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ARTICLE

Organocatalytic vs Ru-based Electrochemical Hydrogenation of Nitrobenzene in Competition with Hydrogen Evolution Reaction

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The electrochemical reduction of organic contaminants allows its removal from water. In this contribution, the electrocatalytic hydrogenation of nitrobenzene is studied using both oxidized carbon fibres and ruthenium nanoparticles supported on unmodified carbon fibres as catalysts. The two systems produce azoxynitrobenzene as main product, while aniline is only observed in minor quantities. Although PhNO₂ hydrogenation is the favoured reaction, the hydrogen evolution reaction (HER) competes in both systems under the catalytic conditions. The H₂ formation occurs in larger amounts when using the Ru nanoparticle based catalyst. While similar reaction outputs have been observed for both catalytic systems, DFT calculations revealed some significant differences related to distinct interactions between the catalytic material and the organic substrates or products, which could pave the way for the design of new catalytic materials.

Introduction

Electrochemical reduction of organic substrates is an important synthetic method but also, an efficient way to remove persistent pollutants^{1–3} and to produce energy vectors based on reversible hydrogenation/dehydrogenation processes.^{4–6} Such processes, when carried out in the presence of proton sources, require electrocatalysts able to hydrogenate organic functionalities.⁷ Such electrocatalytic materials are intended to increase the activity and selectivity of the reduction reaction. Regarding the selectivity, the occurrence of Hydrogen Evolution Reaction (HER) as a parasite process in competition with the hydrogenation of organic reagents is ubiquitously observed.⁸ The characteristics of the electrocatalytic materials will have enormous influence on the reaction output, tipping the balance in favour of one or another process. Thus, a deep understanding of the mechanism underlying both pathways will enable to rationally design electrocatalytic materials capable to hydrogenate organic substrates or to mediate HER. Indeed, a wide range of materials has been already studied due to the need of clean and renewable alternatives to the use of fossil fuels.^{9–11} Although Pt-based catalysts are known to be highly performing for HER, its substitution by cheaper and earth-abundant catalytic materials is highly demanded.^{12–15}

Metal-free catalysts, such as carbon-based materials^{16,17} as well as Ru-based catalysts^{18–20} seem to be ideal alternatives for this purpose.

In a recent report, we explored carbon microfibres (CFs) prepared by the pyrolysis of polyacrylonitrile (PAN) as an alternative electro-organocatalytic material for HER (Fig. 1a, top).²¹ CFs with a graphene-like structure including pyridyl moieties can be easily oxidized to generate carboxylic acid groups at the surface, constituting nicotinic fragments in its structure. The resulting material that will be further referred as ox-CF presents high HER electrocatalytic activity. Indeed, ox-CF acts as catalytic centres for the HER in a way similar to those of NADPH in biological systems^{22,23} and Hantzsch esters in synthetic reduction procedures.^{24–26} In another work, we used pristine CFs as support for Ru-NPs in order to achieve stable and high surface area functionalized electrodes (Fig. 1a, bottom).²⁷ Our results demonstrated the viability of such hybrid material composed by Ru-NPs onto CFs as remarkable electrocatalysts for the HER (referred as Ru-CF). A common feature of both systems (ox-CF and Ru-CF) is the generation of hydride species that can be protonated to form molecular hydrogen. Additionally, they could hydrogenate a variety of substrates, widening the applicability of electrochemical systems usually employed for HER. Remarkably, such electrocatalytic procedures are convenient strategies that avoid the manipulation of H₂ gas or metal hydride derivatives (LiAlH₄ or NaBH₄), commonly used in chemical hydrogenation processes. In this work, we have compared the electrocatalytic HER and the hydrogenation of nitrobenzene (PhNO₂) as model substrate, using modified carbon fibres (ox-CF and Ru-CF) as electrocatalytic materials (see Fig. 1b). The reduction of PhNO₂ is of great interest since nitro aromatic compounds (such as explosives, dyes, agrochemicals or pesticides) are common water contaminants.^{28,29} Although many alternatives have been

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explored,^{30–35} electrochemical procedures are still the most convenient ways to reduce PhNO₂ and related compounds. However, in the presence of protic media, this process would typically be in competition with HER. Again, platinum electrode is often used for electrochemical reduction of nitrobenzene,^{36–38} limiting their applicability for large scale processes.³⁹ Thus, there is a need to find efficient, inexpensive, easy to make and recyclable electrocatalytic materials free of noble metals^{40,41} for the reduction of nitroaryl compounds. This reaction will be deeply presented in this manuscript, considering HER as a competitive process. We will determine the intrinsic properties of ox-CF and Ru-CF as electrocatalysts for both reactions (compare Fig. 1b top and bottom) by means of combination of experimental and theoretical results. This work will provide fundamental understandings on the distinctive catalytic behaviour of metal-based and metal-free electrocatalysts. The obtained fundamental insights can pave the way for the future design of active and selective electrocatalytic materials for HER or hydrogenation of organic substrates.

Experimental

Materials

All reagents, solvents and materials were purchased from commercial sources and used without further purification. Specifically, fabric of carbon fibre (Twill 2x2 3K weight 200 g/m² width 1200 mm, Model HA2301) was purchased from ClipCarbono.

Electrode Preparation

The commercial carbon fibre is prepared in a 6 cm long bunch of fibres. Then, it is joined to a copper wire and tight with a Teflon tape. The hand-made electrodes are modified using two different approaches, namely: 1) oxidative treatment of the carbon fibre and 2) ex-situ deposition of Ru-NPs. For the oxidized CF brushes, they are treated 30 minutes with sulfuric acid (98%) at room temperature with stirring and later they are immersed into a mixture 1:1 of H₂SO₄/H₂O₂. The mixture should be freshly prepared to obtain its stronger oxidative potential and thus, be able to oxidize the carbon fibre. Finally, the electrodes are washed and sonicated in distilled water to neutralize its surface, later washed in ethanol and dried with a heat gun. Characterization of this material was previously reported and confirms that the oxidation process changes the chemical features of the CF surface (generation of carboxylic groups, transforming pyridinic fragments into nicotinic ones) whereas keep its bulk properties and morphology.²¹ For the Ru-based CF, 2 cm of CF electrodes were soaked overnight in a THF (10 mL) crude dispersion of RuPP NPs^{27,42} inside a Fisher-Porter bottle under an Ar atmosphere. Then, the supernatant was removed through cannula and the resulting CF materials were rinsed with pentane (3x10 mL) and dried under vacuum. RuPP@pCF. TEM: $\varnothing = 1.8 \pm 0.3$ nm. ICP(Ru%): 0.47%.

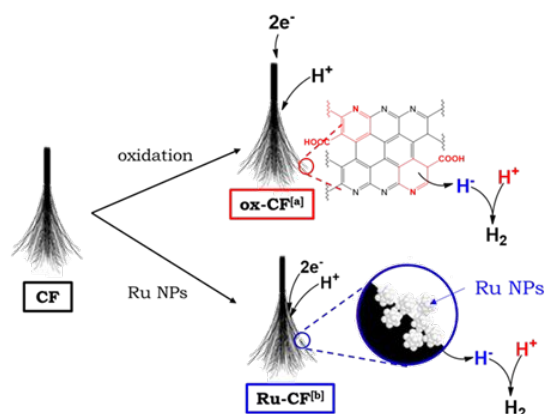
Electrochemistry

Electrochemical experiments were performed under an argon atmosphere at room temperature in CH₃CN. Sodium perchlorate (NaClO₄) was used as supporting electrolytes. Measurements were carried out using an Ivium CompaqStat potentiostat interfaced with a computer. A standard three-electrode electrochemical cell was used with Ag/AgCl reference electrode. The working electrode was carbon fibre brush: pristine, oxidized and modified with inorganic nanoparticles. The counter electrode was a pristine carbon fibre brush.

Gas Chromatography

The evolution of the nitrobenzene during the electrocatalytic reaction was monitored by gas chromatography, by injecting samples of the intern atmosphere to an Agilent 7820A GC system equipped with a mass spectroscopy detector (5977B MSD). For gas chromatography quantification of nitrobenzene and its derivatives, the solvent of the working electrode solution is reduced at low pressure and then it is solved with 1 mL of CHCl₃ which is able to solve the nitrobenzene and its derivatives but not the inorganic salt of the electrolyte. An aliquot of 0.2 mL of the solution is mixed with 0.2 mL of methyl-naphthalene as

a) Previous work: Carbon Fiber-based Electrocatalyst for HER



b) This work: Electrocatalytic HER vs PhNO₂ Reduction

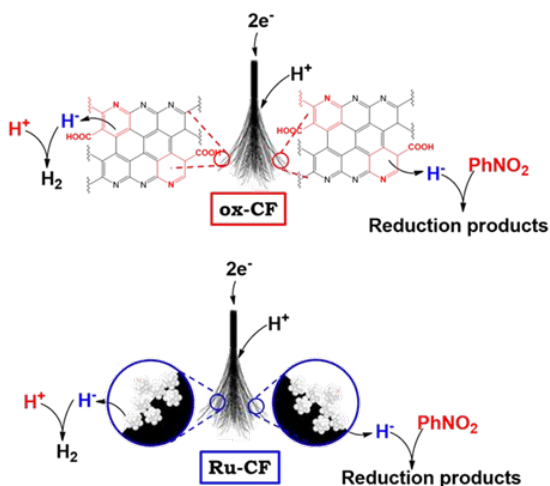


Fig. 1 Schematic representation of a) Carbon Fiber-based electrocatalysts for HER (previous work)^{21,27} and b) HER vs hydrogenation of PhNO₂ using same electrocatalysts (this work).

standard. A calibrate of nitrobenzene, nitrosobenzene, azoxynitrobenzene, diphenylazobenzene and aniline was carried out enabling the quantification of the products.

Computational Details

Quantum chemistry calculations were carried out using the density functional theory (DFT). For the organocatalytic system, geometry optimizations were performed using the M06-2X functional⁴³ in combination with the 6-311G** basis set.⁴⁴ For comparison some selected PBE-D2 calculations were also carried out for this system (see S.I.).^{46,48} Solvent effects were included with the solvation model density (SMD)⁴⁵ and considering acetonitrile ($\epsilon=37.5$) as solvent. Graphitic surface was modelled using a fragment composed by 4 fused aromatic rings (1 pyridine + 3 benzenes) as a compromise between performance and computational cost a carboxylic group in the meta position versus pyridine nitrogen. All optimizations were performed without any geometrical constraint and harmonic vibrational frequencies were used to characterize minima and transition states in the potential energy surface. Transition states were connected to products by optimization of geometries slightly modified from the transition states. All the calculations were performed using the Gaussian09 program.⁴⁶

For modelling the reactivity with Ru-NPs, we used the PBE⁴⁷ functional as implemented in the VASP code.^{48,49} Grimme (D2) empirical correction was added to account for dispersion interactions.⁵⁰ The core electrons were described by ultrasoft pseudopotential^{51,52} and the external ones by plane wave basis set, with a kinetic energy cutoff of 500 eV. With the aim of minimizing replica interactions, a cubic cell of 25 Å was employed. The k point grid includes the Γ point only, as a consequence of the discrete nature of the system. The energy convergence criteria were fixed to 10^{-5} and 10^{-4} eV for electronic and geometry relaxations, respectively. Solvent effects were included during the optimization with the implicit continuum model implemented in VASPsol⁵³ and using acetonitrile as solvent ($\epsilon=37.5$). Transition states were located by using climbing image nudged elastic band (CI-NEB) method without including solvent effects.^{54,55} Six or eight images per NEB were used. The highest in energy image was used for locating the final transition state by performing a gas-phase geometry optimization with the quasi-Newton algorithm implemented in VASP. Convergence was considered to be achieved when forces were smaller than 0.02 eV/Å. Solvent effects at transition state were included with a single-point calculation at the optimized structure. For the case of the hydronium ion, the transition state was located by performing VASPsol restricted optimizations, in which the O-H distance of hydronium was fixed in each step. The highest in energy point was used as starting point for localizing the transition state. The energies reported along the text are all given in kcal mol⁻¹.

Results and discussion

Experimental Results

Details on synthesis and characterization of the electrocatalytic materials used in this comparative study are reported elsewhere.^{21,27} Previous mechanistic studies revealed that both, ox-CF and Ru-CF, generate hydrides that after protonation, lead to HER. Herein, we studied if these systems are capable to transfer the hydride to the organic substrate: PhNO₂. Although the product typically formed from this process is simply aniline, several other species can be generated. Therefore, as previously reported, a more complex mechanism should be considered for hydrogenation of nitrobenzene (see Fig. 2).⁵⁶

The electrochemical behaviour of nitrobenzene has been analysed by cyclic voltammetry (Fig. S1). A reduction signal is observed at $E_{1/2} = -1.1$ V vs Ag/AgCl, which is associated to a reversible electron transfer process. According to this result, -1 V vs Ag/AgCl was chosen as the limit potential for all electrochemical experiments in order to achieve electrocatalytic hydrogenation and avoid electrochemical electron transfer. The choice of an adequate proton source is determinant for the efficiency of the reaction. Also, in order to understand such effect, some factors have to be considered: 1) Electrocatalytic hydrogenation of nitrobenzene will compete with HER and 2) Hydride regeneration on the catalytic centres involves injection of two electrons into the electrocatalytic material and further protonation. Combination of both factors will determine the effect of the proton source in the output of the electrocatalytic PhNO₂ hydrogenation. In order to optimize the composition of our systems, we have compared linear sweep voltammetry results of ox-CF and Ru-CF using water (1 M), trifluoroacetic acid (TFA, 20 mM) and a mixture of both as proton sources (Fig. S2) in acetonitrile. Maximized electrochemical response is observed for both catalytic systems when a mixture of water and TFA is used. Fig. 3 presents the linear sweep voltammeteries recorded in the absence (top) and in the presence (bottom) of nitrobenzene at a scan rate of 10

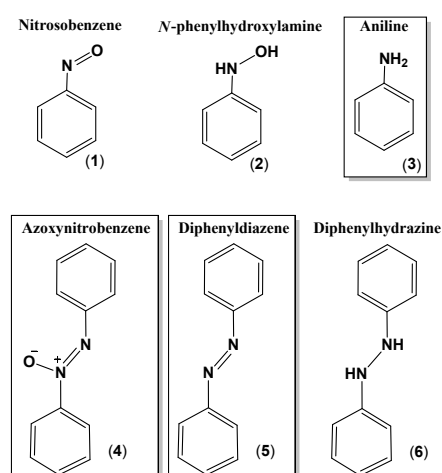


Fig. 2 Possible species that can be generated from hydrogenation of nitrobenzene with species detected in this work highlighted inside the frames.

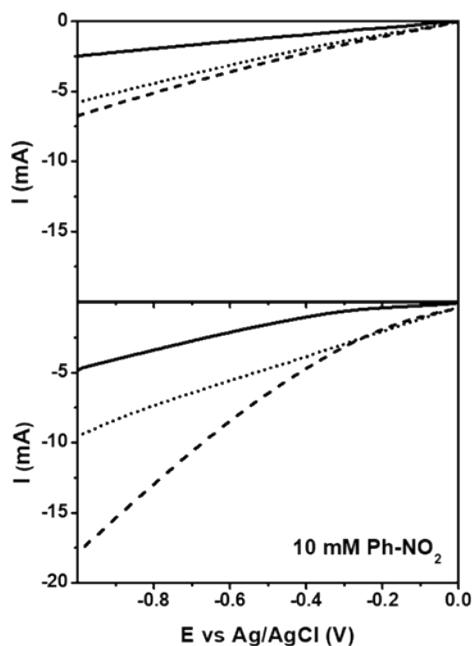


Fig. 3 Linear sweep voltammeteries measured using pristine (solid line), oxidized (dashed line) and Ru-based (dotted line) carbon fibre electrodes in the absence (top) and in the presence (bottom) of 10 mM of nitrobenzene. In all cases, solvent is acetonitrile containing H₂O (1 M), TFA (20 mM) and NaClO₄ (0.2 M).

mV/s. Measurements were performed in acetonitrile using NaClO₄ (0.2 M) and TFA (20 mM) and water (1 M) mixture.

The current intensity values at -1 V vs Ag/AgCl are presented in Table 1. Electrochemical responses of the two materials (ox-CF and Ru-CF) are much higher than that of the pristine fibre (CF), which demonstrates their catalytic properties, either for the proton reduction or for the nitrobenzene hydrogenation (see -2.48 vs -6.76 and -5.77 mA; -4.85 vs -17.89 and -9.31 mA). Current intensity is greatly enhanced upon addition of PhNO₂ when using ox-CF (see -6.76 vs -17.89 mA). However, such an effect is less pronounced for the Ru-CF (see -5.77 vs -9.31 mA). PhNO₂ hydrogenation is clearly facilitated with the purely organic electrocatalyst while larger competition between the nitrobenzene hydrogenation and the HER seems to take place when using the inorganic catalyst.

With the aim of determining the amount and nature of the final product, a 5 h electrolysis was performed at a constant potential of -1 V vs Ag/AgCl for the two electrocatalysts in the presence of water and TFA mixture (Fig. S3). The reaction outputs have been analysed by gas chromatography (GC). As expected from the current observed in the LSV, higher conversion was found for oxidized carbon fibres (Fig. 4a). It is important to note that the concentration of active sites is difficult to determine accurately. Thus, the activity observed

Table 1 Current intensities at -1 V vs Ag/AgCl in 1 M H₂O + 20 mM TGA corresponding to the linear sweep voltammeteries of Fig. 3.

[PhNO ₂] (mM)	I of CF (mA)	I of ox-CF (mA)	I of Ru-CF (mA)
0	-2.48	-6.76	-5.77
10	-4.85	-17.89	-9.31

cannot be uniquely related to the intrinsic properties of the active sites but also to their relative concentration on the electrode surface.

Furthermore, we investigated the reaction output after a longer reaction time (5 vs 15 h, Fig. 4a and 4b). After 15 h, the consumption of nitrobenzene is almost complete for both electrocatalytic materials. The pristine carbon fibre electrode was also tested for 15 h. In these conditions, no significant amounts of products were found, corroborating that the catalytic behaviour observed with the two other materials results from either the oxidation of carbon fibres or the presence of Ru-NPs (Fig. S3).

