902
O,-0.2089903411,2.5448126752,2.7451513905
H,-0.0880209295,2.6166185911,3.6963897187
H,-2.2255708629,4.884831277,1.9321569601
O,-1.9149157276,4.1884513235,1.3459530985
H,-1.3863461152,3.5867214741,1.9150116018
H,-0.813920998,1.367094468,-2.3406605214
H,1.4188643228,1.2452707283,-1.8047499343
O,0.4631165133,4.7614790731,-0.1526025455
H,-0.3691364547,4.6547200756,0.3391251731
H,1.0957532497,4.2012594171,0.3247968228

TS23-H E = -2169.997106
C,1.95797,0.97348,-0.20158
C,0.89738,1.37119,0.56767

H,0.83254,1.10482,1.6267
C,-0.23757,2.56253,-1.11587
C,-1.39829,3.50202,-1.21918
H,-1.46315,4.17231,-0.35436
H,-1.32814,4.09582,-2.13434
O,-2.66842,2.79509,-1.39058
O,-0.14296,2.12706,0.23792
H,0.66778,3.12464,-1.37999
Au,1.73469,-1.14781,-0.13967
P,1.3726,-3.45282,-0.18253
O,-2.32148,-0.00512,-0.90114
H,0.71864,-3.95353,-1.33509
H,2.47824,-4.34071,-0.10276
H,0.54721,-3.98043,0.8411
S,-2.03318,-1.1062,0.06965
O,-1.47113,-0.64459,1.36829
O,-1.4144,-2.31762,-0.52772
C,-3.7336,-1.70337,0.55738
F,-4.37004,-0.75244,1.25334
F,-3.64485,-2.78886,1.31926
F,-4.46225,-1.99176,-0.51994
C,-3.37102,2.30917,-0.44644
C,-3.03561,2.39677,0.97704
H,-2.51133,1.45856,1.23827
H,-2.37085,3.22776,1.22621
H,-3.9598,2.43634,1.56453
C,-4.65515,1.74231,-0.87991
H,-4.62044,1.43362,-1.92816
H,-4.96281,0.92419,-0.22149
H,-5.39973,2.54908,-0.76582
H,3.05565,0.94821,0.48492
O,4.1918,1.12168,1.18517
H,4.19029,0.42425,1.84848
H,3.54286,2.54608,1.75844
O,3.0424,3.37383,2.00677
H,3.63677,3.87996,2.56635
H,2.39345,5.34643,-0.42158
O,1.77041,4.70539,-0.06965
H,2.25705,4.26123,0.65773
H,-0.35826,1.69222,-1.77872
H,2.00054,1.35575,-1.2275
O,5.49422,0.23982,-1.03398
H,6.34586,0.68087,-1.08583
H,5.08358,0.57913,-0.20038

I3H E = -2170.015674
C,2.1637764806,1.7161269344,-0.7637305389
C,0.995067213,1.7320047422,-0.0214301897
H,1.0155401874,1.6861424775,1.0863445531
C,-0.468280039,2.0873886421,-1.8591387195
C,-1.8180465329,2.7264581674,-1.9902547612
H,-1.9292961247,3.5456938483,-1.2702527955
H,-1.9591019422,3.0998726587,-3.0084537359
O,-2.9049938313,1.7619440933,-1.836286582
O,-0.2350564694,1.851844699,-0.4762319812

H,0.2680737239,2.8035101921,-2.2519966741
Au,2.135988997,-0.4686521669,-0.5111413157
P,2.4148062268,-2.788360722,-0.3321829558
O,-1.987057948,-0.7676510257,-0.9657200673
H,1.9448944878,-3.5996610112,-1.3922519588
H,3.7508973991,-3.2524260846,-0.2113804523
H,1.8138515975,-3.3999632786,0.7938984241
S,-1.2787462767,-1.6380431609,0.0205079205
O,-0.5581901558,-0.909002768,1.0984148773
O,-0.5509033749,-2.7827194256,-0.5908468256
C,-2.6753141296,-2.4604741762,0.9443569961
F,-3.3691205822,-1.5470946023,1.6323664611
F,-2.2019964066,-3.3617531109,1.7996033057
F,-3.505448429,-3.0660803212,0.0957529533
C,-3.3836668059,1.3821694491,-0.7181315881
C,-2.9264606688,1.8467996733,0.5943008547
H,-2.205704264,1.0992326895,0.972906669
H,-2.3948633945,2.8029392717,0.5882597788
H,-3.7771627578,1.8603520793,1.2856938993
C,-4.5555582991,0.5030723457,-0.8298352557
H,-4.5969257726,0.0124802186,-1.8058071871
H,-4.5653298927,-0.2224456203,-0.010988004
H,-5.4415236467,1.1490638644,-0.7061900336
H,3.070146558,1.9133742229,-0.1826628307
O,1.1832219959,1.8141434522,3.0217510547
H,0.8287877062,0.9822590352,3.3441961334
H,0.0741719691,2.7764744549,2.6453928113
O,-0.6463751632,3.4395396222,2.3174687045
H,-0.849089771,3.9913357857,3.0763948154
H,-0.1690062856,5.6321376657,0.072124974
O,-0.4075701696,4.7151145781,-0.0858762642
H,-0.4360871705,4.3013364662,0.8083958591
H,-0.3992796144,1.1379881032,-2.4125769587
H,2.1741880996,1.9506204579,-1.8295157392
O,3.6115680438,1.6140065536,2.0557693516
H,4.2377447807,1.786374709,2.7623733509
H,2.702632419,1.6762497939,2.4870132426

TS34-H E = -2169.995846
C,1.7249448174,-2.2601016001,-0.6040525156
C,1.8475800334,-1.2049306578,0.288997823
H,1.9955386103,-1.3943518263,1.3557036577
C,1.7331774049,0.5870127722,-1.2823614388
C,2.7048828221,1.7084695715,-1.4159328164
H,3.2876312505,2.0331384804,-0.554644343
H,3.0075003298,2.0110945167,-2.4119642455
O,1.5425633717,3.1800010481,-1.3996661562
O,1.8476662418,0.081243312,0.0534719996
H,1.982604035,-0.1823123786,-2.0180656064
Au,-0.418384877,-2.3475330673,-0.1879578549
P,-2.7235666819,-2.615801306,0.1639459254
O,-2.8996423369,0.101821097,-0.9692126684
H,-3.5789596864,-2.5192261541,-0.9584920149
H,-3.1426552386,-3.8547731649,0.716400885
H,-3.3070643358,-1.6953655237,1.066156525

S,-2.0449377321,1.0918067847,-0.2568862783
O,-1.3454365533,2.071686931,-1.1362938833
O,-1.2038694426,0.5284583124,0.8391772963
C,-3.2775292504,2.1492535424,0.6591645114
F,-4.1336234296,2.7119711953,-0.191430653
F,-2.6462656436,3.1169149534,1.3284755172
F,-3.9637669514,1.4082804869,1.5287878762
C,0.9543737056,3.6072976038,-0.3936784783
C,1.1110990389,3.0090589433,0.9524426182
H,0.4034458506,2.165348195,1.0289860675
H,2.1228899225,2.617094477,1.1104922905
H,0.8478958413,3.735053118,1.7299328032
C,0.0559534853,4.7773808298,-0.5429300285
H,-0.0813808338,5.0436494305,-1.5950261793
H,-0.9092175549,4.5405773426,-0.0742710554
H,0.4907262791,5.6227535488,0.0118607775
H,2.0586961719,-3.2249130952,-0.2146222911
H,4.1345455098,-0.9054865362,2.0370245056
O,4.9257714648,-0.5561104462,0.5428861131
H,5.828053877,-0.8828647563,0.5152619811
H,5.015278529,0.7483130204,-1.9778255042
O,4.2686383252,0.2538345584,-1.6239219706
H,4.6334697235,-0.1811055355,-0.5505089868
H,0.6943942999,0.9140753007,-1.4365051048
H,1.8313543075,-2.1130987961,-1.6797930894
O,4.5223573358,2.0347997817,1.3014842244
H,4.7235917444,1.0889248142,1.1075947379
H,4.2676522304,2.0245190228,2.2280480453
O,3.5635844131,-1.0554194215,2.8303197649
H,4.1118676824,-0.8654872788,3.5955677827

I4 E = -1747.760728
C,2.6915108718,0.8263502805,-1.3924291067
C,2.8936518875,1.5973818781,-0.2567334451
H,3.8160319023,1.4941020115,0.3221562686
C,0.8118613249,2.7145531381,-0.358383201
C,-0.0476944928,3.4704892232,0.6169427012
H,0.4604756632,4.3959726403,0.9255712677
H,-0.9699220863,3.7613063947,0.0823863194
O,-0.3169015689,2.7305638047,1.7802356334
O,2.1055117348,2.506571995,0.2499385073
H,0.9473371473,3.2658054201,-1.3007317903
H,3.5769537395,0.3151789794,-1.776803854
H,-0.8418184081,1.943041426,1.5385030207
Au,1.7855505242,-0.7220987638,-0.1260635341
P,0.6946839306,-2.4102236031,1.0811671626
H,-0.3802732537,-1.9775655616,1.8919530091
H,0.1047742386,-3.449451573,0.3249773982
H,1.48003958,-3.1488926185,2.0040396258
O,-1.7072061655,0.3621226482,1.1582871199
S,-2.0384120349,-0.078376223,-0.2342576278
O,-1.768622996,0.9355687852,-1.287128813
O,-1.6107406865,-1.4696353799,-0.5514547958
C,-3.8986900326,-0.1952537475,-0.1996021172
F,-4.4260531643,0.9900101766,0.1009542424

F,-4.2916250141,-1.0813378302,0.7140387675
F,-4.3569553902,-0.5786402252,-1.3895964062
H,0.3624379805,1.7330560686,-0.5756153752
H,1.9224657687,1.0915276558,-2.1202549774

TS5 E = -1747.7253710
O,-0.985044623479,1.870324581529,-1.417503570585
C,-2.559216024825,1.687248466304,-0.394815387644
O,-2.691233891037,3.009421426050,-0.226418577320
C,1.437228141793,3.653125540714,0.012000216572
C,-0.648098124522,3.248987816580,-1.218846649626
C,-2.237895923268,0.760157346844,0.673701446633
Au,1.368317049695,-1.066486198953,0.064527097666
P,-0.329759123648,-3.075527105828,-0.594841542284
O, 1.916122391546,-1.058744026142,-1.025660677732
S,1.988351831161,-0.087920474753,0.099437982871
O,1.855163250461,-0.656775838904,1.462636027541
O,1.212089977761,1.180175575578,-0.125570630161
C,3.745831780488,0.529016154036,0.037581878273
F,4.003527240239,1.074912626832,-1.149380318304
F,4.588239174802,-0.483135549779,0.234762475260
F,3.947789768861,1.444918422281,0.982531536910
H,-3.241322184742,1.324463523866,-1.171876397515
H,-0.976424073319,3.804270370285,-2.104477642012
H, 0.434249219024,3.346248723428,-1.082048315136
H,-1.625101350724,4.727511652371,0.087330015942
H,-3.224807657369,0.423352541318,1.041823529581
H,-0.266790052089,1.337798910581,-0.980078910878
H, 0.169514368165,-3.130753494030,-1.920214186210
H, 0.817276220018,-3.475210887489,0.135205964822
H,-1.083725654261,-4.279978160523,-0.561741235251
H,-0.972193999395,3.287192598217,0.939117797447
H,-1.684686388117,1.234405379791,1.495472831752