As shown on Fig. 4 and S4, regardless of the reaction time (5 or 15 h), the major product of the nitrobenzene reduction after bulk electrolysis at -1 V is azoxynitrobenzene dimeric species (4). In addition, residual amounts of aniline (3) and diphenyldiazene (5) are also observed. Interestingly, amounts of aniline (3) at 15 h are equal or even lower than those detected at 5 h. In contrast, the amounts of azoxynitrobenzene (4) and diazobenzene (5) are significantly superior at 15 h than at 5 h. These observations indicate that, a) the generation of aniline (3) corresponds to short reaction times, b) the formation of dimeric species (4 and 5) needs accumulation of monomeric species produced over the electrochemical process, thus requiring longer reaction times. Remarkably, although the nature of the two catalytic systems studied is very distinct, similar product compositions are observed. However, faradaic yields after 15 h electrolysis are approximately 75% for ox-CF and 65% for Ru-CF, thus indicating that HER is the minor process but it is more significant for Ru-CF, in agreement with voltammetry data (see Fig. 3).

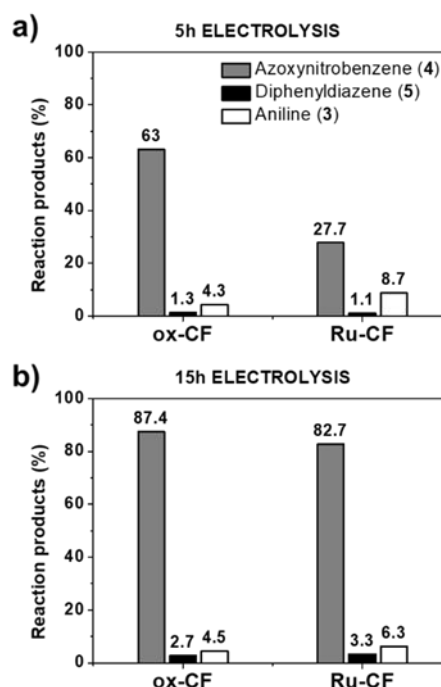


Fig. 4 Reaction products of the electrocatalytic reduction of nitrobenzene at -1 V vs Ag/AgCl after a) 5 h and b) 15 h of reaction using ox-CF and Ru-CF as electrodes in a mixed solution of 1 M of water and 20 mM of TFA in NaClO₄ (0.2 M, acetonitrile).

Theoretical Calculations

Methodological Strategies. In order to get a deep understanding of the processes occurring in the electrocatalysis, we performed a computational DFT study. Two sets of calculations were carried out. The full catalytic process involving the organocatalytic system (ox-CF) was represented with a molecular model from a previous work.²¹ The hybrid M062X functional⁴³ was used and atoms were represented with the 6-311G** basis sets⁴⁴ including solvation effects of acetonitrile ($\epsilon = 37.5$) by means of solvation model density (SMD).⁴⁵ The protonation steps of the PhNO₂ hydrogenation were studied also at this level of theory without including any of the two catalysts in the calculations. The reactivity of Ru-NPs was studied with VASP.^{48,49} For saving computational time, the exploration was limited to the thermodynamics of all steps and the transition states that appeared to be key for the organocatalytic system. VASP includes periodic boundary conditions and defines the basis set with plane wave. Thus, interaction with neighbour images was avoided by using a 25 Å edge cubic unit cell. These calculations were performed with the PBE GGA functional⁴⁷ and an energy cut-off of 500 eV. Dispersion forces were taken into account with Grimme D2 empirical correction⁵⁰ (see Computational Details section for further information). Remarkably, values for the Ru-NPs do not include thermal corrections. However, since all steps are unimolecular, ΔE and ΔG values calculated for ox-CF system using M062X and PBE-D2 functionals show little variations, except for the HER, where H₂ is formed (see details in S.I.). In any case, it is worth to note that since the methodologies used for modelling the two catalytic processes differ significantly, we have performed some selected calculation with PBE-D2 for the ox-CF system. Results are reported in the S.I. and show the PBE-D2 underestimates the energy barriers as it is well-known in the literature.⁵⁷ Thus, comparison should be made with caution.

Initial Considerations. As reported previously,²¹ the electro-organocatalytic behaviour of ox-CF is initiated by the injection of two electrons on the carbon material that contains randomly distributed nicotinic fragments. It is known that the value for the work function of highly orientated pyrolytic graphite (HOPG) in air is c.a. 4.8 eV,⁵⁸ which is expected to be close to that of the carbon fibre material. Thus, it should allow stabilization of injected electrons through the graphitic π -electron density. However, considering the reduced size of the molecular model used in our calculations to simulate the graphenic region, the stabilization energy after injection of two electrons (3.13 eV) is underestimated. After injection of two electrons, the negative charge increases the basicity of the

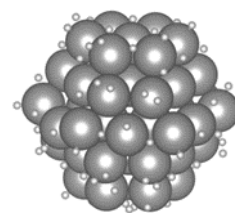


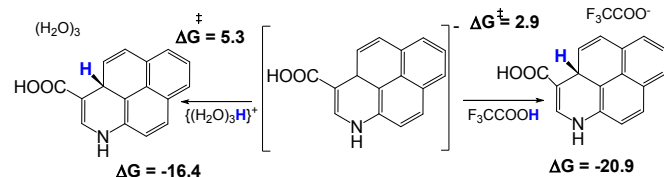
Fig. 5 Ru₅₇H₈₈ model used for representing the Ru-NPs.

pyridinic nitrogen atom and results in its barrierless protonation. Thus, we considered as the starting point the negatively charged species shown in Scheme 1 (centre) that contains a protonated pyridinic nitrogen atom. Further evolution of this reduced species consists in its protonation in the *para*-position with respect to the nitrogen atom. The corresponding species can transfer the hydride that is responsible for the observed reactivity. Taking into account the nature of the reaction medium, we have considered two possible protonation agents: TFA molecule and hydrated proton modelled as [H₃O(H₂O)₃]⁺ according to previous report.⁵⁹ Very similar results have been found using both species, being slightly more favourable the protonation with TFA ($\Delta G = -20.9$ kcal mol⁻¹; $\Delta G^\ddagger = 2.9$ kcal mol⁻¹) than with [H₃O(H₂O)₃]⁺ ($\Delta G = -16.4$ kcal mol⁻¹; $\Delta G^\ddagger = 5.3$ kcal mol⁻¹).

In order to study the processes mediated by Ru-NPs, we used a model that includes 57 ruthenium (44 at the surface) and 88 hydrogen atoms (Ru₅₇H₈₈, Fig. 5). We have considered this structure as a good representation of the active species generated under reductive potentials in acidic media, able to act as an efficient hydride transfer agent. The model choice and the number of hydrogen atoms is based on Comas-Vives *et al.* results.⁶⁰ Their work showed that a) this model is a good compromise between accuracy and computational cost and b) the number of hydrogen atoms per surface ruthenium is close to the double of surface ruthenium atoms in pristine nanoparticles.

Hydride Transfer to PhNO₂ vs Hydride Protonation. Once the active species able to perform hydride transfer processes are generated, two potential reactions can take place: hydride transfer to nitrobenzene and HER. Fig. 6 shows the comparison of the kinetics and thermodynamics of these processes in presence of model systems for a) ox-CF and b) Ru-CF. Fig. 7 shows some optimized structures.

Regarding the reactivity in presence of the ox-CF, calculations show that the hydride transfer to PhNO₂ is slightly endergonic ($\Delta G = +3.6$ kcal mol⁻¹) but this is clearly compensated by the subsequent protonation of PhNO₂H, which leads to PhNO (1) and a water molecule (origin of the exergonicity; $\Delta G = -108.9$ kcal mol⁻¹). The competitive H₂ formation is also thermodynamically favourable both from TFA and hydronium type molecule [H₃O(H₂O)₃]⁺, obtaining computed ΔG values of -12.4 and -6.2 kcal mol⁻¹, respectively. From a kinetic point of view, the hydride transfer to PhNO₂ is favoured with respect to HER by at least 9.2, kcal mol⁻¹. HER reaction is more favourable when TFA is used as proton source. These results are in accordance with the high faradaic yields found for nitrobenzene reduction (see above).



Scheme 1 Generation of the species able to transfer hydrides in the ox-CF organocatalytic system (energy values are given in kcal mol⁻¹).

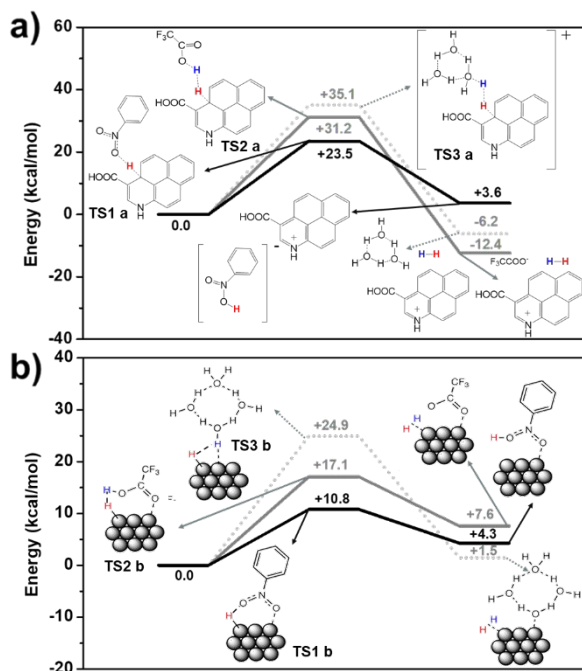


Fig. 6 Comparison of energetics for the hydride transfer to PhNO₂ (black line) and HER (grey lines) using a) ox-CF and b) Ru-CF electrocatalytic models. Hydride protonation can be carried out by TFA (solid grey line) or by [(H₃O)(H₂O)₃]⁺ (dashed grey line). Energies are given in kcal mol⁻¹.

Nitrobenzene hydrogenation and H₂ formation on Ru-NPs start with the adsorption of the reacting substrates to the nanoparticle surface (Table S2). This adsorption is more

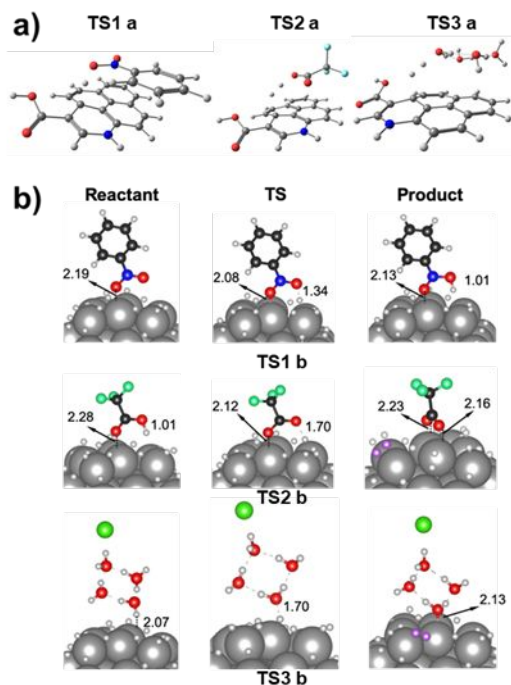
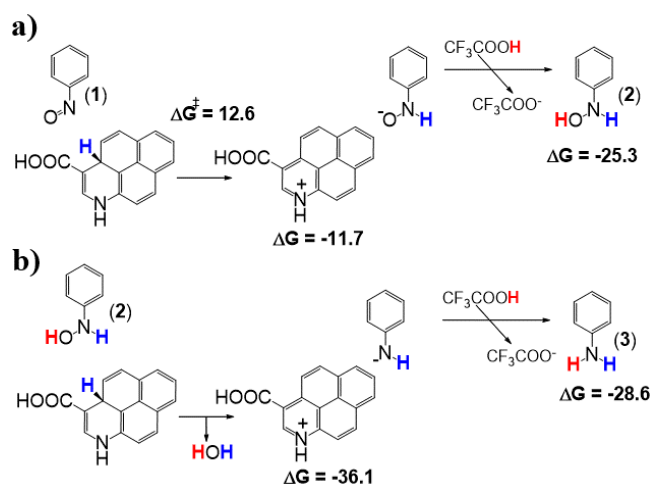


Fig. 7 Optimized structures found for PhNO₂ hydrogenation and HER using TFA and hydronium ion as source of protons: a) transition states shown in Figure 6a for ox-CF model system and b) the starting materials, transition states and final products using Ru-CF as catalytic model system as shown in Figure 6b. Cl atom (green) has been added to balance charge in periodic calculations. Distances are given in Å.

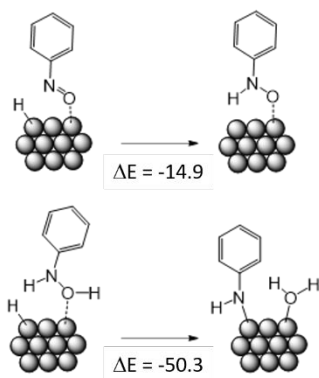
favourable for nitrobenzene and TFA than for hydronium ion [(H₃O)(H₂O)₃]⁺ (see S.I. for further details). Remarkably, two adsorption isoenergetic modes are found for nitrobenzene: a parallel adsorption mainly controlled by dispersion forces and a perpendicular one mainly controlled by the Ru...O interactions (see S.I. for further details). However, only the perpendicular orientation can account for the observed process. As found for the carbon fibres, the hydride transfer to the adsorbed nitrobenzene is slightly unfavourable ($\Delta E = 4.3$ kcal mol⁻¹), but the high exothermicity of the protonation step makes the formation of PhNO + H₂O largely favourable. The energy barrier for the hydride transfer to the adsorbed PhNO₂ species is computed to be 10.8 kcal mol⁻¹, thus suggesting it is kinetically easy.

The hydride protonation in presence of Ru-NPs is easier when involving TFA than [(H₃O)(H₂O)₃]⁺. The energy barrier is computed to be 17.1 kcal mol⁻¹ from adsorbed TFA. This value is higher than that computed for the PhNO₂ hydride transfer. The energy difference between the two processes is slightly smaller than for the ox-CF, indicating that HER (which is in both cases kinetically less favoured) could be a better competing reaction when using Ru-CF rather than when using ox-CF. Similar conclusions can be inferred from PBE-D2 calculations on the organic system. These results agree with the experimentally measured faradaic yields for both systems. A potential explanation of the large difference between the HER energy barriers when involving TFA and [(H₃O)(H₂O)₃]³⁺ could derive from the nature and the strength of the substrate-Ru-NP interaction. Indeed, the Ru...O interaction increases the acidity of TFA favouring the hydride protonation.

From PhNO (1) to PhNH₂ (3). Evolution of PhNO species formed from the first hydrogenation process (hydride transfer + protonation) to aniline consists of two consecutive hydrogenation steps (Scheme 2). Every hydrogenation step has been considered as an initial hydride transfer with a non-negligible energy barrier, followed by the protonation process, which is generally very favourable, mainly barrier-less and does



Scheme 2 Catalytic evolution of PhNO (1) consisting in two consecutive hydrogenation and protonation steps: a) forming hydroxylaniline (2) and b) aniline (3). Energy values are given in kcal mol⁻¹.



Scheme 3 Catalytic evolution of Ph-NO to aniline through two successive hydrogenation/protonation steps with Ru-NPs. Energies in kcal mol⁻¹

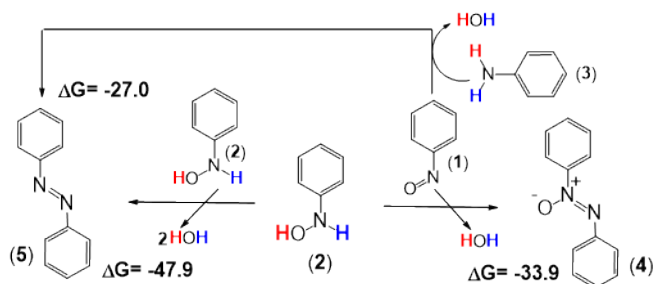
not involve the electrocatalyst. The hydride transfer to PhNO (**1**) results in deprotonated hydroxyaniline. This process is exergonic in presence of ox-CF by -11.7 kcal mol⁻¹. Moreover, the energy barrier is low ($\Delta G^\ddagger = 12.6$ kcal mol⁻¹), which indicates that the process is kinetically favourable (Scheme 2a). In addition, the protonation of deprotonated hydroxyaniline is also very favourable, suggesting that once PhNO (**1**) is formed, it easily evolves to PhNHOH (**2**).

Calculations for the second hydrogenation step indicate that hydride transfer to the OH group of hydroxyaniline to generate a water molecule and deprotonated aniline is very exergonic (-36.1 kcal mol⁻¹, Scheme 2b). In this case, transition state has not been located, indicating that this reaction is barrierless or proceeds through a very shallow barrier. Further protonation of deprotonated aniline is very favourable. Consequently, nitrobenzene hydrogenation (Fig. 6) seems to be the rate-determining step. Once PhNO (**1**) is generated, its reduction to aniline (**3**) should consecutively occur.

With the aim of analysing if these two steps are also straightforward in presence of Ru-NPs, we computed the corresponding reaction energies. Results are reported in Scheme 3 and show that PhNO (**1**) hydrogenation is similar to that found for the ox-CF and it is favourable by -14.9 kcal mol⁻¹. On the other hand, the hydrogenation of PhNHOH shows larger differences. The resulting products are the same for the two catalytic systems. However, the strong Ru-NPs-H₂O interaction and the Ru-PhNH makes the reaction even more exothermic ($\Delta E = -50.3$ kcal mol⁻¹). The ability of Ru-NPs to coordinate the reacting substrates changes the thermodynamics in comparison with the ox-CF system. In any case, the initial PhNO₂ hydrogenation to PhNO (**1**) appears to be the more challenging step also when using Ru-NPs (Fig. 6b).

Overall, calculations suggest that aniline (**3**) should be easily formed with the two catalytic systems. However, according to the experimental data, aniline (**3**) is only a minor product detected in the reaction outcome. Justification of this observation is found in the next section.

Dimerization process. The major product observed in the electrolysis experiments (see Experimental Results section above) is the dimeric compound azoxynitrobenzene (**4**). Therefore, we decided to evaluate the thermodynamics of its



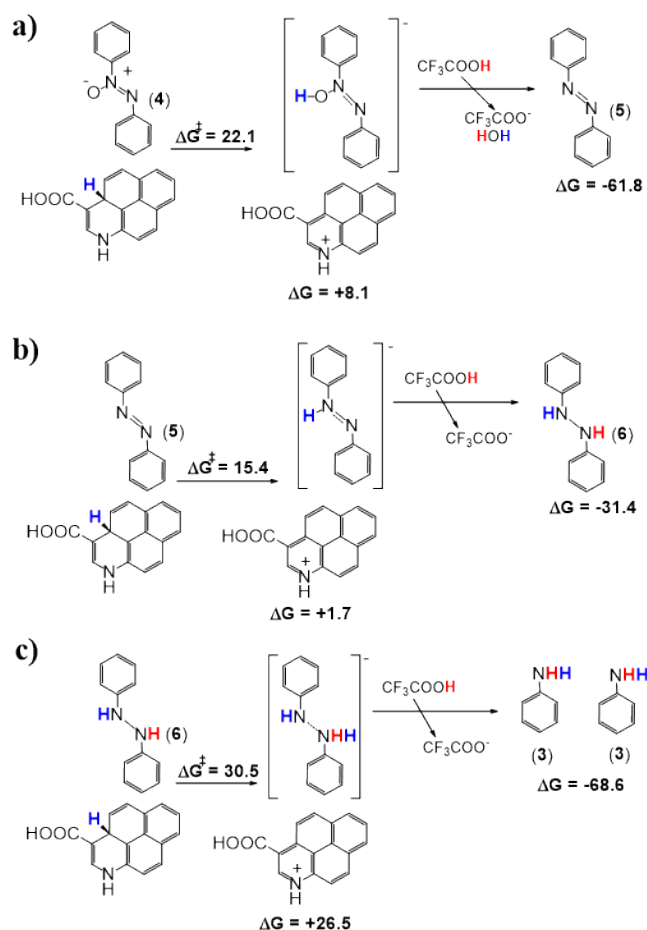
Scheme 4 Dimerization processes towards formation of azoxynitrobenzene (**4**) and azobenzene (**5**) (energy values are given in kcal mol⁻¹).

formation from the reaction of nitrosobenzene (**1**) and hydroxyaniline (**2**) intermediates. Effectively, condensation of such compounds is highly favoured, as it should be expected for the formation of a water molecule, which serves as an efficient driving force of the process (Scheme 4). Thus, while hydroxyaniline (**2**) is slowly being generated, it efficiently reacts with the excess of nitrosobenzene (**1**) to generate the main final product of this electrocatalytic system, azoxynitrobenzene (**4**).

Furthermore, formation of the diazo compound (**5**) that has been detected in residual amounts can be explained by the dimerization of two hydroxyaniline (**2**) molecules (Scheme 4). Considering that during the reaction, hydroxyaniline (**2**) coexists with an excess on nitrosobenzene (**1**), this alternative process is less probable in agreement with the residual amounts of such species experimentally detected. Finally, condensation of aniline and nitrosobenzene (**1**) could also account for the formation of the diazo compound (**5**), which could be responsible for the disappearance over time of aniline (**3**).

Summarising, dimerization processes require significant concentrations of monomeric species. Therefore, at short reaction times, when concentration of products is still low, direct formation of aniline is plausible through the three consecutive hydrogenation steps presented above. However, after longer times of electrolysis, concentration of products increases, and dimeric structures can appear through exothermic condensations. Thus, the amounts of aniline experimentally found have been firstly formed (Fig. 4) whereas dimeric products have been furtherly produced. The fact that the major product found is the azoxynitrobenzene (**4**) species, indicates that its hydrogenation is unfavourable as is demonstrated in the next section.

Evaluation of possible evolution of azoxynitrobenzene (4**).** The hydride transfer to azoxynitrobenzene (**4**) and to the other dimeric species (diphenyldiazene (**5**) and diphenylhydrazine (**6**)) involving the two catalytic systems are summarized in Schemes 5 and 6. With ox-CF, the hydride transfer to azoxynitrobenzene (**4**) (Scheme 5a) is endergonic ($\Delta G = +8.1$ kcal mol⁻¹) and the computed Gibbs energy barrier is $\Delta G^\ddagger = 22.1$ kcal mol⁻¹. These values indicate that the process is both kinetically and thermodynamically challenging and comparable with the first hydride transfer step. This suggests that azoxynitrobenzene (**4**) would hardly be hydrogenated, even though protonation of the resulting product to form a water molecule and the diazo compound is highly exergonic. Therefore, it agrees with the fact

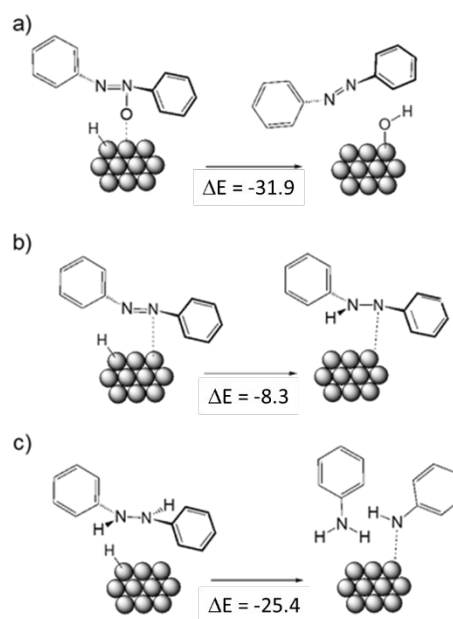


Scheme 5 Catalytic evolution of hydrogenation of azoxynitrobenzene towards a) the diazo compound, b) the diphenyl hydrazine product and c) aniline (energy values are given in kcal mol⁻¹).

that azoxynitrobenzene (**4**) is the major product of nitrobenzene hydrogenation. In addition, the small portions of diazo compound observed experimentally are likely formed by the dimerization processes.

The potential formation of aniline from the diazo compound (**5**) in presence of ox-CF has also been considered (Scheme 5b and 5c). The obtained results indicate that under the reaction conditions, diphenyldiazene (**5**) would easily evolve to diphenylhydrazine (**6**). Finally, the hydride transfer to this hydrazine derivative (**6**) intermediate leading to aniline formation is very endergonic ($\Delta G = +26.5$ kcal mol⁻¹) and kinetically hampered ($\Delta G^\ddagger = 30.5$ kcal mol⁻¹, Scheme 5c). Therefore, although further protonation is calculated to be very exothermic, hydrogenation of diphenylhydrazine (**6**) does not seem the path for the formation of aniline (**3**). Indeed, the observed aniline is expected to be formed by successive hydrogenation of PhNO₂ without dimerization, while the major dimeric product is azoxynitrobenzene (**4**), which presents a high hydride transfer Gibbs energy barrier.

The reactivity of azoxynitrobenzene (**4**) with the Ru-CF has also been explored, considering the thermodynamics of the three potential hydrogenation steps (Scheme 6a to 6c). Furthermore, the transition state for the hydride transfer to azoxynitrobenzene (**4**), which appeared to be a key step in the



Scheme 6 Azoxynitrobenzene conversion to aniline through three successive hydrogenation/protonation steps with Ru-NPs. Energies in kcal mol⁻¹

organocatalytic system, has also been calculated. Fig. 8 shows the optimized structures of azoxynitrobenzene (**4**), diphenyldiazene (**5**) and the transition state connecting these two intermediates.

The hydrogenation pathways found for azoxynitrobenzene (**4**) using Ru-CF are significantly different than those calculated for ox-CF. The resulting products (PhNNPh + Ru-NPs-OH) using Ru-CF are the consequence of the formation of a Ru-OH bond at the nanoparticle surface. Remarkably, despite the large exothermicity of the reaction ($\Delta E = -31.9$ kcal mol⁻¹), the computed energy barrier is high ($+24.9$ kcal mol⁻¹) due to the large electronic reorganization to favour the concerted formation/cleavage of the Ru...O and N...O bonds. Moreover, the two subsequent hydrogenation steps are thermodynamically favourable (Scheme 6), indicating that aniline formation from azoxynitrobenzene (**4**) is thermodynamically feasible. However, as in the case of ox-CF, this is not expected to be the main route for aniline formation. This is due to the large energy barrier of the hydride transfer to azoxynitrobenzene (**4**), which should be the major dimeric species, as found experimentally.

Summarizing, calculations on the evolution of azoxynitrobenzene (**4**) suggest that this species could hardly be

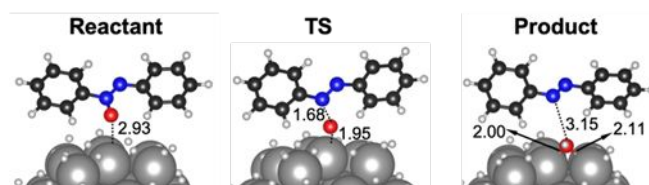
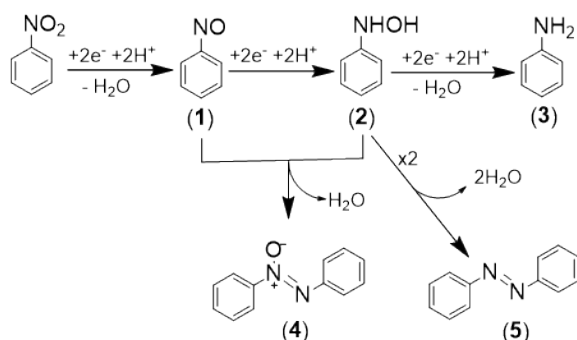


Fig. 8 Optimized structures for azoxynitrobenzene intermediate adsorbed on H₈₈Ru₅₇ nanoparticle, the diphenyldiazene resulting from its hydrogenation and the transition state connecting them. Distances in Å and energies in kcal mol⁻¹



Scheme 7 General scheme for the nitrobenzene reduction reaction proposed for the two electrocatalytic approaches studied.

reduced regardless the nature of the electrocatalyst. Thus, despite the different reactivity expected for ox-CF and Ru-CF, the chemical identity of the final products should not vary, being azoxynitrobenzene (4) the major product.

Overall, our calculations show a reaction mechanism for the nitrobenzene hydrogenation that is consistent with the experimental data. Despite the different reactivities observed for the two electrocatalysts for some particular steps, the mechanisms for the two systems share the main general issues, which are summarized in Scheme 7. First, nitrobenzene is hydrogenated following a first 2-electron and 2 proton transfer steps leading to the formation of nitrosobenzene (1), which is converted to hydroxylamine (2) following a further 2-electron and 2 protons reduction. While this species is being formed, two processes can occur: a) further hydrogenation until aniline product (3) (detected in low amounts) or b) condensation with nitrosobenzene (1) to produce azoxynitrobenzene (4) (observed as main product). This dimeric species can hardly be further reduced, appearing as the final product. In addition, residual amounts of diazo compound (5) found in the reaction outcome seems to be the result of dimerization of residual amounts of hydroxylamine (2). Controversially, according to our theoretical data, diazo species (5) should be easily reduced to hydrazine compound, which should accumulate because its further reduction is unfavourable. However, the known high reactivity of hydrazine compounds can account for its further evolution being impossible its detection under the working conditions.

Conclusions

Two electrocatalytic systems of very different nature result on comparable outputs for PhNO₂ hydrogenation, which is kinetically favoured with respect to HER. Combination of experimental results and DFT calculations indicates that HER is a more significant competitor when Ru-CF are used as catalyst.

The main product experimentally observed for nitrobenzene hydrogenation is the azoxynitrobenzene dimeric species, while aniline is formed in minor quantities during the first stages of the electrocatalytic process. According to DFT results, once the initial hydrogenation rate determining step occurs (from PhNO₂ to PhNO), successive hydrogenation steps to generate aniline (from PhNO to PhNH(OH) and from

PhNH(OH) to PhNH₂) are highly favoured. In parallel to aniline formation, dimeric azoxynitrobenzene compound is generated as a consequence of the highly favourable condensation of PhNO and PhNH(OH).

Overall, this work presents an in-depth understanding of the catalytic behaviour of an organic- and a metal-based material that have been previously used as electrocatalysts for HER. Furthermore, we have shown the efficient competition between hydrogenation of PhNO₂ with HER. Thus, the methodology reported herein can be applied to the electrochemical remediation of an important class of pollutants (nitro aryl compounds). In a more general perspective, these insights may contribute to the future designs of more efficient catalytic systems for hydrogen production, electrochemical waste-water treatments or use of hydrogenation/dehydrogenation based energetic vectors.

Conflicts of interest

There are no conflicts to declare.

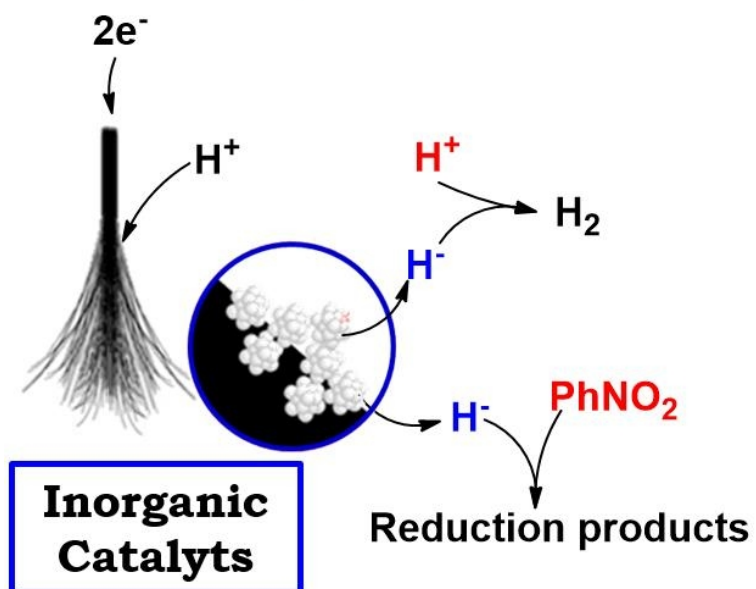
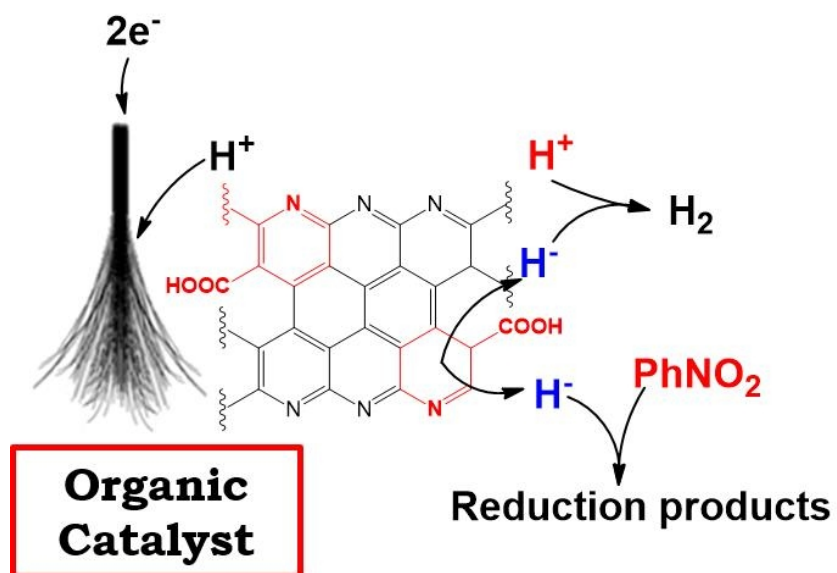
Acknowledgements

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179x260mm (96 x 96 DPI)

SUPPORTING INFORMATION**Organocatalytic vs Ru-based Electrochemical Hydrogenation of Nitrobenzene in Competition with Hydrogen Evolution Reaction**

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1. Experimental Results

1.1. Electrochemical Data

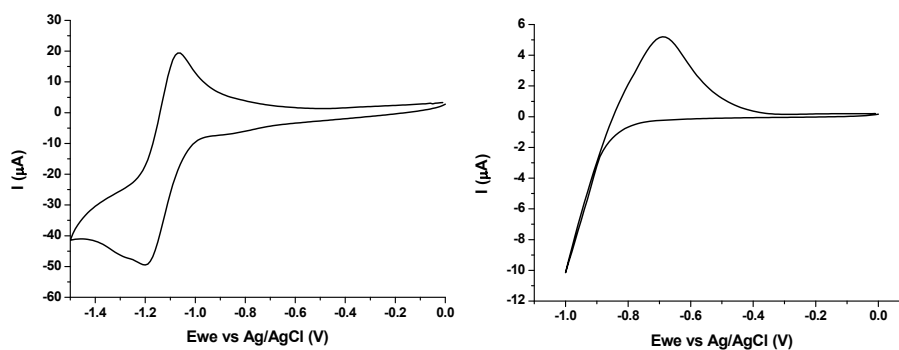


Fig. S1 Cyclic voltammetry of 10 mM of nitrobenzene at a scan rate of 50 mV/s and potential windows of -1.5 – 0 V (left) and -1 V – 0 V (right).