I5 E = -1747.736513
C,-2.0244851124,1.2197625873,0.4240338493
C,-1.3555665664,2.2120384833,-0.4663278336
H,-1.7101304493,2.1587565628,-1.5151864647
C,-0.4761389515,4.2599346377,-0.6661219464
C,0.7102947415,3.3063729902,-0.6088447711
H,1.3446267575,3.3453323701,-1.5041388078
H,1.3311400895,3.4619430989,0.2856616319
O,0.0850827205,2.0198094754,-0.5127422092
O,-1.4960607657,3.5352259643,-0.0047028088
H,-0.7679275453,4.4695544362,-1.7102253977
H,-3.1075826327,1.4163173438,0.3805201274
H,0.7805265762,1.0352403465,0.3887497448
Au,-1.6904477933,-0.7869944182,-0.0810373745
P,-1.2786699769,-3.064703173,-0.5874212854
H,-0.321963395,-3.3538621803,-1.5965581532
H,-0.7755217735,-3.8892834427,0.4539323283
H,-2.3476450144,-3.8866485327,-1.0347013759
O,1.3085520474,0.4077638163,1.0137958145
S,2.0331563692,-0.7413863781,0.2073628654

O,1.6722192345,-0.7276529763,-1.2151887861
O,1.9924088721,-1.9786737698,0.9901898008
C,3.7844866006,-0.1041318211,0.3006249746
F,3.8367199315,1.0982936624,-0.2534529697
F,4.5701907523,-0.9373818525,-0.3638998161
F,4.1726395154,-0.033777803,1.5630131679
H,-0.3075209011,5.2051916518,-0.1392622467
H,-1.6938519406,1.4092925607,1.4598934919

TS6 E = -1747.706160
C,3.707668989916,-2.865136067711,0.146237600244
O,2.309928401938,-3.033572476503,-0.094439547994
C,1.685134386558,-1.768640504763,0.100092771087
O,2.690446726712,-0.818101816208,-0.122760381968
C,3.836243545297,-1.384019982392,0.490375461830
C,0.539984879925,-1.593161528259,-0.862027392519
Au,-1.403136065798,-0.868539224976,-0.092139216150
P,-3.454548179241,-0.183121785435,0.756691946506
O,0.748623509154,0.949928648579,-1.486392622027
S,0.294197847626,2.248368764848,-0.802037008930
O,0.759375996108,3.433465982051,-1.541989819006
C,1.289385538081,2.233014689395,0.777034707731
F,0.969758685107,3.306196674900,1.494637990952
O,-1.111656346996,2.207715293159,-0.343108195257
F,2.585753054515,2.259950420466,0.510921194532
F,1.001607528286,1.141650996691,1.479795108421
H,1.350637132516,-1.703783368051,1.159170293428
H,3.802121246086,-1.219668013668,1.582629186145
H,4.731504585916,-0.904628910087,0.079284816391
H,4.041536302259,-3.520676528907,0.966611383902
H,-0.035111050453,-2.540851541984,-0.853041028797
H,0.383912497386,-0.177618289851,-1.031817824463
H,-4.247919309721,0.588237388963,-0.128972327775
H,-4.397725964231,-1.143831727897,1.200242514634
H,-3.397819223366,0.676728665282,1.881865377185
H,4.260640341583,-3.129317216555,-0.770566900701
H,0.928706021500,-1.555072654984,-1.893137474142

P (1-methyl-dioxolane) E = -307.514756
C,-1.7037002418,-0.3319850482,-0.6004711675
C,-0.2105418062,-0.2560336039,-0.6623920653
H,0.1780363933,-0.5366011665,-1.666906262
C,1.5465946152,0.9095128011,0.204361804
C,1.7076508886,-0.6024701197,0.40706073
H,2.3407190925,-1.0456090558,-0.3815905539
H,2.1097621283,-0.8793165403,1.3880981444
O,0.3820096316,-1.0935684564,0.30038217
O,0.2404741557,1.0475483275,-0.3465226798
H,2.3041503771,1.3161797982,-0.483461748
H,-2.1430782294,0.3635360945,-1.3266383432
H,-2.0403018306,-1.3484466651,-0.8415005099
H,1.5858026102,1.4725339283,1.1475470987
H,-2.0441676845,-0.0645000437,0.4087324524

acetone E = -193.048355
 O,1.5750421698,4.1662365542,0.6400415727
 C,2.5656341089,3.5796630772,0.2379410399
 C,2.7017193501,3.141277239,-1.189490152
 H,2.6810998386,2.0410811621,-1.2293730042
 H,1.8868113191,3.5440566607,-1.8004126199
 H,3.6755307291,3.4510523126,-1.5959296801
 C,3.7164209533,3.2558885128,1.143018574
 H,3.4687395004,3.4836678032,2.1852816718
 H,4.0023146891,2.1990828197,1.0385750224
 H,4.5915253418,3.8492418584,0.8355425754

I2-OH E = -2170.047156
  C,-0.885722637348,-1.017607177978,-1.344215156475
  C,0.041644392970,-1.973487815513,-1.156499990372
  H,-0.109034334143,-2.826808692138,-0.486917199932
  C,1.788319206756,-0.966661971166,-2.444430977254
  C,3.290050289955,-0.974792838442,-2.366252784486
  H,3.685177257526,-1.990816155970,-2.492462510684
  H,3.700306806713,-0.345655360096,-3.166957258151
  O,3.740384041624,-0.384639556449,-1.139141265851
  O,1.299276965285,-2.059097732622,-1.680712210192
  H,1.460456358175,-1.059178841475,-3.493368814006
  Au,-2.672528647479,-0.981023866205,-0.338411075272
  P,-4.724720844503,-0.895912081888,0.830525596210
  O,1.722800551240,2.450369463661,1.173052229532
  H,-5.558405819469,0.235857208322,0.627024999417
  H,-5.677393678001,-1.927609969887,0.616540696834
  H,-4.692004457853,-0.906344828077,2.250785938130
  S,1.220362735487,3.081165771129,-0.096876849705
  O,0.970921195756,2.103956949037,-1.190235426803
  O,1.898600971440,4.343392201689,-0.470635250258
  C,-0.497896659499,3.617990589359,0.386863339330
  F,-1.204677526855,2.563209821433,0.798827111816
  F,-1.121833571707,4.168850679027,-0.652209154745
  F,-0.450594681282,4.508151957150,1.377202883705
  C,4.242743633775,-1.132188491630,-0.106626651670
  C,5.116096458156,-2.306259734304,-0.464231777596
  H,5.516578615692,-2.756550461292,0.453441833211
  H,4.563577823306,-3.080562040383,-1.007715573031
  H,5.957790462539,-1.955627291716,-1.074696878771
  C,4.879739336828,-0.169801440758,0.863253935360
  H,4.182769796232,0.645166067575,1.097685006724
  H,5.177750109969,-0.682342660641,1.787113058023
  H,5.776416190313,0.260314192125,0.399613152442
  H,1.415414625108,-0.009069210345,-2.047505387876
  H,-0.652306068034,-0.209940273277,-2.047462199880
  O,3.042398094339,-1.750801764872,0.589339259994
  H,3.245252993854,-2.145336464766,1.509614015138
  H,2.284955673198,-1.070303339616,0.696702884640
  O,1.072351527192,-0.170586792896,1.041776875744
  H,0.409816496956,-0.226185148826,0.325005182652
  H,1.302887972930,0.786103732350,1.135010145366
  O,3.246265608885,-2.735047992295,2.939909542734

H,2.307211948340,-2.569726097962,3.190547517812
H,3.785915437327,-2.306187077000,3.612708626971
O,0.625731238458,-2.115961782878,2.973585714396
H,0.583582460866,-1.306328519595,2.430384331896
H,0.002321714342,-1.989677221735,3.694466089312

TS23-OH E = -2170.041937
C,0.271703336436,-0.838103061707,0.814101158504
C,-0.566538395466,-1.906204191773,0.979693572207
H,-0.373048352898,-2.861395267668,0.477936566368
C,-2.270049727716,-0.813062116706,2.265730206396
C,-3.777274253238,-0.811829621653,2.097515725931
H,-4.131127680564,-1.840394805650,1.918876477990
H,-4.236866555102,-0.470923213901,3.035071057233
O,-4.231037916194,0.092339672258,1.110171822514
O,-1.718326569466,-1.979256638974,1.626124480407
H,-1.987411904545,-0.862635208384,3.326594504308
Au,2.254420235133,-1.116676798863,0.240017745575
P,4.507964019697,-1.413241367315,-0.347378209582
O,-0.197041583171,2.417025969045,-1.771519166025
H,5.401074316607,-0.332095733745,-0.131487075925
H,5.221042608707,-2.453077950476,0.303410977729
H,4.813865182692,-1.717693040589,-1.699087708069
S,-0.559315673705,3.107557852367,-0.479822058262
O,-1.144265858948,2.194176717880,0.535301215281
O,-1.213946861305,4.423210692954,-0.657237202433
C,1.115776506121,3.535581100141,0.220418021945
F,1.842369543281,2.430975831716,0.389467508343
F,0.979945356785,4.140415279068,1.399108965295
F,1.767359984626,4.351924715598,-0.605642224769
C,-4.314657951921,-0.345276215564,-0.236999831388
C,-5.389652851940,-1.400606665918,-0.414434753570
H,-5.474990442400,-1.668104699596,-1.476558515817
H,-5.162332275891,-2.315551812874,0.150021740041
H,-6.355012810238,-1.007397834452,-0.071474495215
C,-4.600571993772,0.906966173052,-1.032205420776
H,-3.776854150003,1.621293782064,-0.900044583867
H,-4.699888303749,0.660038644206,-2.096966856183
H,-5.530183207030,1.374021018579,-0.683462245818
H,-1.862127316539,0.105092644151,1.825837844228
H, 0.020440525862,0.071263067376,1.370246301717
O,-3.065753935019,-0.857651441501,-0.667265797192
H,-3.067804599478,-1.839365429362,-0.710365261073
H,-1.635739763233,-0.227384222315,-1.324108145071
O,-0.669504854722,-0.163781022887,-1.551069418402
H,-0.140687594927,-0.525855638625,-0.489186851917
H,-0.463119210503,0.806451227969,-1.691982264828
O,-2.728113174275,-3.538042910593,-1.071201662079
H,-1.895744487569,-3.456120590330,-1.579739855928
H,-3.353713779161,-3.959353416584,-1.667903588155
O,-0.281325031016,-2.900486311353,-2.227227066719
H,-0.247847866352,-1.934431834092,-2.312777936195
H, 0.043513874296,-3.246130355005,-3.064363868190

I3-OH E = -2170.093604
C,0.12357,0.69582-1.48035
C,-0.56255,0.18012,-0.3902
H,-0.05082,-0.47179,0.32576
C,-2.65286,1.14059,-0.95473
C,-4.06217,0.96398,-0.46465
H,-4.13342,1.29111,0.58148
H,-4.73858,1.58295,-1.07724
O,-4.39309,-0.40606,-0.57285
O,-1.81931,0.36317,-0.08003
H,-2.33618,2.19489,-0.91347
Au,0.90261,2.26566,-0.16682
P,1.83739,4.01034,1.08363
O,1.67852,-2.67201,-1.05456
H,3.10853,4.48038,0.67146
H,1.10436,5.22119,1.14789
H,2.07029,3.75511,2.45743
S,2.52992,-1.77159,-0.21436
O,1.89289,-1.34604,1.06242
O,3.22754,-0.69762,-0.97055
C,3.91411,-2.89517,0.33232
F,3.42742,-3.92721,1.01909
F,4.76799,-2.22874,1.11008
F,4.57566,-3.35975,-0.72607
C,-5.09767,-0.99408,0.55092
C,-6.50401,-0.44204,0.61034
H,-6.48849,0.63806,0.80993
H,-7.02359,-0.62417,-0.33969
H,-7.06008,-0.93104,1.42142
C,-5.05771,-2.48088,0.27272
H,-4.01611,-2.83357,0.26513
H,-5.60649,-3.01738,1.05757
H,-5.52035,-2.70491,-0.69823
H,-2.53855,0.76735,-1.98268
H,-0.41043,1.17362,-2.30326
O,-4.46688,-0.67107,1.7457
H,-3.60292,-1.13684,1.8064
H,-3.37164,-1.43205,-1.69358
O,-2.67595,-1.85548,-2.23355
H, 1.06725,0.19696,-1.72194
H,-3.14012,-2.42531,-2.8544
O,-2.03761,-1.94668,2.05983
H,-2.00521,-2.66552,2.69819
H,-1.6235,-2.30523,1.24207
O,-1.02454,-2.94275,-0.26543
H,-1.53952,-2.64299,-1.03804
H,-0.08642,-2.88024,-0.52179