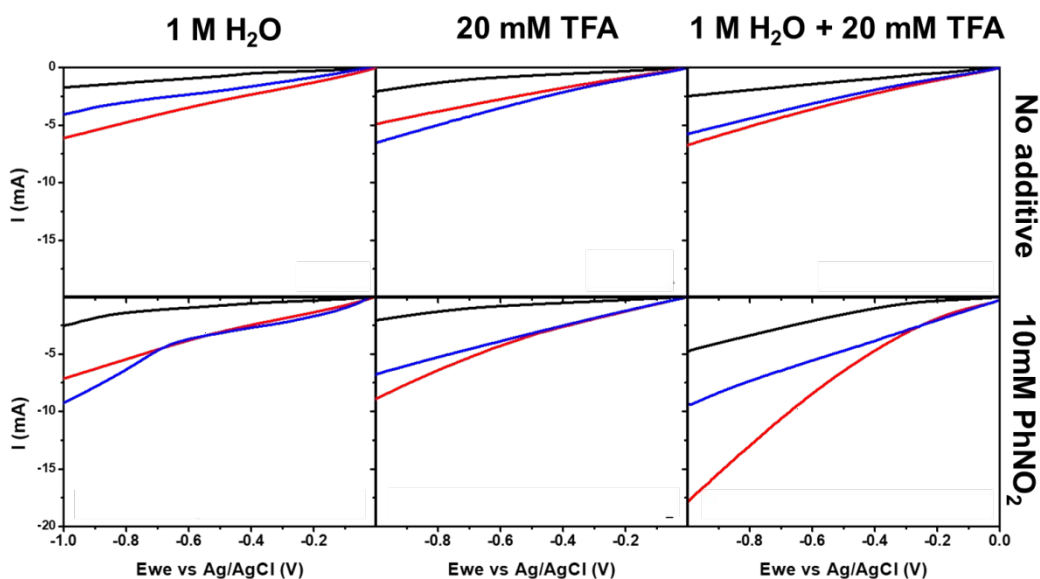
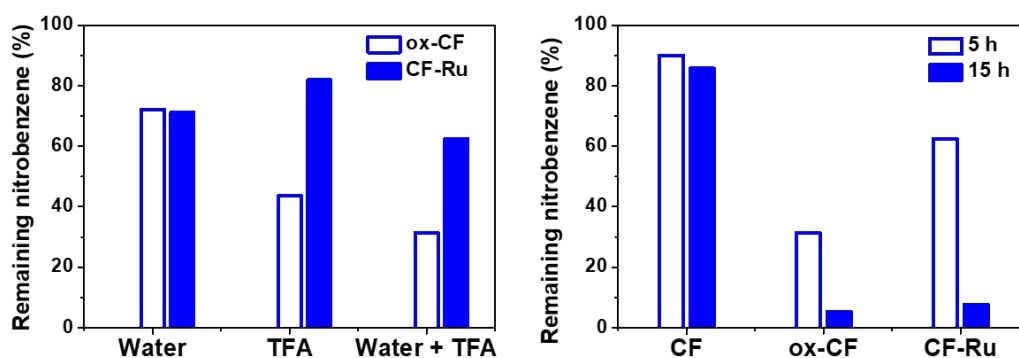


Fig. S2 Linear voltammetry measured using pristine (black), oxidised (red) and Ru-based (blue) carbon fibre electrodes in the absence (top) and in the presence (bottom) of 10 mM of nitrobenzene using as electrolyte: 0.2 M of NaClO_4 in CH_3CN with different proton sources: 1 M of H_2O (left), 20 mM of TFA (middle) and their mixture (right).

Table S1. Current intensities at -1 V vs Ag/AgCl corresponding to the linear sweep voltammeteries of Fig. S2.

[PhNO ₂] (mM)	Proton Source	I of CF (mA)	I of ox-CF (mA)	I of Ru-CF (mA)
0	1 M H ₂ O	-1.72	-6.13	-4.08
	20 mM TFA	-2.08	-4.92	-6.53
	1 M H ₂ O + 20 mM TFA	-2.48	-6.76	-5.77
10	1 M H ₂ O	-2.53	-7.14	-9.24
	20 mM TFA	-2.05	-8.93	-6.78
	1 M H ₂ O + 20 mM TFA	-4.85	-17.89	-9.31

**Fig. S3** Comparison of the electrocatalyst for the nitrobenzene conversion a) during 5 h electrolysis in solutions of 1 M of water, 20 mM of TFA and the mixture of both proton source and b) during electrolysis at 5- and 15-hour reaction using 1 M of water and 20 mM of TFA as proton source.

1.2. Chromatography Data

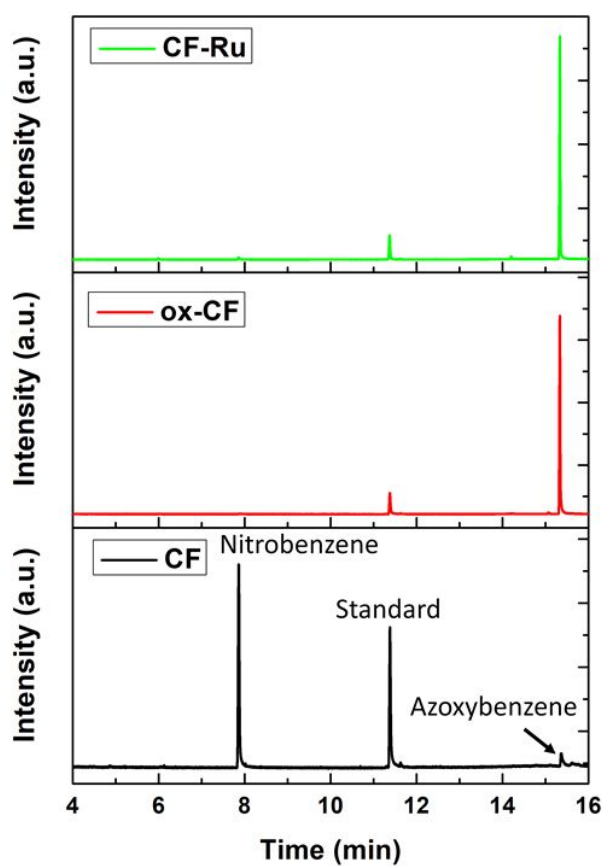


Fig. S4 Gas chromatograms of electrocatalytic nitrobenzene reduction using pristine carbon fibre (black curve), oxidised carbon fibre (red curve) and Ru-modified carbon fibre (green curve).

2. Computational Details

2.1. Adsorption Energies of Reagents on $H_{88}Ru_{57}$ NPs

Table S2. Adsorption energies (in kcal·mol⁻¹) of the different reagents on the $H_{88}Ru_{57}$ nanoparticle model.

Species	E_{ads}
PhNO ₂ (perpendicular)	-10.5
PhNO ₂ (parallel)	-10.6
CH ₃ COOH	-9.0
(H ₃ O)(H ₂ O) ₃ Cl	-3.3
PhNO	-18.0
PhNHOH	-8.4
PhNONPh	-10.8
PhNNPh	-11.1
PhNHNHPh	-8.8

2.2. Comparative Energy Data of ox-CF and Ru-CF catalyst models

Table S3 Electronic energies (in kcal·mol⁻¹) of the hydride transfer to PhNO₂ using ox-CF as catalyst.

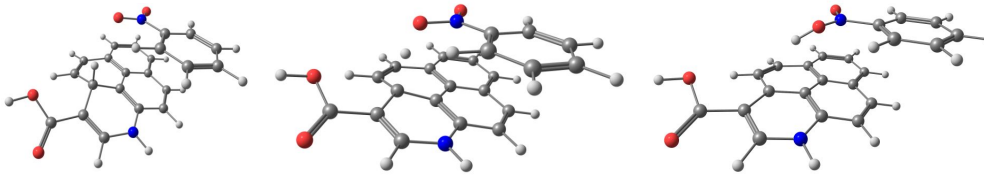
				
M062X	ΔG	0.0	$E_a = +23.5$	+3.6
	ΔE	0.0	$E_a = +25.5$	+5.7
PBE-D2	ΔG	0.0	$E_a = +7.0$	+0.6
	ΔE	0.0	$E_a = +8.7$	+1.0

Table S4 Electronic energies (in kcal·mol⁻¹) of the catalytic hydride transfer to PhNO₂ using Ru-CF catalyst model.

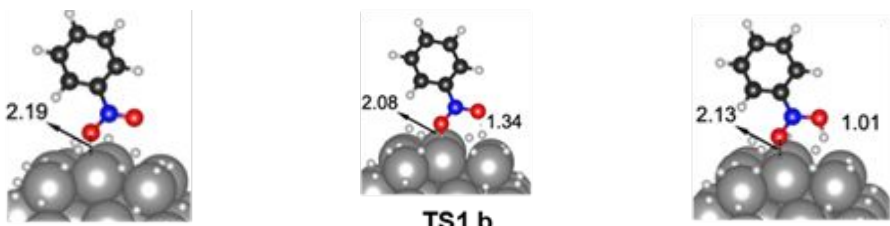
				
ΔE	0.0	$E_a = +10.8$	+4.3	

Table S5 Electronic energies (in kcal·mol⁻¹) of the catalytic hydride transfer to TFA using ox-CF catalyst model.

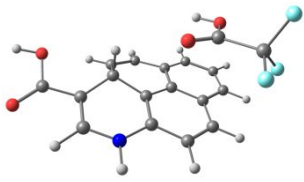
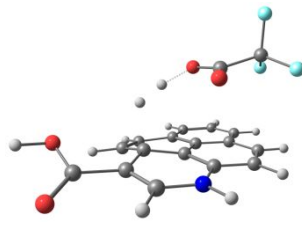
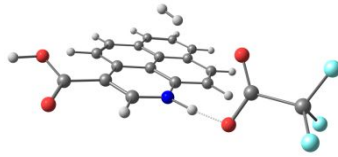
				
M062X	ΔG	0.0	$E_a = +31.2$	-12.4
	ΔE	0.0	$E_a = +38.7$	-3.9
PBE-D2	ΔG	0.0	$E_a = +19.2$	-18.3
	ΔE	0.0	$E_a = +23.7$	-10.7

Table S6 Electronic energies (in kcal·mol⁻¹) of the catalytic hydride transfer to TFA using Ru-CF catalyst model.

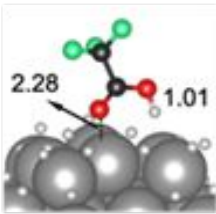
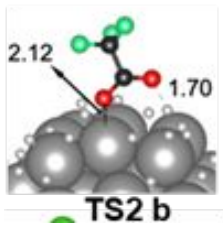
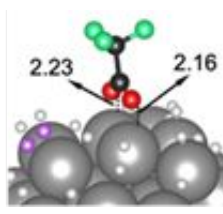
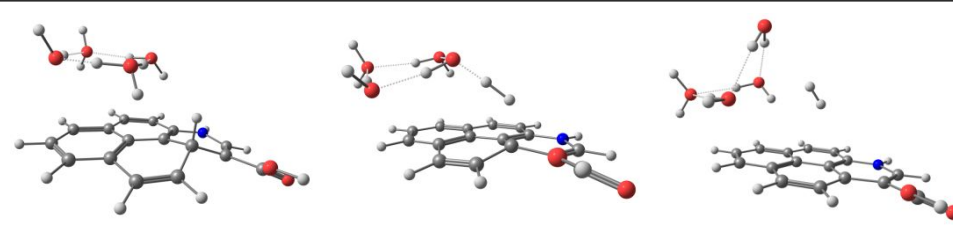
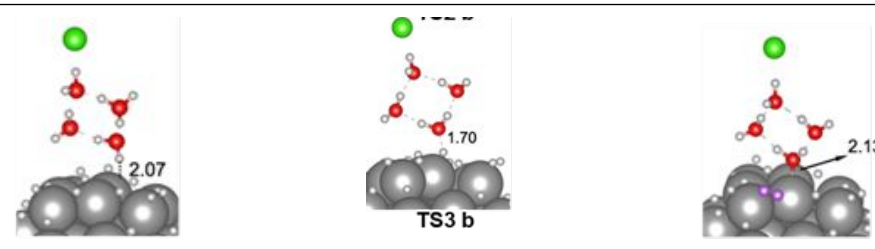
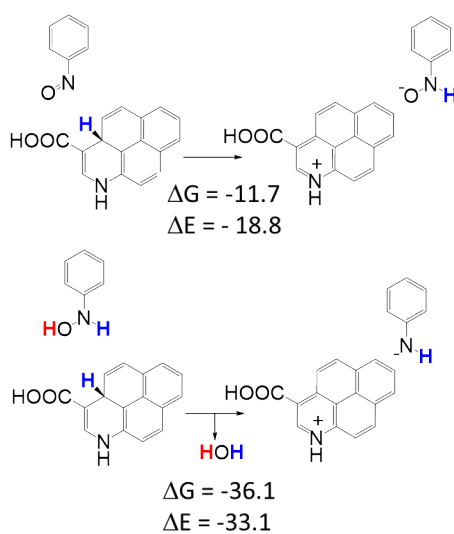
				
ΔE	0.0	$E_a = +17.0$	+7.3	

Table S7 Electronic energies (in kcal·mol⁻¹) of the catalytic hydride transfer to [(H₃O)(H₂O)₃]⁺ using ox-CF catalyst model.


M062X	ΔG	0.0	$E_a = +35.1$	-6.2
	ΔE	0.0	$E_a = +40.1$	+0.7
PBE-D2	ΔG	0.0	$E_a = +19.2$	-6.0
	ΔE	0.0	$E_a = +23.7$	-0.3

Table S8 Electronic energies (in kcal·mol⁻¹) of the catalytic hydride transfer to [(H₃O)(H₂O)₃]⁺ using Ru-CF catalyst model.


ΔE	0.0	$E_a = +24.9$	+1.5
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**Fig. S5** Catalytic hydrogenation of PhNO using ox-CF (M062X). Energy values are in kcal·mol⁻¹.

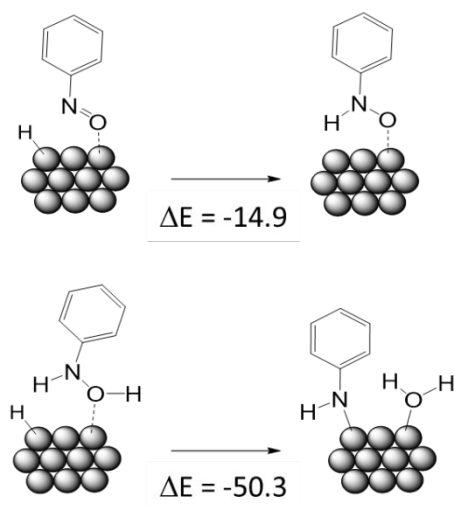


Fig. S6 Catalytic hydrogenation of PhNO using Ru-CF. Energy values are in kcal·mol⁻¹.

Table S9 Electronic energies (in kcal·mol⁻¹) of the catalytic hydrogenation of azoxynitrobenzene using ox-CF catalyst model.

M062X	ΔG	0.0	$E_a = +22.1$	+8.1
	ΔE	0.0	$E_a = +23.2$	+8.1
PBE-D2	ΔG	0.0	$E_a = +6.7$	+0.8
	ΔE	0.0	$E_a = +8.2$	+0.5

Table S10 Electronic energies (in kcal·mol⁻¹) of the catalytic hydrogenation of azoxynitrobenzene using Ru-CF catalyst model.

ΔE	0.0	$E_a = +24.9$	-31.9

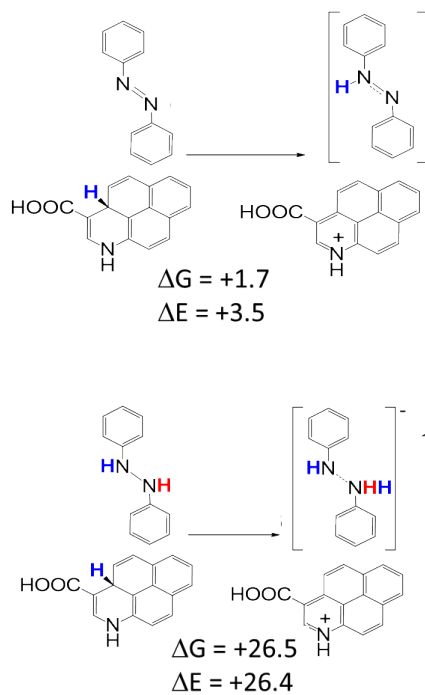


Fig. S7 Catalytic hydrogenation of PhNONPh using ox-CF (M062X). Energy values are in $\text{kcal}\cdot\text{mol}^{-1}$.

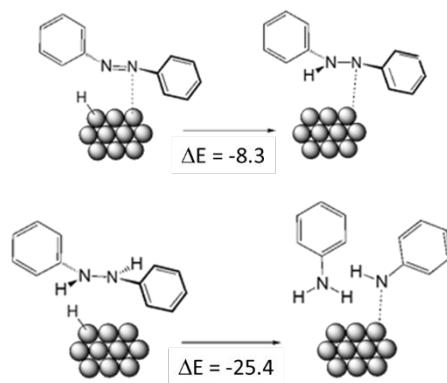
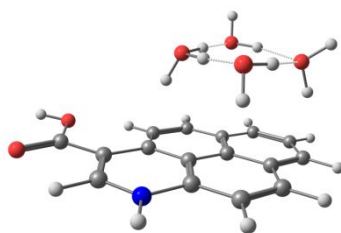


Fig. S8 Catalytic hydrogenation of PhNONPh using Ru-CF. Energy values are in $\text{kcal}\cdot\text{mol}^{-1}$.

2.3. M062X optimized geometries associated with the Organic Catalyst: ox-CF

2.3.1. Hydride generation

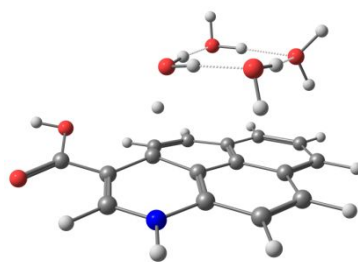


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1126.899548

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6	-2.595785000	-1.302848000	-1.658548000
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6	-0.953892000	0.357371000	-0.866327000
6	-2.009493000	1.331717000	-0.753872000
6	-3.338805000	0.947485000	-1.112017000
6	-0.188081000	-1.888391000	-1.428716000
6	0.393117000	0.705778000	-0.529587000
6	1.449916000	-0.266175000	-0.613273000
6	1.118998000	-1.533745000	-1.088456000
6	2.807565000	0.190953000	-0.194265000
6	2.974853000	1.500925000	0.169501000
6	0.642336000	2.032713000	-0.093979000
6	-1.692267000	2.619636000	-0.285161000
1	-2.479405000	3.358399000	-0.184978000
1	-0.392738000	-2.893767000	-1.780345000
1	-4.610827000	-0.614058000	-1.832913000
1	-2.819883000	-2.307898000	-1.997698000
1	-4.130562000	1.686677000	-1.060340000
1	1.891555000	-2.281924000	-1.189906000
1	3.949283000	1.871548000	0.462140000
6	4.011287000	-0.610169000	-0.075692000
8	5.124730000	-0.186982000	0.216218000
8	3.837642000	-1.928485000	-0.296617000
1	4.698415000	-2.358711000	-0.180157000
7	1.979618000	2.388054000	0.204788000
1	2.172335000	3.338174000	0.491523000
1	-0.135066000	3.960957000	0.372634000
8	0.028101000	-1.427358000	1.887076000
1	-0.363687000	-0.479335000	2.131687000
1	-0.798205000	-2.038326000	1.658089000
1	0.577844000	-1.337464000	1.082355000
8	-1.070542000	0.719546000	2.473224000
1	-0.821376000	1.465711000	1.907556000

1	-1.996439000	0.496722000	2.235194000
8	-2.030431000	-2.712436000	1.372533000
1	-2.689958000	-1.990374000	1.453661000
1	-2.249558000	-3.357019000	2.056539000
8	-3.416583000	-0.375309000	1.644698000
1	-3.598648000	0.004258000	0.763646000
1	-4.243915000	-0.313826000	2.136727000
6	-0.376194000	2.958818000	0.030075000



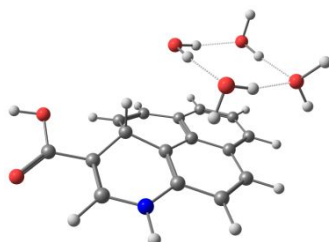
(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1126.891048

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6	-1.075593000	0.399892000	-0.796257000
6	-2.140672000	1.335993000	-0.613762000
6	-3.473996000	0.932294000	-0.933476000
6	-0.234512000	-1.766340000	-1.638984000
6	0.263483000	0.754856000	-0.463751000
6	1.322268000	-0.262111000	-0.487551000
6	1.032629000	-1.430619000	-1.272673000
6	2.709565000	0.279465000	-0.277426000
6	2.875769000	1.587927000	0.051654000
6	0.511561000	2.064913000	-0.047229000
6	-1.837996000	2.623688000	-0.129027000
1	-2.638591000	3.339420000	0.019705000
1	-0.430865000	-2.705343000	-2.144373000
1	-4.732676000	-0.621659000	-1.667248000
1	-2.878481000	-2.227454000	-2.047712000
1	-4.282350000	1.641142000	-0.789615000
1	1.840978000	-2.114843000	-1.498915000
1	3.861158000	1.992016000	0.248637000
6	3.914647000	-0.527318000	-0.186732000
8	5.061317000	-0.105377000	-0.122635000
8	3.676513000	-1.853490000	-0.140928000
1	4.530901000	-2.304921000	-0.063424000
7	1.848552000	2.449957000	0.203088000
1	2.039886000	3.414466000	0.433379000
1	-0.285527000	3.988796000	0.457777000
8	0.551116000	-1.303114000	1.804298000
1	0.031854000	-0.543371000	2.196031000
1	-0.132836000	-2.006293000	1.592561000
1	0.956020000	-0.891462000	0.770262000
8	-1.037349000	0.639601000	2.620212000
1	-0.930309000	1.433656000	2.080222000
1	-1.872145000	0.232209000	2.316099000

8	-1.409732000	-2.946229000	1.230398000
1	-2.139835000	-2.308256000	1.351157000
1	-1.548238000	-3.622406000	1.903684000
8	-3.157985000	-0.857681000	1.702704000
1	-3.547543000	-0.475893000	0.900967000
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6	-0.525791000	2.984439000	0.122465000

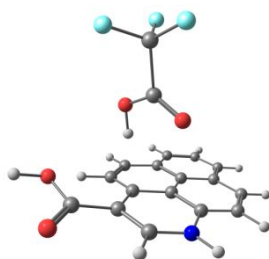


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6	-0.910754000	-1.373256000	-1.181258000
6	-0.752882000	0.012377000	-0.864393000
6	-1.838688000	0.900892000	-1.072175000
6	-3.094415000	0.377058000	-1.480212000
6	0.287262000	-2.213028000	-1.186007000
6	0.506212000	0.500641000	-0.432778000
6	1.577196000	-0.473822000	0.040672000
6	1.455966000	-1.789137000	-0.699704000
6	2.940467000	0.196849000	-0.025737000
6	3.044082000	1.547343000	-0.060262000
6	0.698618000	1.867081000	-0.383040000
6	-1.621317000	2.292276000	-0.896540000
1	-2.448521000	2.979470000	-1.039658000
1	0.204911000	-3.192754000	-1.646870000
1	-4.202402000	-1.359426000	-2.032849000
1	-2.251632000	-2.886542000	-1.850359000
1	-3.925384000	1.062487000	-1.616248000
1	2.329609000	-2.425420000	-0.756139000
1	4.009562000	2.035241000	-0.007959000
6	4.189707000	-0.516600000	0.229005000
8	5.311307000	-0.065165000	0.078697000
8	3.999903000	-1.754096000	0.716830000
1	4.868660000	-2.151962000	0.882329000
7	1.971173000	2.371339000	-0.113775000
1	2.118423000	3.369993000	-0.168142000
1	-0.185590000	3.833683000	-0.515914000

1	1.354105000	-0.707683000	1.095570000
8	-0.815036000	-1.698306000	2.077402000
1	-0.798673000	-0.737398000	2.227300000
1	-1.704979000	-1.844833000	1.715919000
8	-1.076292000	1.087485000	2.376693000
1	-0.501645000	1.556474000	1.762110000
1	-1.968849000	1.163626000	1.993471000
8	-3.572747000	-1.761900000	1.392010000
1	-3.664078000	-0.793611000	1.345153000
1	-3.893761000	-1.986057000	2.272658000
8	-3.739235000	1.048211000	1.559797000
1	-4.047063000	1.560040000	0.802358000
1	-4.312277000	1.306469000	2.292046000
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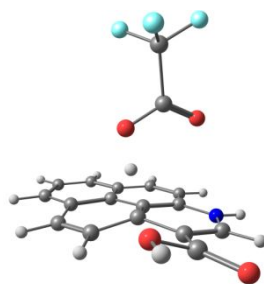


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Sum of electronic and thermal Free Energies= -1347.558819

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6	-2.525992000	-0.297639000	-1.559435000
6	-2.381704000	-0.047747000	-0.148852000
6	-3.298852000	-0.645225000	0.785528000
6	-4.323169000	-1.502039000	0.285854000
6	-1.628175000	0.344329000	-2.442622000
6	-1.333817000	0.807558000	0.315433000
6	-0.389597000	1.381252000	-0.607475000
6	-0.603562000	1.159556000	-1.969006000
6	0.704039000	2.205928000	-0.011482000
6	0.681886000	2.447835000	1.337168000
6	-1.262193000	1.070788000	1.703101000
6	-3.151351000	-0.357461000	2.157479000
1	-3.837555000	-0.801799000	2.870005000
1	-1.739418000	0.188614000	-3.510287000
1	-5.214157000	-2.399684000	-1.432699000
1	-3.667422000	-1.361126000	-3.056856000
1	-5.015724000	-1.954487000	0.987390000
1	0.059997000	1.618688000	-2.689084000

1	1.456658000	3.044449000	1.802959000
6	1.897685000	2.680539000	-0.679056000
8	2.741237000	3.431832000	-0.198291000
8	2.065552000	2.206472000	-1.932425000
1	2.897270000	2.571615000	-2.270202000
7	-0.249932000	1.956731000	2.155748000
1	-0.189148000	2.151731000	3.145598000
1	-2.047530000	0.729874000	3.654863000
6	-2.147756000	0.498724000	2.598088000
6	1.931286000	-1.200899000	0.274719000
8	1.515208000	-0.778521000	1.315317000
8	1.549476000	-0.893513000	-0.938781000
1	0.825690000	-0.218199000	-0.922956000
6	3.057188000	-2.248401000	0.217725000
9	3.471920000	-2.558439000	1.438811000
9	2.632140000	-3.363171000	-0.380019000
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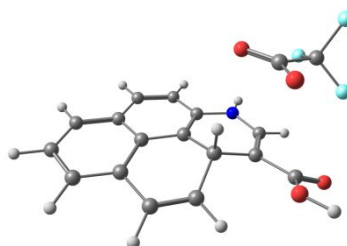
(Transition state)

Charge = -1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1347.554150

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6	-2.275807000	0.010669000	-0.141849000
6	-3.210346000	-0.575812000	0.767589000
6	-4.256631000	-1.394051000	0.245655000
6	-1.572970000	0.558300000	-2.447733000
6	-1.192020000	0.798057000	0.343872000
6	-0.155631000	1.275164000	-0.578769000
6	-0.522363000	1.280039000	-1.967098000
6	0.833888000	2.229540000	0.032544000
6	0.784942000	2.480143000	1.369911000
6	-1.137412000	1.061760000	1.714240000
6	-3.068867000	-0.319859000	2.146912000
1	-3.771298000	-0.761542000	2.845153000
1	-1.763934000	0.508441000	-3.514123000
1	-5.174747000	-2.211290000	-1.491898000
1	-3.625719000	-1.106635000	-3.082292000
1	-4.953290000	-1.853931000	0.938709000
1	0.118166000	1.800419000	-2.668764000
1	1.520524000	3.121176000	1.840346000
6	2.013200000	2.743558000	-0.637269000
8	2.797626000	3.572157000	-0.190995000
8	2.227086000	2.199401000	-1.853767000
1	3.039358000	2.589056000	-2.210894000
7	-0.129373000	1.933147000	2.193122000
1	-0.103283000	2.150304000	3.178805000
1	-1.969103000	0.734868000	3.660468000
6	-2.059709000	0.506231000	2.602752000
6	1.819141000	-1.251221000	0.307914000
8	1.652401000	-0.771818000	1.408338000
8	1.314129000	-0.898307000	-0.814974000
1	0.645330000	0.059707000	-0.711833000
6	2.759628000	-2.463094000	0.141808000
9	3.310290000	-2.822204000	1.298762000

9	2.095552000	-3.518554000	-0.343395000
9	3.748628000	-2.183803000	-0.715664000

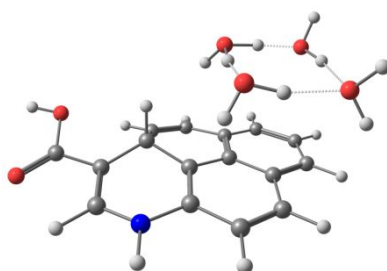


Charge = -1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1347.592203

6	-5.309173000	0.050073000	-0.902684000
6	-4.507335000	1.213690000	-0.901333000
6	-3.201004000	1.173806000	-0.466227000
6	-2.647472000	-0.066409000	-0.017421000
6	-3.484709000	-1.209222000	0.074215000
6	-4.817013000	-1.130698000	-0.407159000
6	-2.391952000	2.382832000	-0.297522000
6	-1.295613000	-0.126483000	0.401097000
6	-0.348185000	1.012839000	0.047319000
6	-1.095441000	2.329744000	0.017635000
6	0.865978000	0.964709000	0.960075000
6	1.183471000	-0.168878000	1.634205000
6	-0.858316000	-1.261992000	1.051541000
6	-2.959516000	-2.387355000	0.666321000
1	-3.587225000	-3.269653000	0.731652000
1	-2.898451000	3.338484000	-0.394099000
1	-6.328791000	0.105745000	-1.266286000
1	-4.931244000	2.159320000	-1.224067000
1	-5.440632000	-2.017739000	-0.364173000
1	-0.534897000	3.242371000	0.176261000
1	2.100700000	-0.237397000	2.206704000
6	1.890231000	2.006990000	0.972333000
8	2.801393000	2.098940000	1.775872000
8	1.765426000	2.882826000	-0.038037000
1	2.491040000	3.523081000	0.024727000
7	0.414685000	-1.280625000	1.616834000
1	0.722063000	-2.106009000	2.111894000
1	-1.297221000	-3.284519000	1.669389000
6	-1.691832000	-2.401793000	1.177162000
6	2.157161000	-0.556463000	-1.472858000
8	1.222333000	-1.367550000	-1.530283000
8	2.291475000	0.563199000	-1.989958000
1	-0.004406000	0.839073000	-0.987217000
6	3.396438000	-1.020470000	-0.657291000
9	3.124355000	-2.005888000	0.210120000
9	4.356069000	-1.482761000	-1.482378000
9	3.947014000	-0.019931000	0.047832000

2.3.2. *Hydrogen Evolution Reaction*

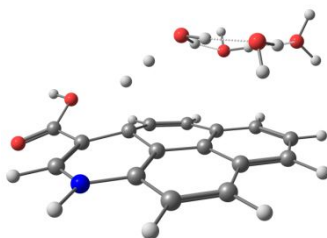


Charge = 1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1127.359239

6	3.194606000	0.920883000	-1.783206000
6	2.096804000	1.801067000	-1.657893000
6	0.870030000	1.346433000	-1.226881000
6	0.707598000	-0.034422000	-0.893486000
6	1.789979000	-0.929198000	-1.092642000
6	3.042859000	-0.416726000	-1.520933000
6	-0.323256000	2.195454000	-1.217062000
6	-0.547455000	-0.511644000	-0.436994000
6	-1.605611000	0.472013000	0.045127000
6	-1.486654000	1.783733000	-0.704541000
6	-2.973044000	-0.190528000	0.002641000
6	-3.082544000	-1.540817000	-0.011751000
6	-0.743158000	-1.876102000	-0.358831000
6	1.571126000	-2.316393000	-0.885413000
1	2.395522000	-3.008131000	-1.022105000
1	-0.243316000	3.170599000	-1.687767000
1	4.151979000	1.306163000	-2.114333000
1	2.211782000	2.846003000	-1.926771000
1	3.869587000	-1.107663000	-1.654586000
1	-2.357005000	2.425098000	-0.752157000
1	-4.049433000	-2.023516000	0.059534000
6	-4.215050000	0.534054000	0.264631000
8	-5.340063000	0.089020000	0.128334000
8	-4.010399000	1.772805000	0.743475000
1	-4.874241000	2.179521000	0.913824000
7	-2.013406000	-2.370010000	-0.066318000
1	-2.165119000	-3.369094000	-0.099254000
1	0.136769000	-3.846761000	-0.459018000
1	-1.373531000	0.707854000	1.100130000
8	1.205379000	1.582739000	2.022991000
1	1.046153000	0.550126000	2.111264000
1	2.227981000	1.693071000	1.724844000
1	0.625610000	1.956284000	1.342106000

8	1.103781000	-0.882671000	2.298845000
1	0.465048000	-1.385525000	1.777830000
1	1.990626000	-1.142816000	1.973272000
8	3.570469000	1.656953000	1.372251000
1	3.803085000	0.703947000	1.368559000
1	4.120294000	2.068550000	2.051078000
8	3.731466000	-1.078408000	1.554265000
1	4.006183000	-1.594673000	0.785987000
1	4.286923000	-1.385059000	2.282241000
6	0.326083000	-2.784043000	-0.568057000



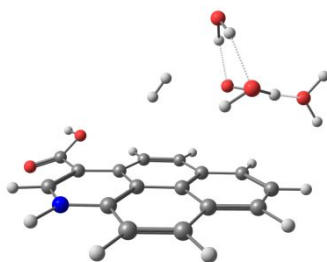
(Transition state)

Charge = 1 Multiplicity =1

Sum of electronic and thermal Free Energies= -1127.303289

6	-3.306205000	0.898714000	-1.264807000
6	-2.516572000	-0.240240000	-1.481535000
6	-1.170108000	-0.243214000	-1.149303000
6	-0.598118000	0.915252000	-0.560946000
6	-1.383359000	2.081374000	-0.387881000
6	-2.748380000	2.048100000	-0.743483000
6	-0.292860000	-1.351360000	-1.474004000
6	0.773668000	0.917254000	-0.194911000
6	1.541195000	-0.325016000	-0.228952000
6	0.993340000	-1.384127000	-1.087037000
6	2.971337000	-0.155562000	-0.040929000
6	3.466604000	1.050988000	0.371266000
6	1.338489000	2.097116000	0.276181000
6	-0.763925000	3.255614000	0.136305000
1	-1.367193000	4.146801000	0.271629000
1	-0.701521000	-2.159257000	-2.070565000
1	-4.356248000	0.881175000	-1.533110000
1	-2.951931000	-1.126617000	-1.931339000
1	-3.348305000	2.940720000	-0.601591000
1	1.630211000	-2.213872000	-1.355842000
1	4.521404000	1.190422000	0.569855000
6	3.955488000	-1.256287000	-0.078810000
8	5.151912000	-1.093831000	-0.169533000
8	3.399775000	-2.460440000	0.058969000
1	4.099633000	-3.133680000	0.042786000
7	2.679266000	2.117434000	0.570039000
1	3.096570000	2.985032000	0.892815000
1	1.042778000	4.168603000	0.823844000
1	1.168503000	-0.961399000	1.159693000
8	-0.831163000	-1.737605000	1.789056000
1	-1.446716000	-0.964472000	1.903826000
1	-1.245557000	-2.290163000	1.079220000
1	0.339345000	-1.297377000	1.450650000
8	-2.684866000	0.137087000	2.031812000

1	-2.512178000	0.999643000	1.638169000
1	-3.396711000	-0.261307000	1.496705000
8	-2.334637000	-3.088181000	0.019694000
1	-3.159367000	-2.598532000	0.200792000
1	-2.501491000	-3.986231000	0.327953000
8	-4.504713000	-1.460522000	0.670265000
1	-5.050372000	-1.140789000	-0.058247000
1	-5.122157000	-1.870122000	1.288915000
6	0.562069000	3.274280000	0.444090000