TS34-OH E = -2170.044497
C,0.26903,0.81767,-1.48093
C,-0.44345,0.28634,-0.41534
H,0.05491,-0.35834,0.31876
C,-2.54429,1.19885,-1.03928
C,-3.96529,0.96097,-0.60281
H,-4.05446,1.24946,0.45729

H,-4.62541,1.61408,-1.201
O,-4.32551,-0.38622,-0.73932
O,-1.71336,0.42937,-0.15046
H,-2.26496,2.2612,-0.95269
Au,0.98277,2.39968,-0.14854
P,1.87616,4.17077,1.09465
O,1.36185,-2.79115,-1.00982
H,3.14617,4.64878,0.68852
H,1.12835,5.37333,1.13254
H,2.09667,3.93704,2.47423
S,2.36059,-1.98497,-0.22935
O,1.8236,-1.44355,1.04916
O,3.15831,-1.04059,-1.05106
C,3.59742,-3.26744,0.3164
F,2.99972,-4.19415,1.06138
F,4.55747,-2.69094,1.03629
F,4.14972,-3.85735,-0.74044
C,-4.96244,-1.03097,0.68942
C,-6.37828,-0.48748,0.64328
H,-6.36918,0.60492,0.75918
H,-6.89731,-0.75228,-0.28829
H,-6.93729,-0.91072,1.49153
C,-4.88494,-2.50548,0.33934
H,-3.84371,-2.85321,0.36506
H,-5.44796,-3.06684,1.09916
H,-5.32533,-2.72338,-0.64405
H,-2.37055,0.86401,-2.07235
H,-0.24549,1.29005,-2.31909
O,-4.25558,-0.63637,1.69415
H,-2.80681,-1.23231,1.84232
H,-3.40451,-1.18918,-1.38676
O,-2.64565,-1.76806,-1.88686
H,1.23026,0.33717,-1.68895
H,-3.06981,-2.39567,-2.48206
O,-1.87151,-1.62064,1.94332
H,-1.89828,-2.16484,2.73509
H,-1.40363,-2.38715,0.63474
O,-1.22671,-2.81133,-0.2642
H,-1.91379,-2.31691,-1.10017
H,-0.26093,-2.8109,-0.47362

TS2-W E = -1593.9300763

C,	-1.094768326802	1.742131168245	-0.549274340717
C,	0.016185638968	1.446228313175	-0.012878723549
H,	0.703491323368	0.840450749888	0.577971015454
O,	1.449873529041	2.797260075327	-0.414404870119
Au,	-2.378901395444	0.172179557236	-0.008612493708
P,	-3.872352519533	-1.544146877927	0.540703003175
O,	2.254903981182	0.003145741214	1.485689942501
H,	-3.692040676374	-2.793380018839	-0.103519265691
H,	-3.925244637508	-1.947969349227	1.898058841808
H,	-5.244589392242	-1.305460807547	0.280275329895
S,	3.537271358566	0.093903968711	0.726900491903
O,	4.741494296197	-0.417434382842	1.416516483529
O,	3.722962156463	1.401068962097	0.012354792554

C,	3.273621477588	-1.097676423366	-0.680683221576
F,	3.088941777130	-2.329110994400	-0.210413574388
F,	4.327077430064	-1.100173149150	-1.492123481705
F,	2.194125542961	-0.740390137984	-1.378534934736
H,	-1.419181833763	2.573093513165	-1.169682415159
H,	2.315146637664	2.343237535197	-0.251624756136
H,	1.387755632648	3.486711556981	0.258700174710

I2-W E = -1593.954885

Au,	2.693367228733	-0.001559005048	0.021907882007
P,	5.006282164232	-0.474695478001	0.090475532176
H,	5.744758739331	-0.438848176435	-1.122122255511
H,	5.835939195030	0.354254920403	0.891430599166
H,	5.414115606996	-1.746747663445	0.572071118165
C,	0.683831321592	0.392716574964	-0.030944174311
C,	0.161136392297	1.603883814845	-0.219779607579
H,	-0.043923004163	-0.419976157866	0.109395570988
O,	-1.224876003900	1.809055373146	-0.239047299693
H,	-1.426663261639	2.729681068226	-0.442753231280
H,	-2.115553137692	0.658589855723	-0.887147132627
O,	-2.706888658877	-0.059911433490	-1.284752736293
S,	-3.417526526080	-0.888251237334	-0.130936968251
O,	-4.000629573128	-2.086878361987	-0.730829896872
O,	-2.589634998784	-0.938062371153	1.077690309182
C,	-4.831865463426	0.265622815518	0.260345214759
F,	-5.593068176837	0.418920415927	-0.809531272726
F,	-5.542350567277	-0.253711134828	1.247679072358
F,	-4.334226274868	1.437416383058	0.629642269238
H,	0.725932291642	2.528063658072	-0.366061065752

TS23-W E = -1593.948561

Au,	-2.433026894134	-0.175735479408	-0.154548310522
P,	-4.546020700286	-1.040232404617	0.450364587986
H,	-4.748014919734	-1.436022168292	1.799289601911
H,	-5.689947634562	-0.216841712118	0.276428180528
H,	-5.001122983516	-2.212969743573	-0.208354728362
C,	-0.593124411515	0.559808082094	-0.673152488172
C,	-0.095870733629	1.729863788832	-0.252727612496
H,	0.068430839799	-0.015234487006	-1.340445253703
O,	1.183326262045	2.132741068805	-0.597776143683
H,	1.379108868898	2.984764499323	-0.192090510651
H,	1.446349087299	0.285749585654	0.406840064872
O,	2.033346583282	-0.337122365360	0.898853920442
S,	3.110668359611	-0.989650652774	-0.091374780314
O,	3.496418155918	-2.281223848513	0.472071193401
O,	2.709790273224	-0.821955696659	-1.489140336226
C,	4.550219317099	0.161432680134	0.211553973142
F,	4.886217310148	0.110704690934	1.488409561126
F,	5.561927813437	-0.243347900886	-0.538353542716
F,	4.208089954822	1.394113837111	-0.117475325005
H,	-0.627113748407	2.431175576828	0.398226389990

I3-W E = -1593.953981

Au,	-1.761956620771	0.101782467310	-0.129560824852
P,	-3.271908298934	-1.702612558528	0.037832978815
H,	-3.087350772003	-2.647427712678	1.081168684653
H,	-4.650541898281	-1.416106764325	0.219303404700
H,	-3.356951774925	-2.586151515293	-1.070076792271
C,	-0.455894113348	1.679250904106	-0.332979073555
C,	-0.302321030560	2.674451621012	0.559057509642
H,	0.066818875527	1.843698296188	-1.287480957122
O,	0.453802576585	3.777401012972	0.295243727595
H,	0.484938853597	4.346714189805	1.072580654037
H,	0.796923733686	0.685439018574	0.722938055451
O,	1.548648805634	0.292002012706	1.280944862488
S,	2.211055819943	-0.993890256221	0.622834494924
O,	3.070158547827	-1.611440186989	1.632531513538
O,	1.246055431812	-1.773808557006	-0.157425740626
C,	3.344286490830	-0.181898494246	-0.620907131802
F,	4.222371642997	0.581361479272	0.005716329585
F,	3.972580788134	-1.133592394042	-1.291736466432
F,	2.620152941666	0.552721411506	-1.450962679773
H,	-0.759231943323	2.665979138336	1.555488132803

TS34-W E = -1593.951873

C,	-0.521032363131	1.029376052829	-0.663211131379
C,	-0.663945966639	2.269665594669	-0.135808622849
O,	-0.290842925314	3.378706336355	-0.792565197800
Au,	-1.787930079714	-0.535247827766	-0.106488050117
P,	-3.240044538133	-2.286410197406	0.460447897815
O,	1.311179991148	0.067926414417	0.982793205756
S,	2.445216442866	-0.680179442300	0.230162970358
C,	3.518861276067	0.751844146599	-0.292850169493
F,	2.806245812553	1.596066714087	-1.029147239353
O,	3.262024193612	-1.462075285741	1.169193305542
O,	1.978262452250	-1.290728885156	-1.025843536939
F,	3.981433027515	1.385354275829	0.776410205081
F,	4.536850040283	0.292269927947	-1.008562384944
H,	-3.286642085701	-2.692095998406	1.819371119582
H,	-4.625293256936	-2.109821609779	0.208321605155
H,	-3.031745723565	-3.541644673353	-0.166817642583
H,	-0.088823318716	1.027220115126	-1.675418559056
H,	-0.394614040230	4.157986385896	-0.231299953103
H,	0.458717145024	0.455687787087	0.277009331658
H,	-1.054248533385	2.439085348914	0.874880272353

I4-W E = -1594.005129

Au,	1.877047806397	-0.280647242624	-0.053906497121
P,	1.057851259246	-2.470240261886	0.113051745026
H,	-0.071763367294	-2.722494659044	-0.703976765439
H,	1.899691361071	-3.564564346751	-0.208865438965
H,	0.580253179119	-2.852878831342	1.390017035166
C,	2.542039918045	1.814981393853	-0.215278217770
C,	1.184653170148	2.090959865994	-0.178043619796
H,	3.075266868448	1.939872461692	-1.160947499401
O,	0.478198941007	2.318834193119	-1.257607497218
H,	-0.484299947227	2.226087314466	-1.026806796191

H,	3.105682067179	1.946183405419	0.710660922814
O,	-1.345547054628	-0.422212360439	1.070240790182
S,	-1.992074369341	0.145167063118	-0.143838503366
O,	-1.878607418468	1.641785234783	-0.262866474817
O,	-1.745912431952	-0.592731264145	-1.408906049571
C,	-3.815386510772	-0.081215666133	0.173888499706
F,	-4.179639766532	0.569357021573	1.275905623440
F,	-4.523653433120	0.381250354821	-0.852934329075
F,	-4.083309132587	-1.375691604203	0.332019341285
H,	0.650860251070	2.153824607935	0.779121652406

Table EMS2. PCM(UFF)-M06/VDZ optimized cartesian coordinates, in Å, of the species involved in hydrolysis steps by considering three explicit water molecules (route H, blue line in Figure 1) of the gold catalysed reaction of DMDO with acetylene. Energies in solution in hartree are given as well.