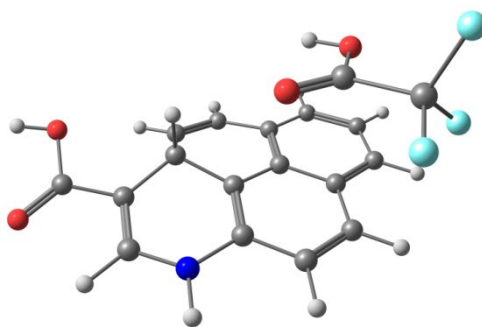


Charge = 1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1127.369125

6	-2.934456000	1.372643000	-1.410944000
6	-2.249943000	0.201095000	-1.712355000
6	-0.918628000	0.033173000	-1.311457000
6	-0.280841000	1.064318000	-0.583662000
6	-0.982481000	2.256834000	-0.277820000
6	-2.310626000	2.390393000	-0.698228000
6	-0.172334000	-1.149053000	-1.612020000
6	1.065345000	0.896587000	-0.164112000
6	1.782552000	-0.300775000	-0.450167000
6	1.116979000	-1.314567000	-1.210350000
6	3.120482000	-0.385511000	0.023830000
6	3.669962000	0.682944000	0.695231000
6	1.674207000	1.948602000	0.551221000
6	-0.312491000	3.289078000	0.454697000
1	-0.858381000	4.197789000	0.683824000
1	-0.661702000	-1.931325000	-2.182105000
1	-3.964316000	1.491411000	-1.726082000
1	-2.737075000	-0.595045000	-2.265173000
1	-2.849746000	3.299689000	-0.456271000
1	1.645318000	-2.218931000	-1.466934000
1	4.687805000	0.670814000	1.060176000
6	4.047579000	-1.548653000	-0.123057000
8	5.246828000	-1.433389000	-0.054455000
8	3.433684000	-2.711741000	-0.288583000
1	4.100560000	-3.413694000	-0.371905000
7	2.960436000	1.789563000	0.942917000
1	3.407777000	2.549146000	1.454372000
1	1.493623000	3.926377000	1.408053000
1	-0.154364000	-1.198218000	1.484765000
8	-2.866499000	-2.484807000	2.759454000
1	-3.002174000	-1.531320000	2.639756000
1	-2.769648000	-2.777609000	1.838198000
1	-0.739737000	-1.523033000	1.807908000
8	-3.092628000	0.118656000	1.653903000
1	-2.248382000	-0.012217000	1.206079000
1	-3.753906000	-0.140538000	0.988744000

8	-2.690910000	-2.672358000	-0.038143000
1	-3.504147000	-2.159737000	-0.193746000
1	-2.818821000	-3.500588000	-0.512745000
8	-4.891704000	-0.979963000	-0.198967000
1	-5.153187000	-0.543880000	-1.018196000
1	-5.708396000	-1.321851000	0.184147000
6	0.977309000	3.148661000	0.857698000

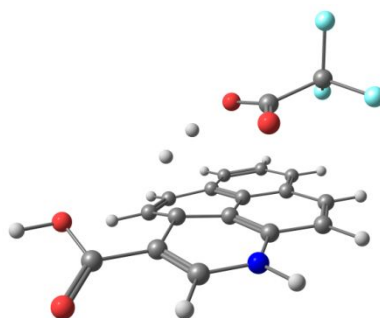


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1348.026567

6	2.168104000	-3.043656000	0.695892000
6	0.928822000	-3.325295000	0.077192000
6	-0.083694000	-2.390863000	0.060046000
6	0.130680000	-1.111087000	0.662805000
6	1.348388000	-0.859868000	1.348833000
6	2.367596000	-1.847049000	1.334645000
6	-1.428367000	-2.693376000	-0.434944000
6	-0.878513000	-0.120671000	0.598793000
6	-2.039695000	-0.283401000	-0.373443000
6	-2.363718000	-1.750077000	-0.569715000
6	-3.196631000	0.599369000	0.071144000
6	-2.971086000	1.667975000	0.871794000
6	-0.716043000	1.034703000	1.335957000
6	1.505957000	0.383707000	2.015726000
1	2.439303000	0.593674000	2.526927000
1	-1.656341000	-3.732339000	-0.653233000
1	2.951427000	-3.792665000	0.683988000
1	0.758818000	-4.300617000	-0.367702000
1	3.304876000	-1.634054000	1.837643000
1	-3.358317000	-2.012545000	-0.904536000
1	-3.768556000	2.360495000	1.110621000
6	-4.536382000	0.543714000	-0.520966000
8	-5.513926000	1.138653000	-0.123153000
8	-4.589835000	-0.220398000	-1.631366000
1	-5.501261000	-0.184239000	-1.962113000
7	-1.753464000	1.963273000	1.387924000
1	-1.656621000	2.764040000	1.997118000
1	0.585108000	2.232155000	2.574125000
1	-1.680270000	0.080612000	-1.352173000
6	0.485826000	1.294096000	2.037996000
6	3.236917000	1.344141000	-0.778048000
9	2.908926000	2.475450000	-0.168433000
9	3.904859000	0.575964000	0.081258000
9	4.061894000	1.635063000	-1.788957000
6	1.979885000	0.642234000	-1.324546000

8	0.931546000	1.201210000	-1.426963000
8	2.280650000	-0.589547000	-1.689400000
1	1.479225000	-1.042646000	-2.008855000



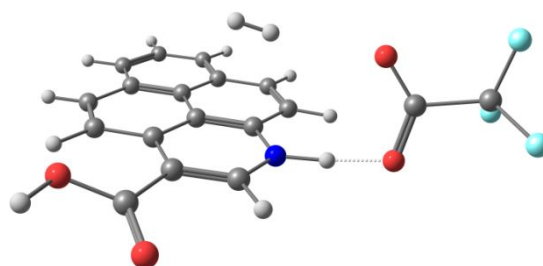
(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1347.974330

6	-2.256312000	3.582511000	-0.066897000
6	-0.976696000	3.674389000	-0.629124000
6	-0.025099000	2.690714000	-0.392330000
6	-0.359230000	1.588539000	0.435558000
6	-1.636948000	1.519317000	1.038972000
6	-2.581753000	2.525063000	0.760284000
6	1.328948000	2.780501000	-0.900110000
6	0.598264000	0.565415000	0.669886000
6	1.824278000	0.518578000	-0.114509000
6	2.215920000	1.780314000	-0.755220000
6	2.798783000	-0.453146000	0.342635000
6	2.446826000	-1.377091000	1.288837000
6	0.288131000	-0.444955000	1.575691000
6	-1.927835000	0.426117000	1.911872000
1	-2.915007000	0.364052000	2.357008000
1	1.621350000	3.695563000	-1.404521000
1	-2.988202000	4.354695000	-0.271416000
1	-0.715652000	4.523487000	-1.251936000
1	-3.566305000	2.457852000	1.210526000
1	3.217943000	1.871690000	-1.146157000
1	3.140324000	-2.142128000	1.611997000
6	4.136975000	-0.660272000	-0.253743000
8	5.017302000	-1.303822000	0.261194000
8	4.265940000	-0.104379000	-1.465172000
1	5.158668000	-0.304772000	-1.791847000
7	1.234037000	-1.392160000	1.856577000
1	1.007845000	-2.126808000	2.519286000
1	-1.197804000	-1.342400000	2.867616000
1	1.319304000	-0.187638000	-1.491678000
6	-0.989412000	-0.517534000	2.195991000
6	-2.642572000	-1.854140000	-0.772407000
9	-2.928734000	-2.551789000	0.329316000
9	-3.275893000	-0.680040000	-0.683582000

9	-3.177647000	-2.513951000	-1.813885000
6	-1.114858000	-1.700826000	-0.978254000
8	-0.384138000	-2.521308000	-0.463744000
8	-0.831896000	-0.709077000	-1.727110000
1	0.417620000	-0.458724000	-1.675684000



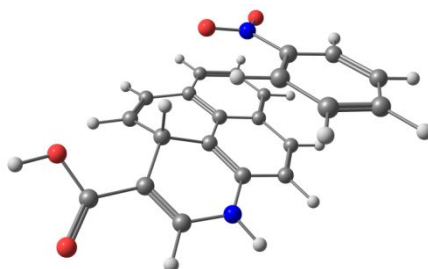
Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1348.045083

6	-3.970466000	-3.572466000	-0.190061000
6	-4.541824000	-2.311593000	-0.314733000
6	-3.756858000	-1.160767000	-0.183448000
6	-2.374064000	-1.292184000	0.080364000
6	-1.795863000	-2.579215000	0.211022000
6	-2.611137000	-3.707499000	0.070221000
6	-4.303886000	0.157398000	-0.299015000
6	-1.569448000	-0.127980000	0.214399000
6	-2.126228000	1.174668000	0.063855000
6	-3.537331000	1.273122000	-0.183077000
6	-1.238880000	2.273051000	0.198472000
6	0.092010000	2.032135000	0.492194000
6	-0.195300000	-0.289217000	0.494976000
6	-0.392612000	-2.687116000	0.488697000
1	0.037572000	-3.677538000	0.590134000
1	-5.368680000	0.254338000	-0.483604000
1	-4.588081000	-4.456348000	-0.293438000
1	-5.602487000	-2.206026000	-0.515162000
1	-2.167300000	-4.692207000	0.169463000
1	-3.993867000	2.245284000	-0.275976000
1	0.795693000	2.847177000	0.605361000
6	-1.570140000	3.722091000	0.046552000
8	-0.859893000	4.602127000	0.457516000
8	-2.700897000	3.958498000	-0.620128000
1	-2.824778000	4.921606000	-0.672054000
7	0.581439000	0.803741000	0.634978000
1	1.687867000	0.656894000	0.779605000
1	1.443813000	-1.662235000	0.857078000
1	0.007992000	0.726076000	-2.442134000
6	0.387360000	-1.586097000	0.630443000
6	4.970150000	-0.461091000	-0.189842000
9	5.746134000	0.516401000	0.300740000
9	5.129357000	-1.526912000	0.613811000
9	5.455913000	-0.792492000	-1.387891000

6	3.482466000	-0.039299000	-0.243452000
8	3.071975000	0.394467000	0.871573000
8	2.883951000	-0.186695000	-1.296082000
1	0.670767000	0.589001000	-2.132482000

2.3.3. *Hydride Transfer processes*

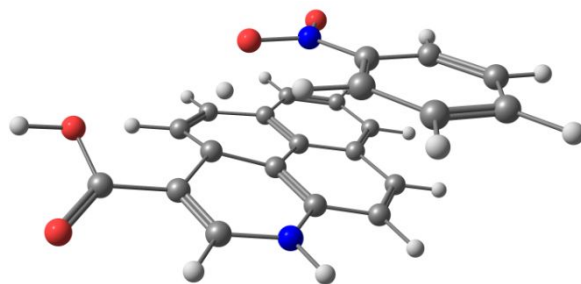


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1257.874819

6	-2.466094000	3.215396000	0.753161000
6	-1.221471000	3.491054000	0.142834000
6	-0.209955000	2.556924000	0.141827000
6	-0.426466000	1.283975000	0.755337000
6	-1.649217000	1.038947000	1.433956000
6	-2.670551000	2.024032000	1.400304000
6	1.135499000	2.854661000	-0.350547000
6	0.589816000	0.295933000	0.719920000
6	1.787004000	0.454614000	-0.211082000
6	2.085165000	1.920692000	-0.445131000
6	2.941793000	-0.390148000	0.307323000
6	2.698161000	-1.456404000	1.106863000
6	0.421702000	-0.842903000	1.480603000
6	-1.804329000	-0.185743000	2.133829000
1	-2.740402000	-0.386223000	2.644642000
1	1.356075000	3.888460000	-0.599453000
1	-3.249780000	3.963868000	0.726849000
1	-1.049131000	4.460941000	-0.312830000
1	-3.610224000	1.817367000	1.902209000
1	3.078594000	2.191919000	-0.777045000
1	3.491991000	-2.135356000	1.392636000
6	4.301211000	-0.316491000	-0.224449000
8	5.277202000	-0.873261000	0.246103000
8	4.393283000	0.403144000	-1.355114000
1	5.317654000	0.388543000	-1.648669000
7	1.461648000	-1.768702000	1.564797000
1	1.355222000	-2.555568000	2.190799000
1	-0.878260000	-2.015708000	2.744900000
1	1.487704000	0.054114000	-1.195006000
6	-0.782342000	-1.091586000	2.183752000
8	-0.584979000	0.522384000	-2.384373000
8	-2.540600000	1.085216000	-1.724464000
6	-1.850636000	-1.073821000	-1.297857000
6	-0.805005000	-1.984873000	-1.364216000

6	-3.082972000	-1.380521000	-0.736970000
6	-1.006393000	-3.253294000	-0.836155000
6	-3.268279000	-2.656287000	-0.220425000
6	-2.233210000	-3.586829000	-0.266251000
1	0.139549000	-1.704748000	-1.812509000
1	-3.869646000	-0.638304000	-0.703770000
1	-0.203130000	-3.979283000	-0.870787000
1	-4.220890000	-2.919975000	0.222450000
1	-2.383495000	-4.579087000	0.143360000
7	-1.644742000	0.275162000	-1.842616000



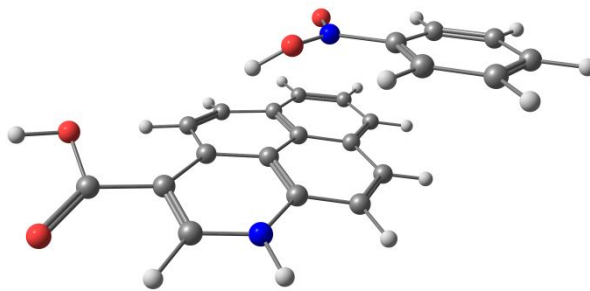
(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1257.837384

6	2.668044000	3.443618000	-0.182413000
6	1.359469000	3.683194000	0.264410000
6	0.341309000	2.770104000	0.020515000
6	0.652295000	1.558723000	-0.657684000
6	1.971550000	1.326450000	-1.124551000
6	2.970024000	2.294122000	-0.879522000
6	-1.032553000	3.017037000	0.398691000
6	-0.348722000	0.567385000	-0.821298000
6	-1.649519000	0.712939000	-0.153964000
6	-1.983967000	2.066015000	0.276568000
6	-2.656971000	-0.286779000	-0.558088000
6	-2.273391000	-1.377042000	-1.272379000
6	-0.028368000	-0.591102000	-1.530610000
6	2.247710000	0.117329000	-1.824828000
1	3.254465000	-0.054903000	-2.190735000
1	-1.286488000	3.997348000	0.787072000
1	3.441665000	4.177051000	0.013293000
1	1.127822000	4.603590000	0.790099000
1	3.976972000	2.111459000	-1.239398000
1	-3.001985000	2.281494000	0.569206000
1	-2.969007000	-2.168419000	-1.517953000
6	-4.048944000	-0.326026000	-0.076182000
8	-4.922306000	-1.018579000	-0.556218000
8	-4.266171000	0.448296000	0.991249000
1	-5.193574000	0.349582000	1.260287000
7	-0.995659000	-1.559077000	-1.686382000
1	-0.760398000	-2.400649000	-2.199263000
1	1.469319000	-1.723461000	-2.593795000
1	-1.224859000	0.215412000	1.095074000
6	1.266504000	-0.805544000	-2.052402000
8	-0.675471000	-0.304424000	2.003261000
8	1.262431000	0.731431000	2.137679000
6	1.209581000	-1.433389000	1.268827000

6	0.437028000	-2.555212000	0.931071000
6	2.596488000	-1.424372000	1.075546000
6	1.067486000	-3.654567000	0.372685000
6	3.204195000	-2.544576000	0.524807000
6	2.448150000	-3.655778000	0.160826000
1	-0.631288000	-2.551471000	1.102612000
1	3.171006000	-0.553061000	1.358839000
1	0.476323000	-4.522331000	0.102442000
1	4.277172000	-2.543293000	0.371064000
1	2.929041000	-4.522819000	-0.276144000
7	0.603024000	-0.292997000	1.829149000

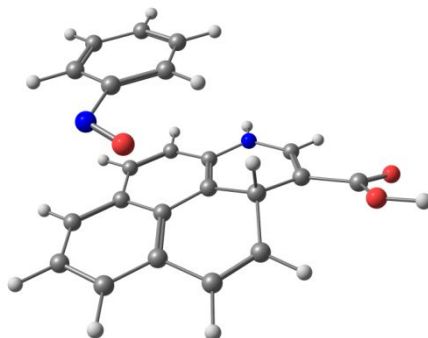


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1257.756958

6	-1.785793000	3.249003000	0.886830000
6	-0.506934000	3.461835000	0.323669000
6	0.416813000	2.441648000	0.256167000
6	0.068227000	1.144151000	0.748192000
6	-1.188558000	0.954253000	1.381429000
6	-2.113185000	2.029867000	1.421801000
6	1.798508000	2.655755000	-0.179439000
6	0.985096000	0.072362000	0.629391000
6	2.334576000	0.336070000	0.109495000
6	2.648408000	1.643117000	-0.366766000
6	3.244162000	-0.816349000	0.102750000
6	2.897250000	-1.918655000	0.808727000
6	0.695140000	-1.116967000	1.266664000
6	-1.479375000	-0.317593000	1.941684000
1	-2.443782000	-0.479288000	2.411068000
1	2.126516000	3.682929000	-0.307466000
1	-2.497272000	4.066128000	0.916079000
1	-0.235140000	4.448917000	-0.036723000
1	-3.081520000	1.866172000	1.882670000
1	3.672895000	1.837464000	-0.654651000
1	3.620665000	-2.698744000	1.010500000
6	4.601707000	-0.839235000	-0.449675000
8	5.508114000	-1.551598000	-0.077161000
8	4.759656000	0.000993000	-1.493122000
1	5.674177000	-0.093679000	-1.803102000
7	1.641996000	-2.139045000	1.269117000
1	1.453577000	-2.972485000	1.809117000
1	-0.748076000	-2.281485000	2.371641000
1	0.664489000	-0.327593000	-1.579010000
6	-0.547132000	-1.317700000	1.915586000
8	-0.284546000	-0.554556000	-1.797688000
8	-1.456817000	1.368712000	-1.947970000
6	-2.511315000	-0.662992000	-1.137207000
6	-2.438870000	-2.028599000	-0.814407000
6	-3.738489000	-0.003571000	-0.954064000
6	-3.552536000	-2.710053000	-0.326359000

6	-4.852505000	-0.684481000	-0.466053000
6	-4.764812000	-2.041143000	-0.149838000
1	-1.500832000	-2.558434000	-0.947917000
1	-3.817630000	1.051531000	-1.196879000
1	-3.472819000	-3.765841000	-0.083535000
1	-5.790923000	-0.153841000	-0.332638000
1	-5.632646000	-2.571877000	0.230403000
7	-1.279887000	0.090102000	-1.676758000

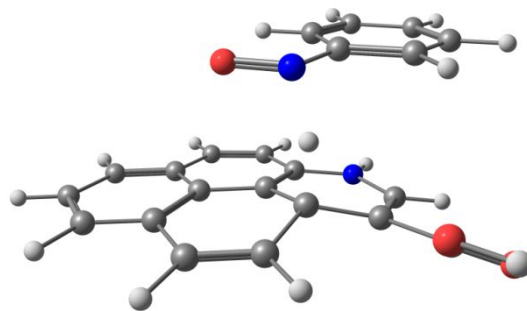


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= 1182.672835

6	-2.335260000	3.294362000	0.513606000
6	-1.034961000	3.549011000	0.025390000
6	-0.050144000	2.588628000	0.104007000
6	-0.357058000	1.316138000	0.678128000
6	-1.625847000	1.105783000	1.274312000
6	-2.619904000	2.109406000	1.146688000
6	1.343949000	2.851133000	-0.259221000
6	0.618096000	0.289573000	0.679629000
6	1.835839000	0.419487000	-0.224713000
6	2.249624000	1.872790000	-0.337815000
6	2.914031000	-0.548815000	0.231332000
6	2.602035000	-1.611050000	1.013925000
6	0.371888000	-0.851703000	1.411035000
6	-1.860187000	-0.117208000	1.957864000
1	-2.830632000	-0.289698000	2.411774000
1	1.631132000	3.885584000	-0.421725000
1	-3.099745000	4.056781000	0.416414000
1	-0.801214000	4.518842000	-0.401885000
1	-3.604056000	1.927313000	1.566686000
1	3.283359000	2.099809000	-0.564977000
1	3.345142000	-2.360040000	1.258865000
6	4.256160000	-0.570170000	-0.343254000
8	5.188741000	-1.249488000	0.048802000
8	4.382395000	0.222024000	-1.421723000
1	5.291663000	0.143911000	-1.749852000
7	1.359303000	-1.832296000	1.502501000
1	1.196887000	-2.632549000	2.098354000
1	-1.034962000	-1.984465000	2.597337000
1	1.513391000	0.127185000	-1.240879000
6	-0.873969000	-1.057822000	2.055743000
8	-1.254203000	0.970677000	-2.224752000
6	-2.294352000	-0.809553000	-1.361613000
6	-1.159073000	-1.621205000	-1.393734000
6	-3.501442000	-1.263974000	-0.836594000

6	-1.244110000	-2.906884000	-0.883736000
6	-3.576379000	-2.551107000	-0.320108000
6	-2.448172000	-3.367503000	-0.345301000
1	-0.237157000	-1.240636000	-1.817650000
1	-4.356989000	-0.597146000	-0.835476000
1	-0.374875000	-3.554326000	-0.899492000
1	-4.506555000	-2.918694000	0.096187000
1	-2.505704000	-4.374301000	0.053024000
7	-2.317837000	0.536699000	-1.859463000



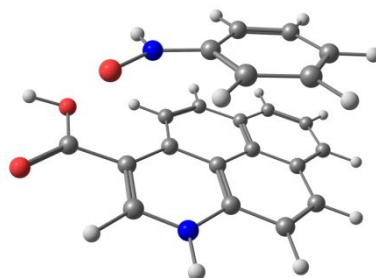
(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1182.652759

6	4.844068000	0.140425000	0.350808000
6	4.051351000	1.275301000	0.617626000
6	2.709015000	1.293134000	0.297896000
6	2.118204000	0.148579000	-0.313113000
6	2.927407000	-0.971200000	-0.629908000
6	4.297165000	-0.958318000	-0.265319000
6	1.874781000	2.466357000	0.507963000
6	0.737065000	0.155268000	-0.648840000
6	-0.147120000	1.250710000	-0.201194000
6	0.563357000	2.480507000	0.218630000
6	-1.434952000	1.305854000	-0.924506000
6	-1.833173000	0.245859000	-1.683511000
6	0.230498000	-0.912587000	-1.386693000
6	2.340624000	-2.068527000	-1.315241000
1	2.956022000	-2.930738000	-1.548871000
1	2.357645000	3.367562000	0.872069000
1	5.893275000	0.146412000	0.622461000
1	4.498660000	2.150843000	1.076553000
1	4.904498000	-1.827916000	-0.493433000
1	-0.016312000	3.381002000	0.365898000
1	-2.808093000	0.226421000	-2.153955000
6	-2.472593000	2.319285000	-0.687037000
8	-3.446670000	2.492366000	-1.390087000
8	-2.277564000	3.018553000	0.437487000
1	-3.009109000	3.647892000	0.540620000
7	-1.064554000	-0.843007000	-1.867676000
1	-1.421629000	-1.613937000	-2.419361000
1	0.586712000	-2.853436000	-2.260195000
1	-0.500180000	0.891927000	1.011087000
6	1.031666000	-2.035543000	-1.703645000
8	0.670823000	-0.286718000	2.294892000
6	-1.365706000	-0.935699000	1.528867000
6	-2.689274000	-0.572101000	1.264559000
6	-0.906068000	-2.225622000	1.253689000

6	-3.553125000	-1.499558000	0.699018000
6	-1.777697000	-3.144900000	0.687793000
6	-3.093554000	-2.780465000	0.396691000
1	-3.018988000	0.433247000	1.508192000
1	0.120910000	-2.481864000	1.481682000
1	-4.579773000	-1.224554000	0.486090000
1	-1.432447000	-4.147913000	0.463302000
1	-3.767186000	-3.503156000	-0.049936000
7	-0.513780000	0.083586000	2.063714000

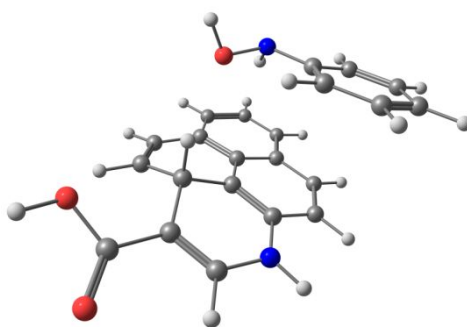


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1182.697115

6	-4.031507000	0.696633000	1.445388000
6	-2.914705000	1.455196000	1.798109000
6	-1.626980000	0.967350000	1.577333000
6	-1.461238000	-0.310221000	0.988772000
6	-2.598694000	-1.079935000	0.638461000
6	-3.880340000	-0.557030000	0.876285000
6	-0.449518000	1.717944000	1.910731000
6	-0.148793000	-0.808782000	0.743789000
6	1.012334000	-0.028485000	1.048750000
6	0.802187000	1.246557000	1.673894000
6	2.275179000	-0.600295000	0.728091000
6	2.326725000	-1.876712000	0.211610000
6	-0.029449000	-2.089718000	0.177310000
6	-2.409848000	-2.369277000	0.046241000
1	-3.285827000	-2.949429000	-0.223142000
1	-0.579393000	2.690567000	2.374354000
1	-5.025198000	1.092640000	1.619958000
1	-3.039025000	2.436124000	2.244550000
1	-4.748093000	-1.146833000	0.601147000
1	1.655986000	1.844321000	1.949315000
1	3.265620000	-2.350286000	-0.038315000
6	3.607756000	0.063377000	0.792600000
8	4.648401000	-0.523896000	0.589758000
8	3.579088000	1.346146000	1.149606000
1	4.490371000	1.679963000	1.141808000
7	1.221511000	-2.583338000	-0.029881000
1	1.314944000	-3.514540000	-0.428310000
1	-1.011928000	-3.848644000	-0.609497000
6	-1.164925000	-2.869511000	-0.169641000
8	2.741549000	0.650573000	-1.557109000
6	0.438173000	1.182521000	-1.713236000
6	0.126947000	-0.003276000	-2.418800000
6	-0.608611000	2.096468000	-1.428556000
6	-1.185911000	-0.263038000	-2.790587000
6	-1.907093000	1.805830000	-1.802806000
6	-2.219182000	0.620751000	-2.480510000

1	0.925183000	-0.693944000	-2.658678000
1	-0.375154000	3.019078000	-0.906419000
1	-1.406160000	-1.180931000	-3.327324000
1	-2.695156000	2.513804000	-1.565205000
1	-3.240930000	0.400879000	-2.766563000
7	1.693884000	1.432354000	-1.282926000
1	1.879652000	2.303432000	-0.795430000

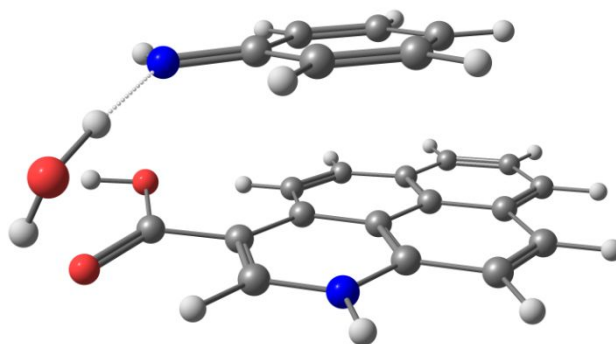


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1183.88852

6	2.315717000	3.100579000	-0.856386000
6	1.054008000	3.391939000	-0.286697000
6	0.056235000	2.443391000	-0.257115000
6	0.304256000	1.142658000	-0.796913000
6	1.534018000	0.886198000	-1.454783000
6	2.544378000	1.882969000	-1.446461000
6	-1.299249000	2.739763000	0.207224000
6	-0.691139000	0.137087000	-0.710475000
6	-1.883639000	0.320161000	0.220411000
6	-2.224554000	1.788958000	0.359019000
6	-3.017941000	-0.590290000	-0.226540000
6	-2.755783000	-1.688293000	-0.976984000
6	-0.499135000	-1.036781000	-1.408660000
6	1.717438000	-0.370735000	-2.087758000
1	2.660345000	-0.579810000	-2.582051000
1	-1.546617000	3.781600000	0.387834000
1	3.090667000	3.858664000	-0.851984000
1	0.861016000	4.381375000	0.115410000
1	3.495342000	1.665678000	-1.922226000
1	-3.226920000	2.053716000	0.668837000
1	-3.533550000	-2.405629000	-1.208098000
6	-4.364296000	-0.534685000	0.336922000
8	-5.329119000	-1.162626000	-0.063036000
8	-4.457799000	0.261312000	1.415807000
1	-5.372488000	0.228993000	1.736274000
7	-1.521486000	-1.986259000	-1.445432000
1	-1.400143000	-2.804315000	-2.026887000
1	0.830604000	-2.247381000	-2.606208000
1	-1.557778000	-0.004441000	1.223960000
6	0.712389000	-1.296617000	-2.096298000

8	0.619632000	0.840866000	2.333863000
6	2.310750000	-0.541881000	1.469048000
6	1.468102000	-1.648408000	1.561747000
6	3.562537000	-0.672061000	0.852843000
6	1.874204000	-2.869974000	1.025988000
6	3.953824000	-1.893095000	0.326470000
6	3.110198000	-3.002383000	0.404699000
1	0.502962000	-1.549799000	2.041570000
1	4.217199000	0.192125000	0.793141000
1	1.207103000	-3.722682000	1.094794000
1	4.923795000	-1.980672000	-0.150843000
1	3.418529000	-3.955067000	-0.009431000
7	1.987537000	0.708097000	2.037320000
1	2.229188000	1.472700000	1.408582000
1	0.582776000	0.914666000	3.295238000

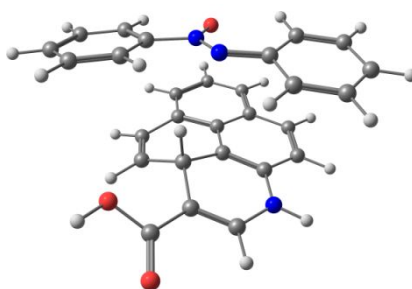


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1183.943104

6	4.755883000	-0.858804000	-0.286716000
6	3.781809000	-1.832717000	-0.481953000
6	2.459940000	-1.604070000	-0.088092000
6	2.120099000	-0.370020000	0.512685000
6	3.118128000	0.612817000	0.727044000
6	4.430756000	0.350416000	0.313920000
6	1.427499000	-2.581552000	-0.264978000
6	0.773203000	-0.120342000	0.889717000
6	-0.252658000	-1.080580000	0.648875000
6	0.137640000	-2.342849000	0.084702000
6	-1.576395000	-0.729750000	1.026587000
6	-1.805451000	0.493536000	1.618407000
6	0.473978000	1.118586000	1.487217000
6	2.755015000	1.851079000	1.347652000
1	3.527359000	2.594996000	1.509732000
1	1.699663000	-3.540216000	-0.694302000
1	5.775305000	-1.046142000	-0.601978000
1	4.038042000	-2.779778000	-0.944666000
1	5.191846000	1.107507000	0.469207000
1	-0.605631000	-3.109664000	-0.063059000
1	-2.795796000	0.818988000	1.901310000
6	-2.817672000	-1.523175000	0.794324000
8	-3.858260000	-1.289002000	1.367358000
8	-2.687572000	-2.517472000	-0.075634000
1	-3.545363000	-2.964411000	-0.163394000
7	-0.811019000	1.358396000	1.838903000
1	-1.035914000	2.256068000	2.264256000
1	1.187603000	3.039502000	2.185611000
1	-3.978344000	0.904539000	-0.522702000
6	1.473890000	2.103441000	1.720052000
8	-4.551765000	1.359373000	0.191674000
6	-1.737619000	0.674210000	-1.769867000
6	-1.387972000	1.983959000	-1.313704000
6	-0.671809000	-0.066118000	-2.371235000

6	-0.102106000	2.481593000	-1.433028000
6	0.609519000	0.452620000	-2.489062000
6	0.923759000	1.729061000	-2.017784000
1	-2.165051000	2.582268000	-0.845402000
1	-0.884507000	-1.070275000	-2.731028000
1	0.112065000	3.479718000	-1.059291000
1	1.383906000	-0.157063000	-2.948077000
1	1.928621000	2.126041000	-2.104433000
7	-2.983819000	0.210261000	-1.592983000
1	-3.063907000	-0.733002000	-1.964476000
1	-4.761861000	0.639106000	0.7954740000

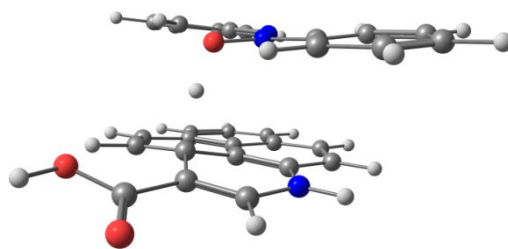


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1468.945955

6	2.588979	-0.012305	2.552357
6	2.092191	-1.224196	2.022234
6	0.826276	-1.295303	1.484139
6	0.000316	-0.128777	1.464639
6	0.472209	1.065542	2.070332
6	1.793549	1.105219	2.587142
6	0.237496	-2.556369	1.031569
6	-1.299177	-0.185406	0.899447
6	-1.717187	-1.370360	0.034801
6	-0.955584	-2.616075	0.432793
6	-3.236428	-1.479802	0.031909
6	-3.991631	-0.385096	0.283672
6	-2.141518	0.890810	1.088461
6	-0.406330	2.177016	2.159487
1	-0.047779	3.097063	2.609134
1	0.794474	-3.466279	1.235551
1	3.596627	0.022496	2.950585
1	2.711837	-2.115798	2.042689
1	2.155101	2.031442	3.021913
1	-1.363842	-3.573059	0.136694
1	-5.068344	-0.413522	0.172285
6	-3.978526	-2.626815	-0.501986
8	-5.173833	-2.802148	-0.410454
8	-3.198960	-3.491456	-1.182971
1	-3.773574	-4.202232	-1.508633
7	-3.462507	0.810463	0.649769
1	-4.087011	1.573456	0.872999
1	-2.386690	2.910404	1.812142
1	-1.388083	-1.142297	-0.992621
6	-1.694152	2.081044	1.712898
8	0.460633	-0.179958	-1.965526
6	0.217732	2.034478	-1.339646
6	-1.112553	1.969784	-1.730917
6	0.789820	3.210149	-0.865828

6	-1.893121	3.116448	-1.639781
6	-0.001507	4.349358	-0.789039
6	-1.340068	4.305052	-1.172536
1	-1.523338	1.035161	-2.089565
1	1.828553	3.228536	-0.566500
1	-2.935057	3.076105	-1.934550
1	0.430594	5.273482	-0.424292
1	-1.950567	5.198297	-1.108628
6	3.042131	-0.243553	-1.015865
6	4.294886	0.043000	-0.446977
6	2.780820	-1.548470	-1.468441
6	5.259920	-0.940004	-0.313693
6	3.761327	-2.527822	-1.325577
6	4.992557	-2.237673	-0.749896
1	4.477098	1.053079	-0.098238
1	1.834321	-1.801467	-1.913770
1	6.216872	-0.699613	0.134491
1	3.549827	-3.533478	-1.670832
1	5.741431	-3.013985	-0.642911
7	2.189707	0.873691	-0.995940



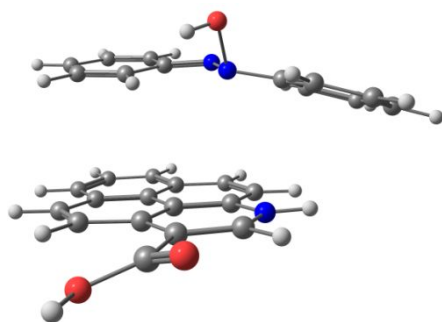
(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1468.910784