I2-H-3w E = -2093.610048
C,1.39972,0.89934,-0.62259
C,0.32395,0.99025,0.17768
H,0.22603,0.4549,1.12605
C,-0.96523,2.33386,-1.28099
C,-2.32666,2.95388,-1.33006
H,-2.54729,3.56123,-0.44453
H,-2.44237,3.55616,-2.23583
O,-3.35852,1.92185,-1.4825
O,-0.81247,1.72051,-0.02289
H,-0.22416,3.13839,-1.4212
Au,2.98636,-0.33949,-0.22324
P,4.80914,-1.78292,0.19172
O,-2.45053,-0.92457,-0.91257
H,5.07656,-2.80547,-0.75705
H,6.11035,-1.22392,0.30336
H,4.79063,-2.56463,1.37684
S,-1.87831,-1.74994,0.19245
O,-1.92587,-1.1019,1.53626
O,-0.62226,-2.47029,-0.13076
C,-3.12295,-3.12852,0.36278
F,-4.33125,-2.63803,0.66127
F,-2.75981,-3.96568,1.33385
F,-3.22044,-3.81598,-0.77517
C,-3.93167,1.3322,-0.50899
C,-3.64194,1.56488,0.90192
H,-2.95384,0.74538,1.19608
H,-3.15264,2.51826,1.12677
H,-4.56305,1.42684,1.48093
C,-5.0182,0.4225,-0.90057
H,-4.91273,0.09292,-1.93748
H,-5.06902,-0.4262,-0.21051
H,-5.95616,0.99363,-0.79307
H,2.20777,2.38498,0.80159
O,2.42267,3.22383,1.25276
H,2.47117,2.99479,2.18667
H,1.05946,4.27772,0.75313
O,0.30367,4.79097,0.39652
H,0.65477,5.66852,0.22066
H,-2.35873,5.18105,2.20899
O,-2.20515,4.51766,1.53141
H,-1.28686,4.66314,1.22476
H,-0.84218,1.59276,-2.08909

TS23-H-3w E = -2093.570010
C,2.11016,1.38888,-0.45523
C,0.95024,1.55623,0.26093
H,0.90202,1.31345,1.32638
C,-0.35907,2.46168,-1.47984

C,-1.65877,3.19561,-1.58844
H,-1.7673,3.92123,-0.77397
H,-1.73403,3.69704,-2.55733
O,-2.7937,2.27168,-1.60603
O,-0.21282,2.05316,-0.12714
H,0.44698,3.15735,-1.75767
Au,2.19937,-0.74408,-0.3227
P,2.218,-3.0798,-0.24141
O,-2.0747,-0.44596,-0.87338
H,1.62721,-3.75924,-1.33483
H,3.46179,-3.76079,-0.15731
H,1.52965,-3.6721,0.84587
S,-1.4954,-1.40146,0.11888
O,-0.89226,-0.76093,1.31926
O,-0.72751,-2.52564,-0.48025
C,-3.00138,-2.24738,0.82503
F,-3.7627,-1.35915,1.47431
F,-2.64064,-3.19735,1.68411
F,-3.73328,-2.79903,-0.14185
C,-3.37086,1.80798,-0.57019
C,-2.98146,2.09732,0.81224
H,-2.37604,1.23251,1.14296
H,-2.37358,2.99896,0.93709
H,-3.88154,2.1215,1.43833
C,-4.5754,1.01672,-0.85652
H,-4.54249,0.59033,-1.86268
H,-4.72745,0.24858,-0.09309
H,-5.4243,1.71899,-0.78925
H,3.0892,1.66968,0.3003
O,3.96466,2.23679,1.2058
H,4.14364,1.55504,1.86032
H,2.77757,3.25193,1.62973
O,2.00453,3.87425,1.81923
H,2.35349,4.53251,2.42521
H,-0.46085,5.67496,1.1831
O,-0.48606,4.7639,0.87822
H,0.37427,4.38867,1.16064
H,-0.32438,1.58104,-2.14081
H,2.10434,1.74065,-1.49329

I3-H-3w E = -2093.623761
C 2.79048,-0.15753,-0.5871
C 2.4525,1.05935,0.22745
H 2.3836,0.82468,1.29938
C 0.97218,2.01421,-1.40414
C 0.30749,3.36371,-1.48647
H 0.70804,4.0551,-0.7338
H 0.43222,3.78826,-2.48694
O -1.15416,3.31687,-1.36022
O 1.22084,1.67396,-0.05866
H 1.90974,2.11175,-1.9744
Au 1.45858,-1.74899,-0.29461
P 0.03438,-3.59532,0.13534
O -2.11452,-1.77216,-0.75734
H -0.7367,-4.14964,-0.91791

H 0.64617,-4.78473,0.62325
H -0.97019,-3.42279,1.12086
S -2.20564,-0.48688,-0.01605
O -2.18738,0.73014,-0.88213
O -1.38492,-0.38368,1.22163
C -3.94964,-0.51059,0.64929
F -4.83612,-0.52501,-0.34494
F -4.1747,0.57398,1.39917
F -4.13976,-1.58976,1.40684
C -1.78646,3.18557,-0.2637
C -1.15305,3.01535,1.0442
H -1.07457,1.92397,1.21872
H -0.14026,3.42866,1.09498
H -1.80537,3.43079,1.8206
C -3.24309,3.34794,-0.37801
H -3.59109,3.13573,-1.39253
H -3.76149,2.73557,0.36596
H -3.45133,4.40483,-0.13671
H 3.78776,-0.49975,-0.26328
O 5.25458,1.03125,2.17256
H 5.22198,1.57696,2.96333
H 4.70369,1.50065,1.52387
O 3.49113,2.06582,0.1503
H 3.96384,1.96077,-0.68575
H 2.84261,5.16424,1.19461
O 2.19436,4.53528,0.86562
H 2.70439,3.73503,0.64573
H 0.35493,1.24385,-1.89545
H 2.87245,0.10534,-1.6563

TS34-H-3w E = -2093.568145
C,2.734586645342,-0.375385543305,-0.617631827277
C,2.234556282352,0.432471981711,0.396103008811
H,2.491347303841,0.215409393300,1.437643610526
C,1.096538171274,1.991725053822,-0.987790191132
C,0.983056302257,3.475774788490,-0.882755823081
H,1.176559352361,3.962295604225,0.065699783881
H,1.132366992883,4.054526393284,-1.785640086835
O,-0.769428024152,3.744419560317,-0.942063343201
O,1.476119920202,1.487947706598,0.302485631491
H,1.867563299998,1.763251638328,-1.728797336599
Au,1.151884069008,-1.844363562258,-0.335243390289
P,-0.426159077426,-3.573806467020,-0.157651600411
O,-2.247406401805,-1.431753783413,-1.076677321634
H,-1.141332870109,-3.930894971958,-1.324922369381
H,0.056215681682,-4.843093324272,0.258077017195
H,-1.474084241323,-3.366004966475,0.770764640160
S,-2.197882820867,-0.201184839992,-0.240459831487
O,-2.279186976549,1.081113558901,-0.995101478153
O,-1.180131711373,-0.211784873984,0.851796051116
C,-3.810057921261,-0.258363019813,0.693780396376
F,-4.838057028637,-0.237416760892,-0.151552823929
F,-3.909310357300,0.794162717204,1.508954477047
F,-3.880136145619,-1.369314119656,1.425747140085
C,-1.549299589086,3.575741759659,0.015112195640

C,-1.120160074242,3.085105124742,1.344003842907
H,-1.051911198987,1.983567444722,1.290939042796
H,-0.134226022618,3.465268290553,1.633006004386
H,-1.863334717737,3.342482788225,2.106253365322
C,-2.972370602061,3.926907314651,-0.190281830144
H,-3.195827401245,4.073146774130,-1.250981756323
H,-3.614190696183,3.150833124799,0.244773843205
H,-3.168142814114,4.857748484868,0.365878932676
H,3.603635497240,-0.970865420102,-0.322728940179
O,4.356604666778,0.283762655135,2.595681281069
H,4.860511472647,0.514458091114,3.380149497498
H,4.529271982475,1.005332027241,1.951277413058
O,4.730759275514,2.134848593478,0.616464120460
H,5.365843404451,1.775203572268,-0.008063273506
H,3.426969632182,4.428574533564,-0.907378205005
O,3.172017569571,3.502001752452,-0.893653150953
H,4.103120927685,2.707825490135,0.043528313263
H,0.144183141251,1.514968641798,-1.267862331184
H,2.701431101900,-0.055504206692,-1.660424697581

I4-H-3w E = -2093.654936
C,1.993783,-0.200676,-1.434644
C,2.754819,0.080936,-0.310911
H,3.703467,-0.432855,-0.129528
C,1.367102,1.837723,0.464473
C,1.456759,2.87382,1.538697
H,1.596344,2.389493,2.518373
H,0.514905,3.44103,1.546593
O,-0.651598,3.907843,-0.818096
O,2.51104,0.971826,0.618201
H,1.40756,2.308489,-0.52873
Au,1.092453,-1.818636,-0.256771
P,-0.095767,-3.511896,0.846836
O,-2.023744,-1.748015,-0.586634
H,-0.919777,-4.313791,0.021932
H,0.610688,-4.503325,1.576316
H,-1.01771,-3.043199,1.812539
S,-2.144503,-0.395251,0.034051
O,-1.69325,0.735298,-0.822092
O,-1.709612,-0.319147,1.457319
C,-3.996239,-0.168629,0.131283
F,-4.530356,-0.186601,-1.090503
F,-4.299217,0.997191,0.706175
F,-4.544415,-1.147438,0.849918
C,-1.806596,3.652461,-0.514964
C,-2.227873,3.53316,0.920515
H,-2.121521,2.475583,1.210439
H,-1.585519,4.145726,1.564252
H,-3.280318,3.811355,1.063592
C,-2.875598,3.466718,-1.545349
H,-2.438046,3.338009,-2.541327
H,-3.509008,2.607108,-1.289181
H,-3.519702,4.36048,-1.539853
H,2.498368,-0.766878,-2.22045
O,5.746176,0.51204,0.164797

H,6.668357,0.683467,0.372226
H,5.379635,1.374065,-0.113555
O,4.382475,2.791604,-0.691691
H,4.778647,3.530986,-1.161512
H,2.694269,4.347881,1.952624
O,2.554476,3.725219,1.232338
H,3.818025,3.190742,-0.003074
H,0.438791,1.249636,0.546667
H,1.168585,0.445948,-1.738833

Table EMS3. PCM(UFF)-M06/VDZ optimized cartesian coordinates, in Å, of all the species located in the reaction between DMDO and propyne in DCM solution catalyzed by [Au(PH_3)]TfO. Energies in solution are also given in hartree.

propyne E = -116.565747
C,-2.0638544675,0.7853908147,0.3787562337
H,-2.4938138417,0.967709819,1.3732340185
H,-2.0621608436,1.7365794408,-0.1710255791
C,-2.8234025289,-0.2260561114,-0.3371912609
C,-3.4564595145,-1.0710613155,-0.9351331461
H,-4.01485766,-1.8170987978,-1.4630467463
H,-1.0204394737,0.4685674302,0.5132314403

RC-p E = -1556.812600
C,2.0473342854,-2.6332497173,-2.0729605763
H,3.1316566444,-2.484274275,-2.1642546815
H,1.7448230649,-3.3830445333,-2.8169131405
C,1.332082755,-1.3837231565,-2.2695158635
C,0.7201758559,-0.3441862762,-2.4113873171
H,0.1852996761,0.5817101103,-2.5276187661
Au,-1.326939306,-0.6953137389,-0.0659296513
P,-1.8987155035,-2.8523269529,-0.5195922111
O,-0.7873867536,1.2896075261,0.474828934
H,-1.69159813,-3.2707128132,-1.8577091081
H,-1.1967878255,-3.8516644774,0.1983916441
H,-3.2426959325,-3.2430800086,-0.3031749233
S,-1.1376837474,2.4943110389,-0.4087469939
O,-1.3056778327,2.1532325108,-1.8391238323
O,-0.3274885693,3.6721038952,-0.0544366047
C,-2.8582610148,2.9160790547,0.1782123349
F,-3.6878760074,1.903382142,-0.054198152
F,-3.2912106801,3.9892266829,-0.4732903286
F,-2.8397867881,3.172335406,1.4805278702
H,1.8489634791,-3.0440008074,-1.072246363

TS1-p E = -1556.808200
C,-3.750234509167,1.999525753011,-0.132049753320
H,-4.289983149188,2.927295674341,0.099705425189
H,-4.255945211918,1.169173827399,0.380321211037
C,-2.366582677668,2.103421942214,0.299760509287
C,-1.212225733867,2.214882432744,0.680802372589
H,-0.206753911463,2.372065323120,1.034619827359
Au,-1.029692580906,-0.226951298520,-0.123230415058
P,-2.330473107401,-2.104461730691,0.153384708334
O,0.923690244340,0.629659740937,-0.990989528424
H,-3.641471519271,-1.919391769754,0.663223364721
H,-2.607583332435,-2.896938882090,-0.988474013912
H,-1.841565271611,-3.087867986818,1.049280392168
S,2.123636530396,0.953715646286,-0.120661558460
O,1.765154908876,1.404023588303,1.248391108631
O,3.162750550696,1.720833627679,-0.837580709194
C,2.903505865501,-0.721040147967,0.147022768436
F,2.056924068260,-1.537877746090,0.772318871220

F,3.998138889171,-0.586945347049,0.889777778096
F,3.237858058921,-1.263046562489,-1.020504748742
H,-3.810413111289,1.827783915410,-1.214904610014

I1-p E = -1556.821675
C,3.7730792457,-1.97023423,0.5136099873
C,2.3693566711,-1.8710272292,0.1428597556
Au,1.3801059232,0.2224213542,-0.0401901357
O,-1.2730541629,0.5982429006,-1.197936917
S,-2.2926571595,-0.4458602511,-0.8718387336
C,-2.6679752622,-0.1173664943,0.9275104175
F,-3.1109042971,1.1296041803,1.0887421434
C,1.178977556,-1.96665119,-0.172017973
P,0.8691175534,2.5017485337,-0.028121344
O,-1.765345889,-1.8435891261,-0.8535987742
O,-3.6091212538,-0.2734647368,-1.5326124481
F,-1.5715360733,-0.2730730342,1.6751482681
F,-3.5999548945,-0.9609584463,1.365773272
H,4.0536404847,-3.030630966,0.5655926148
H,3.9511196604,-1.5108846005,1.4940563531
H,0.1458796399,-2.1813308999,-0.4456567646
H,0.5544801943,3.0575650299,-1.2913190067
H,-0.2927436139,2.8158280274,0.7189253462
H,1.7988942877,3.443229478,0.4782745696
H,4.4103298234,-1.4744619473,-0.2292541986

TS2-term E = -1903.613795
C, -0.538079836284 -2.299508292828 0.083754903257
C, -1.150646253283 -1.270474742651 -0.376548937720
H, -1.063229221803 -0.266038238612 -0.783349854155
C, -3.660000477267 -1.266441113443 -1.570059537144
C, -5.029980045096 -0.683853377001 -1.199639990244
H, -5.175772088882 0.317742581801 -1.631131597735
H, -5.862554080032 -1.325875201392 -1.507199724011
O, -5.022350963329 -0.633538245981 0.221333063310
O, -3.000740421956 -1.390788967959 -0.299322976092
H, -3.080287173691 -0.603644453929 -2.229477901072
Au, 1.462929293599 -1.628911878127 -0.024252156556
P, 3.661118001588 -0.808770295518 -0.081526015721
O, 2.165245807763 1.825923381960 -0.295224897578
H, 4.023224100234 -0.052337222014 -1.222373265628
H, 4.036886673507 0.070380637147 0.962740275912
H, 4.727130358876 -1.745816835103 -0.035612726723
S, 0.700369838604 1.904422202986 -0.033979016276
O, 0.255706709759 1.345633139115 1.272415662154
O, -0.164366057162 1.549525560982 -1.199688572841
C, 0.393961834852 3.733053018438 0.159602025079
F, 1.114158091363 4.222302991278 1.168886190919
F, -0.896237374437 3.959115896551 0.412143581184
F, 0.727948427784 4.382585299514 -0.955284728331
C, -3.690635358134 -0.480856181838 0.630187224937
C, -3.196146414881 0.938568925395 0.459986408433
H, -2.148518868580 1.036729547823 0.774065291101
H, -3.283380641274 1.287160915530 -0.577477042008

H, -3.811460602899 1.590946586157 1.092970795451
C, -3.513993527807 -1.018985279430 2.019437989411
H, -3.881310403814 -2.050861370819 2.073165476898
H, -2.454035245871 -0.983501842216 2.304556622011
H, -4.081396999426 -0.396011345143 2.722267587525
H, -3.707787469095 -2.267292098935 -2.012710780196
C, -0.965925830163 -3.601830524196 0.647748111095
H, -0.640611072812 -3.680770689018 1.694542030847
H, -2.056654053105 -3.722697417978 0.602035048617
H, -0.489409406846 -4.430337610653 0.107296011771

I2-term E = -1903.622381
C,-2.4089135529,-2.5644338504,0.6342769833
H,-2.1342521383,-2.7210321524,1.6885923905
H,-2.352620092,-3.5536639591,0.1581213192
C,-1.4373571839,-1.6271149094,-0.0063509268
C,-1.7645336913,-0.4335486263,-0.4868368318
H,-1.1337285479,0.3243289136,-0.9517510526
C,-3.8965904774,0.2631251678,-1.5911374266
C,-4.8210156721,1.4279583525,-1.2346588059
H,-4.5197525323,2.3584145403,-1.7352975148
H,-5.8691276722,1.2196942993,-1.4683317545
O,-4.7145804763,1.5458988501,0.1798562398
O,-3.1513995895,0.0526345083,-0.352132857
H,-3.182366748,0.4915794189,-2.3915551311
Au,0.5961713722,-2.0243841381,-0.1078407053
P,2.940040043,-2.3063637093,-0.1555844729
O,2.8182014672,0.6991812872,0.3151624747
H,3.6527602977,-1.6086794909,-1.1623462674
H,3.657209943,-1.9002490681,0.9970411911
H,3.4762533768,-3.6110720809,-0.3343652068
S,1.5559116414,1.4796975977,0.1778909615
O,0.6722944341,1.4769670455,1.3776095069
O,0.8581142087,1.326391019,-1.1312228697
C,2.1512405305,3.2460449879,0.1159344858
F,2.8174499812,3.5555694193,1.2289702592
F,1.112886604,4.0777898776,0.0000920329
F,2.9608244806,3.4356495301,-0.9269468763
C,-3.4126416626,1.2933504239,0.5528094784
C,-2.4234710523,2.3682457397,0.192494963
H,-1.4118386574,2.0982237385,0.5234631888
H,-2.4004744114,2.5877834124,-0.8820585956
H,-2.7330176487,3.2773362849,0.7246470184
C,-3.3402938597,0.8165497731,1.9669062147
H,-4.0963774938,0.0443814406,2.1490068696
H,-2.3365991741,0.4285909219,2.1831945245
H,-3.5271410668,1.6700881117,2.6308479583
H,-3.4525056731,-2.2178409092,0.5950804827
H,-4.4171063066,-0.677071768,-1.7989392481

TS2-inter E = -1903.614857
C -2.17061 -1.90132 1.82524
H -2.32320 -1.11711 2.57781
H -1.30795 -2.51149 2.12447

C	-1.87677	-1.35123	0.50427
C	-1.05653	-1.24481	-0.48099
H	-1.25857	-0.70809	-1.40721
C	-4.20403	-0.85576	-0.99302
C	-5.09386	0.35841	-1.28056
H	-4.80490	0.86277	-2.21539
H	-6.15853	0.10475	-1.33003
O	-4.90182	1.21046	-0.16003
O	-3.49411	-0.47051	0.19444
H	-3.49695	-1.06227	-1.80878
Au	0.91823	-1.81292	-0.16448
P	3.21389	-2.11950	0.17336
O	2.84981	0.94781	0.18032
H	4.06302	-1.54106	-0.80173
H	3.73842	-1.55198	1.36051
H	3.75655	-3.43059	0.24904
S	1.51065	1.57602	-0.02168
O	0.5629	1.42186	1.11771
O	0.92027	1.38425	-1.37573
C	1.89858	3.39942	0.00443
F	2.44778	3.74754	1.16942
F	0.78248	4.11228	-0.16453
F	2.75081	3.71268	-0.97284
C	-3.60027	1.00145	0.31461
C	-2.55651	1.70019	-0.52609
H	-1.54793	1.54556	-0.12100
H	-2.57435	1.37547	-1.57449
H	-2.77734	2.77568	-0.50261
C	-3.53504	1.36715	1.76951
H	-4.27083	0.78782	2.34115
H	-2.52554	1.19803	2.16685
H	-3.76149	2.43655	1.87171
H	-3.06173	-2.54313	1.79978
H	-4.76332	-1.76834	-0.75607

I2-inter E = -1903.620290

C	-2.58666	-1.88126	1.52534
H	-2.76062	-1.27847	2.42778
H	-1.75714	-2.57027	1.72003
C	-2.24693	-1.04327	0.35035
C	-1.19085	-0.97052	-0.44377
H	-1.23175	-0.25434	-1.27046
C	-4.20093	-0.33321	-1.13889
C	-4.87655	1.02839	-1.30658
H	-4.42723	1.60817	-2.12437
H	-5.95400	0.94688	-1.47449
O	-4.68410	1.67565	-0.05374
O	-3.41600	-0.14080	0.07264
H	-3.52768	-0.59550	-1.96237
A	0.63363	-1.86834	-0.14962
P	2.84813	-2.60876	0.17027
O	2.80182	0.51919	0.13136
H	3.78705	-2.18075	-0.80234
H	3.48275	-2.14759	1.35181
H	3.17555	-3.98977	0.23960

S	1.65792	1.4668	-0.00616
O	0.7598	1.5528	1.18058
O	0.96745	1.44326	-1.32538
C	2.49331	3.13623	-0.00285
F	3.19274	3.3104	1.12035
F	1.5814	4.10828	-0.08595
F	3.32634	3.25274	-1.03816
C	-3.41636	1.38358	0.40263
C	-2.30017	2.06295	-0.33995
H	-1.32586	1.81388	0.09786
H	-2.28423	1.83224	-1.41082
H	-2.46288	3.14312	-0.22293
C	-3.34146	1.5167	1.88958
H	-4.15721	0.96408	2.36937
H	-2.36714	1.16929	2.25641
H	-3.43394	2.58178	2.13812
H	-4.89917	-1.15178	-0.93527
H	-3.49811	-2.47052	1.34166

I2-term-OH E = -2209.323117

C	0.82062	-0.80813	1.34937
C	0.01844	-1.87577	1.14328
H	0.27330	-2.64078	0.39993
C	-2.06307	-1.23443	2.21341
C	-3.49188	-1.65687	1.9037
H	-3.51408	-2.73892	1.69268
H	-4.12598	-1.48331	2.78353
O	-4.08723	-0.89876	0.86461
O	-1.15500	-2.23194	1.74674
H	-1.93547	-1.11433	3.29998
Au	2.56200	-0.67868	0.22536
P	4.58543	-0.51367	-0.99263
O	-1.01532	2.21342	-1.72241
H	5.29766	0.71197	-0.93699
H	5.63726	-1.40987	-0.66893
H	4.54757	-0.69872	-2.39913
S	-1.57421	2.91631	-0.49535
O	-1.87838	1.97344	0.60806
O	-2.57093	3.95627	-0.81495
C	-0.09053	3.86945	0.10798
F	0.91743	3.03773	0.36312
F	-0.40103	4.52429	1.22265
F	0.29628	4.74418	-0.81525
C	-3.94563	-1.34616	-0.46614
C	-4.77026	-2.58933	-0.73236
H	-4.66064	-2.89367	-1.78217
H	-4.45878	-3.42862	-0.09545
H	-5.82818	-2.37568	-0.53482
C	-4.36134	-0.17436	-1.32348
H	-3.70975	0.68439	-1.10828
H	-4.28874	-0.43639	-2.38661
H	-5.39533	0.11044	-1.09356
H	-1.86243	-0.26805	1.72794
O	-2.57933	-1.62201	-0.75772
H	-2.34667	-2.57746	-0.68000

H	-1.45678	-0.68209	-1.07969
O	-0.56757	-0.20209	-1.27791
H	-0.01211	-0.32709	-0.45267
H	-0.72788	0.81530	-1.46683
O	-1.58535	-4.12402	-0.87831
H	-0.87652	-3.82661	-1.48313
H	-2.07566	-4.79534	-1.36288
O	0.36670	-2.79438	-2.34343
H	0.21964	-1.83854	-2.34415
H	0.60646	-3.01494	-3.24935
C	0.60091	0.22392	2.42928
H	0.07243	1.11096	2.04522
H	0.02641	-0.16611	3.28163
H	1.56364	0.57820	2.82264

TS23-term-OH E = -2209.316656

C,	0.629920424067	-0.667901396945	1.077511986756
C,	0.031321860803	-1.894114745811	0.989514933207
H,	0.366091506678	-2.601220892039	0.219418890145
C,	-1.976412580262	-1.665433184278	2.341481028602
C,	-3.366067512510	-2.113313638265	1.926357584255
H,	-3.326318718966	-3.154628992538	1.568391471949
H,	-4.020138062971	-2.098942677281	2.809715991302
O,	-3.968343059060	-1.242522343299	0.988324724833
O,	-0.988964638470	-2.447313729091	1.648236261234
H,	-1.822397277232	-1.814719793034	3.419326273753
Au,	2.552671771543	-0.591270024134	0.201969771089
P,	4.721691044172	-0.465171074289	-0.683646615981
O,	-1.121815232970	2.404472034584	-1.811653545601
H,	5.425287724544	0.756231472684	-0.518551453198
H,	5.691096706598	-1.378211580696	-0.192979438808
H,	4.884306286043	-0.658779026232	-2.080142266262
S,-1.720419133877		2.972105691584	-0.549157761346
O,-2.063943559344		1.931528535696	0.455445566640
O,-2.714050049990		4.045684373206	-0.769371595183
C,-0.261235969153		3.854603780326	0.205590737169
F,	0.776723964033	3.022971689625	0.306002953811
F,-0.570254600887		4.299076471996	1.421435151631
F,	0.096607027840	4.888920524408	-0.551809183769
C,-3.845921524394		-1.527293687908	-0.395884661755
C,-4.596712305696		-2.789530690860	-0.774563586815
H,-4.537265203102		-2.943812965285	-1.860490895860
H,-4.180530440093		-3.679072296258	-0.281548907257
H,-5.651777067422		-2.692163215891	-0.489116463469
C,-4.385573811679		-0.301094842898	-1.094368500580
H,-3.778363207681		0.572535289845	-0.818125145925
H,-4.349864848256		-0.445068487415	-2.181855140835
H,-5.424456775489		-0.119747084278	-0.791567728032
H,-1.870555005543		-0.602862553517	2.103492957138
O,-2.482465514935		-1.655760798774	-0.756507199705
H,-2.194632489178		-2.594258330080	-0.802575079857
H,-1.324896794309		-0.518669265175	-1.134313756358
O,-0.437072714942		-0.093441584687	-1.296071924585
H,	0.154373579714	-0.298209517846	-0.242521279543
H,-0.611655123237		0.869082213583	-1.507747667498

O,-1.308778111613 -4.076952439601 -1.173781251758
H,-0.634197774690 -3.674173562560 -1.757650883908
H,-1.767482604029 -4.726954064444 -1.714744652126
O, 0.569358332196 -2.506980203153 -2.475721145221
H, 0.334619940827 -1.572632164622 -2.355422537860
H, 0.810094751479 -2.594924963523 -3.403255918881
C, 0.341964351214 0.347599911704 2.169162743912
H,-0.467079699890 1.042025543965 1.893475476386
H, 0.079162658775 -0.130093316632 3.123902063953
H, 1.230059744823 0.963919221108 2.359824587492

I3-term-OH E = -2209.372855
C 0.093424955121 -0.687597740248 1.417205542818
C -0.622370034512 -0.308850418384 0.286676683320
H -0.125532710861 0.358381381006 -0.427795021033
C -2.774712948302 -1.306319135519 0.714047978672
C -4.143901469503 -1.000010911272 0.174295173027
H -4.175134996638 -1.233133566549 -0.899075963577
H -4.891621458440 -1.619822737560 0.696139279253
O -4.391724694778 0.376252151728 0.383754436542
O -1.856721373540 -0.559700714157 -0.097949439473
H -2.544948518134 -2.379999800741 0.631912780263
Au 0.958561363792 -2.187451189410 0.013603132084
P 2.027096344954 -3.871363848261 -1.213041112091
O 1.648910182920 2.672908274503 1.127284302313
H 3.262694801368 -4.342758158960 -0.705934754297
H 1.326089950297 -5.087972117910 -1.400925073707
H 2.381842357884 -3.547737210711 -2.545539076764
S 2.481084995833 1.830380889507 0.212153160779
O 1.801643732174 1.441165747020 -1.054359230926
O 3.236113688339 0.743901428989 0.891593671543
C 3.811890531746 3.010388502536 -0.345827552046
F 3.274403034240 4.048658125187 -0.983277389991
F 4.654606937881 2.392435989591 -1.173373496137
F 4.499193069287 3.461925632344 0.702482937478
C -5.022261806593 1.106552831097 -0.696689956733
C -6.458954965253 0.658961587594 -0.843700150261
H -6.507210755641 -0.394921000895 -1.150031086467
H -6.992641008131 0.781787261141 0.107970960755
H -6.958887631453 1.260844063310 -1.613993569306
C -4.893045148229 2.556112148554 -0.279582537143
H -3.830697663742 2.827344220203 -0.189014156465
H -5.360407378547 3.199621370705 -1.035741919879
H -5.389512756825 2.728285424849 0.685543199445
H -2.684547427157 -0.985889985438 1.758796210873
O -4.376737608572 0.853717231637 -1.900829154289
H -3.471690934814 1.240032502722 -1.878601972897
H -3.445266922617 1.206958889303 1.684705442309
O -2.778614655584 1.521772977415 2.327383518132
H 1.010525271169 -0.089807239706 1.509318317589
H -3.266753685465 2.038992213084 2.974944818267
O -1.834619082284 1.921680282840 -1.926002067809
H -1.676599697657 2.646591990867 -2.537415628062
H -1.536668727319 2.254914930133 -1.048551725066
O -1.108525592461 2.844209120536 0.528833921325

H	-1.604876185352	2.445349544026	1.268603362421
H	0.163527081451	2.794665672793	0.763761749567
C	-0.375689095186	-1.319104032030	2.702539739927
H	0.496301139663	-1.657261316784	3.275316006550
H	-0.908872911351	-0.580785260449	3.320478438531
H	-1.030112174135	-2.185900335404	2.557690405438

TS34-term-OH E = -2209.323956

C	0.258716226129	-0.795620323661	1.463469871165
C	-0.499386389361	-0.373229707508	0.376604058239
H	-0.016752896809	0.295694678755	-0.346957472811
C	-2.651191990495	-1.359918937481	0.851021057965
C	-4.038843647215	-1.052778472419	0.356034046089
H	-4.072188282233	-1.243440689554	-0.729335768734
H	-4.747597312918	-1.736041910655	0.856535654741
O	-4.378206875757	0.288415817120	0.592747490641
O	-1.756585418809	-0.570268832824	0.048409205035
H	-2.409375903455	-2.425621827930	0.711936740618
Au	1.061539553490	-2.259060488874	-0.008055424580
P	2.090078979696	-3.914053526591	-1.308609469013
O	1.333417911220	2.807057995533	1.054236589840
H	3.332702269516	-4.404298571564	-0.837688696972
H	1.378076381204	-5.121281131948	-1.513481485923
H	2.420587744680	-3.557253643779	-2.638714319883
S	2.325715887153	2.008594653708	0.258155971612
O	1.766656630249	1.439539340530	-0.998289983474
O	3.163106982007	1.090597901148	1.070602270240
C	3.526892551285	3.303150425835	-0.335341829122
F	2.898438135300	4.209212106889	-1.080484237736
F	4.479642464062	2.730555605680	-1.068334988173
F	4.094198165915	3.917617086917	0.699498851246
C	-4.994719789616	1.047496923067	-0.767011603555
C	-6.420396187262	0.525277255020	-0.774988811928
H	-6.430003282935	-0.552321011037	-0.989671895308
H	-6.937694059667	0.712856673792	0.176471234967
H	-6.969818623737	1.033240382248	-1.582011069850
C	-4.904867488572	2.491183052150	-0.305187734258
H	-3.860787007163	2.830772532726	-0.305397208647
H	-5.462775591467	3.113654606653	-1.019589999661
H	-5.342740274829	2.638883041694	0.692585641719
H	-2.533901461729	-1.091824857439	1.907572171927
O	-4.289163913799	0.729558962617	-1.802611100474
H	-2.831953568518	1.320604280188	-1.892205320266
H	-3.456261269198	1.014423327339	1.308802960178
O	-2.693219660684	1.536434151750	1.870237333095
H	1.190283350786	-0.216449614576	1.529976139013
H	-3.116531214513	2.117771162619	2.511532711762
O	-1.887169794006	1.694162508251	-1.946441143484
H	-1.881097632589	2.281887808253	-2.706814764571
H	-1.429400004065	2.368600769727	-0.578227996132
O	-1.268963500099	2.721509582177	0.352624631304
H	-1.955376568699	2.144676077531	1.142120134422
H	-0.303483710551	2.743839418589	0.560887892540
C	-0.170212676008	-1.451824382485	2.750452268672
H	0.716691163312	-1.821217124014	3.279297384698

H -0.663363048135 -0.721827246842 3.410043803502
H -0.846934235231 -2.301197671084 2.608811650522

I4-term-OH E = -2209.367402

C,-0.1639850598,0.7232456397,1.4973482948
C,0.6331522298,0.1825075074,0.4936902124
H,0.1427243739,-0.415839993,-0.2830447172
C,2.7907079675,0.9741579181,1.1714037098
C,4.2125973271,0.6563303935,0.8092461932
H,4.3404392877,0.7963850193,-0.2782013259
H,4.8593384807,1.389280031,1.3197851807
O,4.6034524156,-0.6480974313,1.1687903397
O,1.9359005692,0.2131719384,0.3003547391
H,2.582367148,2.044324816,1.0126424272
Au,-0.5713024848,2.2794527746,-0.0395293484
P,-1.1603137895,4.0748521912,-1.423054403
O,-1.9533870571,-2.5941535021,1.1096310536
H,-2.2942283605,4.8335866989,-1.0426903488
H,-0.193584569,5.0955905435,-1.5965432372
H,-1.4774981486,3.7637253949,-2.7680672547
S,-2.7193044297,-1.6160478241,0.2753704871
O,-2.0059211632,-1.1756968874,-0.9548599606
O,-3.3934620612,-0.5366906445,1.0445337418
C,-4.1364141071,-2.6389438089,-0.3744828971
F,-3.6759289403,-3.664114307,-1.0901307466
F,-4.9240077738,-1.8963512442,-1.1523380121
F,-4.8632008972,-3.116515804,0.6350178469
C,4.7398753572,-1.8454616356,-1.3100987227
C,6.2239493903,-1.6663112291,-1.3075404477
H,6.4944885743,-0.6812658742,-1.7045825809
H,6.623514706,-1.7952547103,-0.2937139051
H,6.6747869916,-2.4478765285,-1.9392608868
C,4.2092214979,-3.0905131282,-0.6738292275
H,3.1220536391,-3.0447142548,-0.5375197383
H,4.4498598157,-3.9409936178,-1.3324739983
H,4.7076960449,-3.2817615948,0.2852338813
H,2.5837845688,0.6990240453,2.2132731577
O,4.0108970688,-1.0484664984,-1.8911456206
H,2.2419445249,-1.3044849984,-1.9485627785
H,3.8377421425,-1.1378404971,1.5341085315
O,2.3578405058,-1.902572528,2.2043563772
H,-1.172042878,0.2898822989,1.4598788098
H,2.4594689833,-2.5608253184,2.897358366
O,1.2849391742,-1.5208131293,-1.9883031949
H,1.1460160246,-1.9199758246,-2.851902841
H,0.8471436831,-2.5704268006,-0.554483832
O,0.7260783282,-3.010529603,0.3096123776
H,1.7673294673,-2.3183904629,1.5332163576
H,-0.2195909707,-2.9085585886,0.5277124369
C,0.2085244582,1.3058928878,2.8370066449
H,-0.680106415,1.7654781611,3.286260038
H,0.5464509796,0.5126405048,3.5206376707
H,0.9881378123,2.0736958853,2.7904841821

TS5-term E = -1787.005926

O	-0.926822	1.861474	-1.326666
C	-2.458694	1.747578	-0.283541
O	-2.556476	3.081982	-0.101643
C	-1.296908	3.754177	-0.036283
C	-0.591449	3.252976	-1.278471
C	-1.565979	1.313563	2.056050
C	-2.221687	0.796126	0.786372
Au	-1.401878	-1.034053	0.067198
P	-0.400988	-3.042901	-0.657991
O	1.898272	-1.086148	-0.988876
S	2.000085	-0.137138	0.151829
O	1.835224	-0.720247	1.505147
O	1.273572	1.163331	-0.060717
C	3.780672	0.412484	0.111058
F	4.065401	0.970072	-1.064059
F	4.580015	-0.636878	0.292298
F	4.015460	1.300343	1.074398
H	-0.503318	1.550288	1.902595
H	-1.609963	0.542548	2.835732
H	-3.149516	1.406129	-1.063423
H	-0.985770	3.721901	-2.186956
H	0.497015	3.369286	-1.228294
H	-1.499790	4.829112	-0.047356
H	-3.244331	0.419698	0.990063
H	-0.192839	1.363736	-0.869051
H	0.120831	-3.066750	-1.975446
H	0.724212	-3.486383	0.080996
H	-1.179116	-4.232435	-0.676017
H	-2.070133	2.210880	2.451871
H	-0.749220	3.486340	0.877620

I5-term E = -1787.015880

C,-2.0177007308,1.686876029,1.732845764
H,-1.0414604695,1.4591955559,2.1877565065
H,-2.7627346923,1.0645385639,2.2475034913
C,-2.024054065,1.4068244815,0.2321405626
C,-1.0590355049,2.2796165255,-0.5135622244
H,-1.1057954122,2.1163916297,-1.6080181847
C,-0.0110751987,4.2722536462,-0.519093576
C,0.9780609642,3.294429491,0.0819373341
H,1.9545765481,3.2868408596,-0.4191011952
H,1.112983178,3.4592940019,1.1624848305
O,0.3268908218,2.0378013601,-0.12806864
O,-1.2502596481,3.6490511907,-0.2418717609
H,0.1384206353,4.3712685723,-1.609077733
H,-3.0150462302,1.662383272,-0.1833048949
H,0.8603951465,0.8194886643,0.5936604632
Au,-1.7593160955,-0.6334884631,-0.2362047921
P,-1.4890871353,-2.9491427009,-0.7047325144
H,-0.5209972656,-3.3272886457,-1.6737972073
H,-1.0875460585,-3.7949117614,0.3635814948
H,-2.601377667,-3.6918589537,-1.184618091
O,1.2832063883,0.0344674369,1.1053122668
S,1.9702983598,-0.9930653859,0.1196458196

O,1.6173043431,-0.732387519,-1.280358196
O,1.8756095145,-2.3367465111,0.6950177389
C,3.749385754,-0.463266652,0.3119514696
F,3.8681704443,0.8044837537,-0.0539140206
F,4.4991596469,-1.2265748774,-0.4670861369
F,4.1252350537,-0.6026939669,1.5721387945
H,0.0054989632,5.264311422,-0.0550327767
H,-2.2499045883,2.7404689806,1.9587484076

TS6-term E = -1786.985776

C	-3.88449	-2.46215	-0.37483
O	-2.49745	-2.76088	-0.47526
C	-1.76795	-1.52915	-0.4221
O	-2.69807	-0.54389	-0.06503
C	-3.9266	-0.96907	-0.6283
C	-0.6292	-1.62163	0.57227
Au	1.38776	-0.91133	-0.02911
p	3.52569	-0.26891	-0.6843
O	-0.67469	0.9134	1.38033
S	-0.11328	2.24994	0.85644
O	-0.52122	3.36067	1.73045
C	-1.07486	2.48084	-0.72527
F	-0.67921	3.60975	-1.30543
O	1.29542	2.16963	0.41749
F	-2.37275	2.55161	-0.47678
F	-0.8316	1.46287	-1.54417
H	-1.38158	-1.33063	-1.44488
H	-3.95223	-0.74454	-1.71013
H	-4.74687	-0.44535	-0.12487
H	-4.44455	-3.0483	-1.11609
H	-0.10455	-2.54562	0.23875
H	-0.38383	-0.14597	0.83649
H	4.29256	0.3858	0.3117
H	4.45526	-1.23408	-1.14805
H	3.58735	0.68322	-1.73234
H	-4.24966	-2.71005	0.63675
C	-1.08092	-1.90129	2.00582
H	-1.69108	-1.08377	2.40915
H	-1.67637	-2.82567	2.0525
H	-0.21029	-2.02643	2.66332

P-term E = -346.797222
C,-1.4639453553,1.8220635839,0.6395958807
H,-1.8298718019,1.3852025334,1.5786456616
H,-1.6419631634,2.9049075553,0.6801439529
C,-2.1620142505,1.2095674471,-0.5605878831
C,-1.9104650362,-0.2693183222,-0.7168506086
H,-2.4238789203,-0.6648163669,-1.6181523902
C,-0.1721296787,-1.5501309879,0.0957672412
C,-1.5172940544,-2.117425989,0.4976576497
H,-1.8568406082,-2.8918209214,-0.2137031701
H,-1.5545486791,-2.5150458628,1.5181954143
O,-2.3500319401,-0.9726745476,0.4205951422
O,-0.519991523,-0.5523360149,-0.8557237195

H,0.494185457,-2.2867234032,-0.3726171851
H,-1.8334094534,1.6940325873,-1.493056742
H,-3.2521463897,1.356171566,-0.5013058433
H,-0.3775600869,1.6624099681,0.5873369406
H,0.341563074,-1.0877641453,0.9561528188

I2-inter-OH E = -2209.338516

C	-0.516296323121	-0.969438907045	-1.029001858520
C	0.373693148359	-1.994566206512	-1.036276903682
C	2.105248007182	-0.757907992418	-2.161029862494
C	3.625722406157	-0.746390763594	-2.144855349591
H	3.999996332696	-1.753025725430	-1.894518172324
H	4.011635016196	-0.494258472044	-3.140998195207
O	4.149371107875	0.248064469155	-1.281794443381
O	1.638041328577	-1.951232827702	-1.540139611308
H	1.707602165898	-0.720776522624	-3.187967406569
Au	-2.419767287403	-1.036849531745	-0.247730159350
P	-4.616995251570	-1.067735121121	0.615104005796
O	0.335662978581	2.294649820341	1.667819001636
H	-5.364317606717	0.139119539412	0.582097437152
H	-5.559644829885	-1.944240868846	0.014825948514
H	-4.806047954043	-1.422105232882	1.977454270326
S	0.624211469637	3.090226376352	0.406214623910
O	1.146201661833	2.245200752560	-0.695597023158
O	1.294131720584	4.381138359366	0.661823914772
C	-1.089361625210	3.565518224185	-0.150729247413
F	-1.818596441567	2.475585728890	-0.376012700610
F	-1.013681594111	4.273294316030	-1.274087911328
F	-1.687164546968	4.300039341389	0.783580125630
C	4.328874558017	-0.074354363546	0.083552302075
C	5.541646308681	-0.962156181973	0.278138762428
H	5.676760632968	-1.189983772276	1.344366331839
H	5.440939495912	-1.909548855185	-0.269675277002
H	6.435638590762	-0.441948867540	-0.087973918417
C	4.449432437223	1.251242291696	0.795566497039
H	3.516538733905	1.818427141776	0.668782969758
H	4.641932717346	1.091005447498	1.864076583969
H	5.272605774816	1.834652449026	0.365332207490
H	1.751866698076	0.133331442515	-1.624654797620
H	-0.215860762086	-0.047550671801	-1.541287188546
O	3.178275276066	-0.733741748584	0.600831640559
H	3.283433236758	-1.713129568857	0.634233854222
H	1.809391161148	-0.252052556660	1.066176456610
O	0.837072601879	-0.145030226852	1.367997712142
H	0.273779882817	-0.486616585471	0.596001841774
H	0.616400322403	0.862725626706	1.513047082389
O	3.246803662439	-3.380713670669	1.176667603093
H	2.569354031540	-3.256393211714	1.871950184233
H	4.041918311032	-3.663265219772	1.640421124210
O	1.154629659485	-2.666270502135	2.881348746238
H	0.889786744457	-1.752775262133	2.703992074177
H	1.224202197732	-2.726694981977	3.840545991353
C	0.142745043700	-3.355792425493	-0.467402812178
H	-0.774888892459	-3.381000178949	0.132504328451
H	0.046155684513	-4.085747851242	-1.286492552977

H	1.003222777791	-3.668341370908	0.141702227348

TS23-inter-OH E = -2209.336255

C	-0.372373633048	-0.901888137228	-0.893812507097
C	0.522721261284	-1.932530418395	-1.037914908353
C	2.169490358428	-0.628932881655	-2.220229027766
C	3.689067804156	-0.578518602214	-2.154310322407
H	4.080393532200	-1.577665018362	-1.899922617323
H	4.095410086870	-0.312557215862	-3.138858573212
O	4.159665440766	0.422185418634	-1.273006490334
O	1.713140266996	-1.860256192100	-1.642790041787
H	1.801981748070	-0.590235605395	-3.256030747969
Au	-2.324435747786	-1.112111845482	-0.220231925969
P	-4.555768709841	-1.280697345704	0.505973818736
O	0.052857855543	2.280501988601	1.711236053696
H	-5.353434158976	-0.107456568820	0.465843706201
H	-5.414310963774	-2.179279314701	-0.179868316819
H	-4.798804938057	-1.690615416506	1.843033403991
S	0.413505218798	3.087558169286	0.487726057643
O	1.036192450840	2.279162643087	-0.592250655151
O	1.034663389340	4.396648609343	0.788790887924
C	-1.261731149393	3.534267259071	-0.199582097905
F	-1.938807239974	2.433389280106	-0.521071288125
F	-1.121483096350	4.281839967509	-1.292512505716
F	-1.961778064001	4.221032782504	0.701255373497
C	4.313085251691	0.088550337201	0.099005517532
C	5.571794145483	-0.728794520485	0.312473959897
H	5.692317431649	-0.965565913268	1.378707660111
H	5.541134800093	-1.671277300368	-0.252178160818
H	6.443674047034	-0.151520180611	-0.020256143209
C	4.342288119858	1.410885082135	0.827675192437
H	3.376949574761	1.918919751027	0.693923402240
H	4.526614971242	1.247414108580	1.897412292888
H	5.135107387548	2.050808447071	0.420694940195
H	1.770327721209	0.233508903850	-1.671702549586
H	-0.145377004934	0.012295756175	-1.452702174617
O	3.186161482112	-0.636390364506	0.560914229610
H	3.375117581367	-1.596681401893	0.652933790872
H	1.705721688406	-0.201467316687	1.125668241984
O	0.744115530645	-0.218198758923	1.400064608282
H	0.178275483640	-0.579158921524	0.412174494022
H	0.464485240608	0.730635960541	1.579740248613
O	3.398990842486	-3.277790985995	1.176584502244
H	2.692439597529	-3.199524236865	1.851201698873
H	4.188543386027	-3.548219782947	1.655515090302
O	1.191373880139	-2.724599410809	2.768683053760
H	0.889101627928	-1.833073098456	2.531466550726
H	1.251041963938	-2.721553473062	3.729245069471
C	0.344812904315	-3.288433053675	-0.446116054201
H	-0.443441645823	-3.280613474044	0.314413719792
H	0.047061887379	-3.990083208038	-1.239464547385
H	1.288475206528	-3.652786740150	-0.019723949284

I3-inter-OH E = -2209.387282

C	0.05836	0.96328	-0.74618
C	-0.50140	0.22845	0.30598
C	-2.47133	-0.33822	-0.92192
C	-3.56651	-1.35137	-0.75473
H	-4.06606	-1.20860	0.21442
H	-4.30834	-1.20886	-1.55946
O	-2.98336	-2.63637	-0.81975
O	-1.64720	-0.40915	0.25488
H	-2.87751	0.68281	-1.00064
Au	-0.77819	2.86180	-0.11092
P	-1.61657	4.97324	0.45825
O	3.03900	-1.69028	1.18204
H	-0.92706	6.09708	-0.06084
H	-2.94596	5.27013	0.06714
H	-1.66261	5.29896	1.83648
S	3.37745	-0.80822	0.01966
O	3.27738	0.65075	0.29785
O	2.80630	-1.25649	-1.27744
C	5.21185	-1.08410	-0.17818
F	5.85804	-0.72484	0.93056
F	5.68012	-0.36223	-1.19589
F	5.46496	-2.37049	-0.41901
C	-3.61452	-3.68438	-0.05510
C	-5.00032	-3.96229	-0.59393
H	-5.65740	-3.09592	-0.43871
H	-4.95233	-4.19175	-1.66705
H	-5.43965	-4.81919	-0.06624
C	-2.67215	-4.85970	-0.20998
H	-1.66819	-4.58510	0.14587
H	-3.03985	-5.71113	0.37642
H	-2.60255	-5.16040	-1.26454
H	-1.86417	-0.56434	-1.80856
H	-0.30842	0.80081	-1.76083
O	-3.75269	-3.29571	1.27554
H	-2.86325	-3.24231	1.69130
H	-1.38397	-2.80682	-1.69685
O	-0.46742	-2.57335	-1.93696
H	1.13543	1.13145	-0.64651
H	-0.22833	-3.13012	-2.68404
O	-1.26853	-3.13329	2.46241
H	-1.03287	-3.84156	3.06947
H	-0.55630	-3.12514	1.78188
O	0.67492	-3.12875	0.56862
H	0.43587	-2.89104	-0.34754
H	1.53120	-2.69854	0.74743
C	0.15523	0.09266	1.62947
H	-0.50304	0.49291	2.41264
H	0.29960	-0.97595	1.84015
H	1.12193	0.60607	1.64210

TS34-inter-OH E = -2209.339109

C	0.33485	-0.94620	-0.68366
C	0.54546	-0.03036	0.35381
C	2.06478	1.30666	-0.91756

C	2.56290	2.72109	-0.82145
H	3.00527	2.87484	0.17727
H	3.35170	2.86146	-1.58186
O	1.51937	3.64116	-1.00824
O	1.29174	1.04543	0.26894
H	2.89656	0.58373	-0.94424
Au	1.96310	-2.25830	-0.10581
P	3.67979	-3.76780	0.40071
O	-3.27426	0.27358	1.06024
H	3.56327	-5.06879	-0.14842
H	4.99264	-3.41983	-0.00454
H	3.88952	-4.07085	1.76973
S	-3.33217	-0.72632	-0.06008
O	-2.70110	-2.03493	0.25738
O	-3.01844	-0.15394	-1.39423
C	-5.15048	-1.12806	-0.1474
F	-5.56688	-1.63010	1.01354
F	-5.37284	-2.02589	-1.10573
F	-5.85575	-0.03101	-0.41756
C	1.55015	4.90099	0.08699
C	2.70638	5.73227	-0.43934
H	3.65686	5.20088	-0.29289
H	2.58698	5.98586	-1.50216
H	2.75091	6.66483	0.14317
C	0.19849	5.52167	-0.22218
H	-0.61496	4.87945	0.13998
H	0.13382	6.48245	0.30904
H	0.06540	5.71309	-1.29682
H	1.43743	1.16359	-1.80703
H	0.55299	-0.64745	-1.71057
O	1.71252	4.43054	1.28117
H	0.50120	3.66827	1.89828
H	0.30837	3.12424	-1.30085
O	-0.64511	2.65370	-1.54503
H	-0.54707	-1.57990	-0.54882
H	-1.06262	3.12082	-2.27645
O	-0.29026	3.15920	2.29153
H	-0.59721	3.68681	3.03437
H	-1.41286	2.79829	1.19485
O	-2.00576	2.56160	0.41987
H	-1.36282	2.57530	-0.60668
H	-2.48797	1.72271	0.62133
C	-0.06460	-0.18007	1.69846
H	0.72661	-0.35057	2.44238
H	-0.55477	0.76432	1.97441
H	-0.78397	-1.00537	1.71465

I4-inter-OH E = -2209.378705

C	0.00147	-1.03118	-0.72901
C	0.51700	-0.14517	0.22487
C	2.38702	0.43610	-1.12887
C	3.43099	1.51718	-1.14643
H	3.83978	1.63061	-0.12574
H	4.25387	1.18290	-1.79861
O	2.94798	2.75272	-1.61478

O	1.57837	0.60807	0.05248
H	2.84351	-0.56603	-1.06947
Au	1.11925	-2.76256	-0.05686
P	2.22990	-4.73090	0.55663
O	-3.16530	1.32782	1.11666
H	1.70129	-5.94090	0.04231
H	3.59203	-4.85537	0.18567
H	2.29805	-5.03322	1.93938
S	-3.45153	0.40231	-0.02548
O	-3.21904	-1.03798	0.27218
O	-2.95909	0.87548	-1.34508
C	-5.30618	0.51653	-0.17130
F	-5.88226	0.12941	0.96673
F	-5.74348	-0.26717	-1.15727
F	-5.67510	1.77107	-0.43014
C	3.22711	4.43795	0.42330
C	4.55930	4.83895	-0.12985
H	5.30906	4.06630	0.07727
H	4.50093	5.03875	-1.20669
H	4.87163	5.77164	0.36758
C	2.02844	5.18528	-0.07235
H	1.09912	4.68993	0.23195
H	2.05202	6.19848	0.35954
H	2.05942	5.29886	-1.16323
H	1.74746	0.49545	-2.01955
H	0.28122	-0.90373	-1.77627
O	3.14375	3.60412	1.31988
H	1.57921	3.28089	2.10906
H	1.96800	2.73310	-1.65500
O	0.23344	2.53168	-1.77927
H	-1.03668	-1.32566	-0.54404
H	-0.23960	2.91518	-2.52317
O	0.69517	3.14775	2.51636
H	0.63849	3.80759	3.21434
H	-0.59533	3.22350	1.23042
O	-1.17035	3.19977	0.44126
H	-0.31079	2.74782	-0.98534
H	-1.90614	2.59757	0.66085
C	-0.08982	0.02446	1.56694
H	0.66312	-0.17149	2.34236
H	-0.40608	1.06870	1.68784
H	-0.95156	-0.63767	1.69357

TS5-inter E = -1787.022037

O	0.364403030245	1.973433224410	0.768099206607
C	2.117031716164	2.014000432846	0.167520227328
O	2.047409706702	3.302880007391	-0.248910787201
C	0.773107947217	3.638507320256	-0.791542506601
C	-0.157893909037	3.235778774756	0.333349434436
C	2.198546360573	0.925324394692	-0.815916489751
Au	1.516458867350	-0.973552294804	-0.196906888535
P	0.627447922516	-3.039843052269	0.501762499333
O	-1.695764678789	-0.883270250304	1.186476014255
S	-2.121890904793	-0.482044268425	-0.180792738451
O	-2.468328518811	-1.580455970376	-1.112136311564

O -1.269578582808 0.600717540810 -0.790063041836
C -3.731917057652 0.412990962380 0.106755511589
F -3.525630258855 1.469644708102 0.894096926642
F -4.611149286437 -0.394459335395 0.693873362111
F -4.241782217820 0.834590019737 -1.047806983389
H -0.092694739605 3.932627553041 1.176690186395
H -1.199643299500 3.112740576549 0.017096144278
H 0.774858990261 4.710997094526 -1.005399542183
H 3.283207333491 0.791763924620 -0.980200659802
H -0.136110791189 1.272645691410 0.260719438236
H 0.305232693258 -3.149061400132 1.878674300747
H -0.614482469729 -3.407176386282 -0.076873517520
H 1.364922013603 -4.240616258928 0.322045097984
H 0.568113327371 3.074034789394 -1.714506242815
H 1.743051468940 1.216937716111 -1.772661989051
C 2.902161010009 1.905350072131 1.428252447893
H 3.949039497514 2.145235943657 1.190515925449
H 2.541873187509 2.629550435583 2.167564649151
H 2.857290642299 0.889296034514 1.832937326252

I5-inter E = -1787.026460
C,-2.2145984765,1.4613905332,-0.3521189739
H,-2.3368871031,1.7028113307,-1.4200250405
H,-3.145932426,1.7513768871,0.1611579174
Au,-1.9152700665,-0.6015641283,-0.1630033744
P,-1.5099126882,-2.9345102882,-0.0682385841
H,-0.9044397914,-3.516131823,-1.2138719615
H,-0.627209242,-3.4261118661,0.930849766
H,-2.5875917266,-3.843150347,0.1118152507
O,1.466636379,0.2518933568,1.0982203804
S,2.0858020415,-1.0254869271,0.4068933116
O,2.3305096976,-2.0386800725,1.4343083091
O,1.4051602646,-1.3579595794,-0.8505308325
C,3.7545199377,-0.3442110429,-0.0765126683
F,4.3971915021,0.0633094741,1.0049347934
F,3.5828499266,0.6744625782,-0.9066659283
F,4.4439070389,-1.3006868534,-0.6765777147
C,-1.1079335438,2.3185240942,0.1886883522
C,1.0130827758,3.0256626458,-0.5480562273
C,0.0758300243,4.2109300472,-0.3055386545
H,0.2791195429,4.7019665432,0.6601672646
H,0.1300454071,4.9662977006,-1.097992235
O,-1.2142164448,3.6335493205,-0.3285323203
O,0.1793013092,1.875996273,-0.3589869087
H,1.8542289034,3.0050670685,0.1622366027
H,1.4073694738,2.9928838676,-1.571449543
C,-1.0239519942,2.3399260568,1.7038457735
H,-1.9257351367,2.8210142925,2.1050806404
H,-0.9744997061,1.3175654787,2.099463982
H,-0.1441436513,2.8937274811,2.0608793334
H,0.9031357728,0.833752898,0.4553512894

TS6-inter E = -1786.997961

C	-3.607326043747	-1.262648352374	1.424318261452
O	-2.424746853215	-0.674507635491	0.905580193285
C	-2.168391013287	-1.295352827188	-0.348578236929
O	-3.468383016968	-1.508271086577	-0.894635227161
C	-4.325958719117	-1.828415104711	0.188168458529
C	-1.426601807419	-0.329894299070	-1.248025832751
Au	-0.434607022339	1.343837697083	-0.223309804550
P	0.563610908728	3.137811887204	0.861961503429
O	1.059834747297	-1.195682200052	-1.361966500446
S	2.431545810522	-0.810513840696	-0.772800568052
O	3.515885153883	-1.538757736194	-1.449545436797
C	2.338765964919	-1.560262154750	0.933525965882
F	3.480370675623	-1.328923337157	1.568715515506
O	2.584947624315	0.638204848425	-0.530337163478
F	2.140421612974	-2.869511319672	0.848223082621
F	1.339576673951	-1.011501344645	1.618221685287
H	-4.475285336463	-2.917791682768	0.267271735836
H	-5.300668630995	-1.357979750482	0.004652646219
H	-3.366255772952	-2.053048669341	2.153441459484
H	-2.146222479330	0.454256359675	-1.553927353174
H	0.026633174343	-0.528610127263	-1.147907612895
H	1.608726764615	3.774595224806	0.147212756602
H	-0.213568458734	4.256404780376	1.255402174703
H	1.225407470619	2.832431715396	2.077917819946
H	-4.181270848099	-0.480586099287	1.937339016396
H	-1.200804282880	-0.824071785684	-2.207104681195
C	-1.464059877192	-2.625008202430	-0.152144492354
H	-0.502006804662	-2.480656673630	0.354012699167
H	-2.077059673552	-3.300732928133	0.458980925919
H	-1.284759886760	-3.105325154604	-1.123224707092