6	-3.807437	0.212198	2.001011
6	-3.364923	1.353889	1.320416
6	-2.017235	1.510184	1.005830
6	-1.080205	0.521626	1.432652
6	-1.539832	-0.637460	2.115084
6	-2.923320	-0.778595	2.374715
6	-1.527248	2.634019	0.248876
6	0.308465	0.697051	1.171115
6	0.769206	1.768502	0.279136
6	-0.211835	2.774636	-0.057526
6	2.237343	2.028889	0.348378
6	3.042526	1.111718	0.947574
6	1.205212	-0.244119	1.677372
6	-0.588563	-1.616481	2.510716
1	-0.937898	-2.517950	3.002120
1	-2.241525	3.385068	-0.071778
1	-4.863609	0.099725	2.220927
1	-4.071396	2.117686	1.013567
1	-3.271823	-1.668745	2.887446
1	0.107917	3.635014	-0.627518
1	4.116671	1.242738	0.965804
6	2.961338	3.128774	-0.303355
8	4.129530	3.395378	-0.125279
8	2.215749	3.827788	-1.179016
1	2.786410	4.516061	-1.556982
7	2.570713	-0.020926	1.513215
1	3.221801	-0.681797	1.916762
1	1.484655	-2.132180	2.671484
1	0.635610	0.945694	-0.878652
6	0.754097	-1.405940	2.330181
8	0.570902	0.121603	-1.732768
6	1.445387	-1.912303	-0.995327
6	2.728235	-1.406532	-1.191267
6	1.248231	-3.229357	-0.569489

6	3.824655	-2.227156	-0.948028
6	2.354450	-4.029550	-0.328146
6	3.645995	-3.534944	-0.512626
1	2.864851	-0.388422	-1.529173
1	0.245430	-3.607746	-0.432286
1	4.822556	-1.832390	-1.098845
1	2.205951	-5.050025	0.004873
1	4.503680	-4.168250	-0.319780
7	0.317013	-1.066674	-1.247458
6	-2.013895	-0.881816	-1.374041
6	-3.174210	-1.564759	-0.931919
6	-2.180445	0.316958	-2.111166
6	-4.436571	-1.066004	-1.181062
6	-3.460705	0.798923	-2.352057
6	-4.589614	0.134448	-1.879568
1	-3.037371	-2.490936	-0.385381
1	-1.331526	0.856381	-2.496035
1	-5.307230	-1.602794	-0.821397
1	-3.573435	1.720389	-2.912707
1	-5.578554	0.535582	-2.068392
7	-0.854186	-1.542692	-1.030390

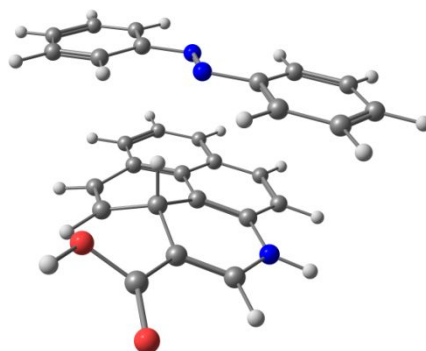


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1468.933017

6	2.972041000	-2.176068000	1.833236000
6	2.105995000	-3.069778000	1.216028000
6	0.795305000	-2.686859000	0.903511000
6	0.352987000	-1.388197000	1.244306000
6	1.233753000	-0.483396000	1.885441000
6	2.546081000	-0.892418000	2.156818000
6	-0.103127000	-3.545275000	0.201551000
6	-0.963374000	-0.983833000	0.903142000
6	-1.851445000	-1.860389000	0.217394000
6	-1.365220000	-3.157579000	-0.136180000
6	-3.147272000	-1.356997000	-0.100490000
6	-3.469008000	-0.061535000	0.234906000
6	-1.363313000	0.326770000	1.249148000
6	0.765196000	0.822348000	2.226863000
1	1.447801000	1.504017000	2.723004000
1	0.246036000	-4.533156000	-0.080865000
1	3.989895000	-2.475541000	2.053056000
1	2.441984000	-4.066708000	0.951003000
1	3.226650000	-0.193911000	2.632165000
1	-2.001825000	-3.834682000	-0.682885000
1	-4.431164000	0.371424000	-0.003101000
6	-4.251838000	-2.092352000	-0.783761000
8	-5.180856000	-1.527805000	-1.310382000
8	-4.146195000	-3.413858000	-0.729065000
1	-4.901122000	-3.806912000	-1.197591000
7	-2.607428000	0.726357000	0.887357000
1	-2.888976000	1.680822000	1.107443000
1	-0.873633000	2.203642000	2.195860000
1	0.107180000	0.889701000	-2.734781000
6	-0.506421000	1.215715000	1.941085000
8	0.464446000	1.764745000	-2.548652000
6	0.020903000	2.895482000	-0.590554000

6	-1.325294000	3.080306000	-0.930622000
6	0.621556000	3.777664000	0.309698000
6	-2.058414000	4.112957000	-0.362346000
6	-0.122077000	4.812105000	0.873821000
6	-1.463484000	4.984292000	0.551383000
1	-1.790419000	2.400361000	-1.634775000
1	1.661035000	3.633688000	0.564166000
1	-3.101717000	4.236929000	-0.632332000
1	0.357497000	5.488262000	1.573614000
1	-2.038297000	5.787183000	0.998320000
7	0.701858000	1.755337000	-1.102429000
6	2.667917000	0.595358000	-1.062013000
6	4.074059000	0.506874000	-0.823593000
6	2.051507000	-0.601426000	-1.536386000
6	4.793728000	-0.646368000	-1.073259000
6	2.792898000	-1.749024000	-1.783001000
6	4.170036000	-1.798609000	-1.568624000
1	4.573984000	1.395788000	-0.450597000
1	0.978552000	-0.633066000	-1.685989000
1	5.862838000	-0.651277000	-0.881127000
1	2.274946000	-2.634029000	-2.144478000
1	4.737294000	-2.697880000	-1.776966000
7	2.074178000	1.785746000	-0.838266000

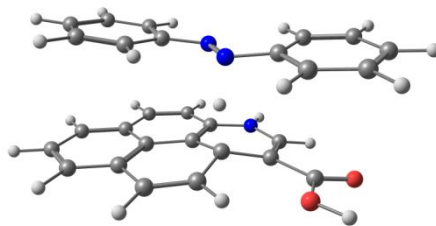


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1393.770166

6	2.995561000	0.566055000	2.326964000
6	2.631740000	-0.740066000	1.929012000
6	1.343934000	-1.023917000	1.532517000
6	0.363491000	0.017466000	1.535816000
6	0.701020000	1.295740000	2.049306000
6	2.050485000	1.558672000	2.403066000
6	0.890344000	-2.385666000	1.237435000
6	-0.952368000	-0.252053000	1.089041000
6	-1.207536000	-1.497455000	0.254416000
6	-0.316755000	-2.631790000	0.720571000
6	-2.696398000	-1.791333000	0.209287000
6	-3.605712000	-0.848538000	0.563074000
6	-1.939945000	0.675513000	1.348016000
6	-0.333184000	2.255464000	2.210010000
1	-0.085598000	3.237934000	2.598146000
1	1.558311000	-3.201771000	1.496820000
1	4.023797000	0.771640000	2.603197000
1	3.372495000	-1.534101000	1.943813000
1	2.315007000	2.550814000	2.754158000
1	-0.645885000	-3.649540000	0.551774000
1	-4.667600000	-1.030051000	0.448172000
6	-3.240108000	-2.975903000	-0.445854000
8	-4.407160000	-3.327548000	-0.437214000
8	-2.313664000	-3.666377000	-1.134248000
1	-2.748559000	-4.428613000	-1.546671000
7	-3.265209000	0.369364000	1.039194000
1	-3.989681000	1.031829000	1.279547000
1	-2.432432000	2.650097000	2.074238000
1	-0.868536000	-1.260235000	-0.769464000
6	-1.629995000	1.937446000	1.912816000
6	-0.399460000	1.824080000	-1.564812000

6	-1.694716000	1.413305000	-1.875806000
6	-0.148243000	3.146059000	-1.184425000
6	-2.747511000	2.317924000	-1.796975000
6	-1.202137000	4.044678000	-1.113786000
6	-2.502027000	3.632943000	-1.413038000
1	-1.860420000	0.381490000	-2.168404000
1	0.861571000	3.450133000	-0.939758000
1	-3.755800000	1.996269000	-2.031029000
1	-1.014742000	5.070506000	-0.817279000
1	-3.320729000	4.340774000	-1.348502000
7	0.596127000	0.807816000	-1.631931000
6	2.727432000	0.147646000	-1.349754000
6	4.010802000	0.546181000	-0.984034000
6	2.459249000	-1.193089000	-1.641357000
6	5.031032000	-0.394212000	-0.891283000
6	3.479663000	-2.126796000	-1.545620000
6	4.764356000	-1.731920000	-1.166061000
1	4.186788000	1.591906000	-0.756952000
1	1.456683000	-1.492331000	-1.920881000
1	6.027727000	-0.085013000	-0.598867000
1	3.275513000	-3.169655000	-1.760795000
1	5.554769000	-2.469680000	-1.085978000
7	1.744202000	1.177163000	-1.339385000



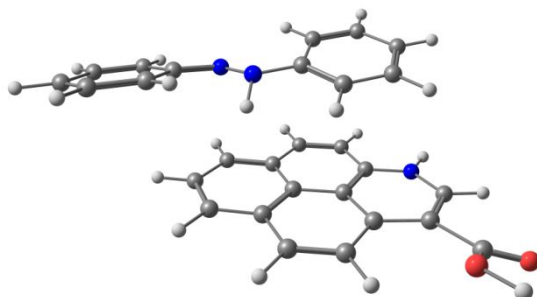
(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1393.745642

6	4.385954000	-1.762067000	-0.464063000
6	3.286974000	-2.296001000	-1.146262000
6	1.988590000	-2.031485000	-0.724566000
6	1.781930000	-1.214287000	0.422227000
6	2.900828000	-0.692046000	1.123853000
6	4.200039000	-0.968677000	0.651108000
6	0.833847000	-2.568028000	-1.405743000
6	0.461520000	-0.917102000	0.854869000
6	-0.697350000	-1.283312000	0.027609000
6	-0.425063000	-2.249984000	-1.039611000
6	-1.995081000	-1.231733000	0.761759000
6	-2.056158000	-0.546295000	1.938920000
6	0.298235000	-0.164270000	2.016705000
6	2.673540000	0.112576000	2.277121000
1	3.528636000	0.521324000	2.805008000
1	1.002463000	-3.243718000	-2.237852000
1	5.389290000	-1.971881000	-0.816999000
1	3.441153000	-2.923173000	-2.018241000
1	5.050107000	-0.552010000	1.181335000
1	-1.259038000	-2.665508000	-1.583983000
1	-2.993838000	-0.427358000	2.465283000
6	-3.297115000	-1.739884000	0.307047000
8	-4.342746000	-1.591161000	0.914440000
8	-3.272045000	-2.406074000	-0.854305000
1	-4.179561000	-2.681187000	-1.059134000
7	-0.978741000	0.014440000	2.520119000
1	-1.092695000	0.515284000	3.392313000
1	1.228088000	0.930301000	3.626174000
1	-0.679031000	-0.132806000	-0.750353000
6	1.407770000	0.347109000	2.729378000
6	-2.134950000	1.366942000	-0.833277000
6	-2.986250000	0.644782000	-1.670570000
6	-2.667908000	2.230834000	0.125282000
6	-4.363893000	0.769164000	-1.541588000

6	-4.046841000	2.349247000	0.248542000
6	-4.899836000	1.616575000	-0.575595000
1	-2.554104000	-0.024387000	-2.408426000
1	-2.001623000	2.791157000	0.767825000
1	-5.018088000	0.195353000	-2.188647000
1	-4.459705000	3.017094000	0.996497000
1	-5.974254000	1.709573000	-0.467008000
7	-0.739660000	1.136938000	-1.012884000
6	1.376634000	1.813400000	-0.575465000
6	2.243095000	2.552056000	0.249462000
6	1.915566000	1.143393000	-1.693270000
6	3.599815000	2.625757000	-0.030337000
6	3.272209000	1.224478000	-1.963067000
6	4.125656000	1.955878000	-1.133708000
1	1.819553000	3.066531000	1.105298000
1	1.260731000	0.574912000	-2.342837000
1	4.250485000	3.204480000	0.616425000
1	3.675274000	0.706273000	-2.826859000
1	5.185773000	2.009923000	-1.353721000
7	0.033855000	1.825134000	-0.222053000

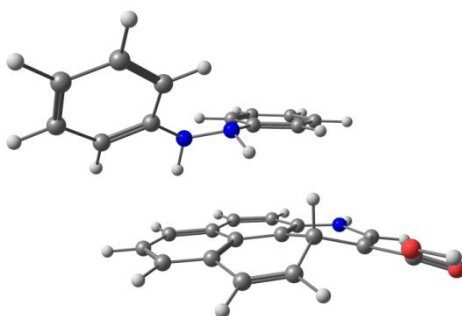


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1393.764744

6	2.361581000	-1.592842000	1.444879000
6	1.479262000	-2.418603000	0.765262000
6	0.129569000	-2.054282000	0.608922000
6	-0.314050000	-0.820990000	1.143453000
6	0.592310000	0.021481000	1.833325000
6	1.930514000	-0.374908000	1.966538000
6	-0.807895000	-2.867595000	-0.085524000
6	-1.661104000	-0.420144000	0.950927000
6	-2.571570000	-1.227464000	0.206820000
6	-2.104784000	-2.481845000	-0.280316000
6	-3.888206000	-0.709018000	0.015044000
6	-4.229646000	0.498230000	0.576404000
6	-2.061524000	0.830148000	1.470522000
6	0.130010000	1.276612000	2.331133000
1	0.837396000	1.921809000	2.841333000
1	-0.470109000	-3.823049000	-0.473761000
1	3.399510000	-1.886252000	1.551160000
1	1.821027000	-3.360415000	0.348429000
1	2.621949000	0.269205000	2.496893000
1	-2.779349000	-3.132342000	-0.814197000
1	-5.218650000	0.922442000	0.467996000
6	-4.984823000	-1.335976000	-0.778821000
8	-6.149585000	-1.061974000	-0.614441000
8	-4.563805000	-2.182204000	-1.710815000
1	-5.335056000	-2.533242000	-2.185660000
7	-3.344584000	1.221298000	1.274347000
1	-3.640187000	2.120034000	1.650673000
1	-1.517138000	2.631849000	2.531810000
6	-1.160815000	1.676436000	2.164463000
6	0.655986000	1.658249000	-1.095912000
6	-0.597444000	1.187843000	-1.541653000
6	0.767613000	3.012765000	-0.729566000
6	-1.690201000	2.036524000	-1.605954000
6	-0.342563000	3.848096000	-0.795365000

6	-1.581387000	3.377396000	-1.225414000
1	-0.695027000	0.144054000	-1.829586000
1	1.723627000	3.383654000	-0.386221000
1	-2.643167000	1.645415000	-1.950488000
1	-0.233840000	4.887131000	-0.500714000
1	-2.439595000	4.037221000	-1.272796000
7	1.731821000	0.804079000	-1.075454000
6	3.903056000	0.355147000	-0.541270000
6	5.093842000	0.593782000	0.221137000
6	3.943730000	-0.778608000	-1.413974000
6	6.189788000	-0.236716000	0.143669000
6	5.066153000	-1.600907000	-1.473288000
6	6.199199000	-1.361251000	-0.701631000
1	5.100616000	1.454816000	0.883274000
1	3.100368000	-0.998090000	-2.057738000
1	7.063516000	-0.012011000	0.749124000
1	5.049552000	-2.452766000	-2.148153000
1	7.063035000	-2.012759000	-0.754167000
7	2.861937000	1.171685000	-0.335894000
1	1.474830000	-0.182087000	-1.029013000

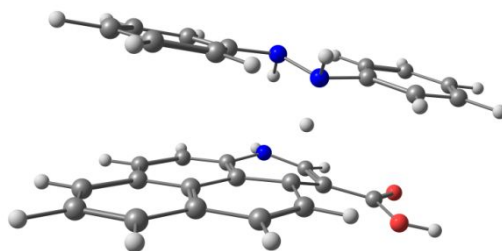


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1394.968254

6	2.119253000	0.013673000	3.087834000
6	1.652160000	-1.210678000	2.556648000
6	0.461070000	-1.274582000	1.865342000
6	-0.303159000	-0.081049000	1.668431000
6	0.125411000	1.128849000	2.275914000
6	1.365374000	1.154891000	2.967054000
6	-0.143547000	-2.545343000	1.459842000
6	-1.512102000	-0.128726000	0.931237000
6	-1.826949000	-1.351235000	0.078092000
6	-1.247122000	-2.599559000	0.710249000
6	-3.313630000	-1.387051000	-0.233191000
6	-4.067564000	-0.265539000	-0.128014000
6	-2.334120000	0.978921000	0.944575000
6	-0.716507000	2.268454000	2.187147000
1	-0.391302000	3.200182000	2.637727000
1	0.308818000	-3.455105000	1.842525000
1	3.062816000	0.038263000	3.620667000
1	2.221261000	-2.120080000	2.720877000
1	1.698688000	2.089471000	3.406223000
1	-1.700121000	-3.553502000	0.473180000
1	-5.103081000	-0.257760000	-0.445666000
6	-3.952199000	-2.508174000	-0.917332000
8	-5.149795000	-2.647985000	-1.091299000
8	-3.071588000	-3.397395000	-1.407549000
1	-3.567446000	-4.101516000	-1.853727000
7	-3.584830000	0.910696000	0.335284000
1	-4.203992000	1.706698000	0.406063000
1	-2.599408000	3.042067000	1.530200000
1	-1.288469000	-1.234001000	-0.879787000
6	-1.931779000	2.187335000	1.567218000
6	0.395306000	1.635179000	-1.404266000
6	-0.872453000	1.501952000	-1.990403000
6	0.828063000	2.899842000	-0.994833000
6	-1.690110000	2.610300000	-2.147450000

6	-0.002510000	4.004795000	-1.163978000
6	-1.264507000	3.872883000	-1.732562000
1	-1.207695000	0.522051000	-2.317049000
1	1.805147000	3.011680000	-0.542677000
1	-2.670075000	2.486000000	-2.596006000
1	0.345973000	4.978603000	-0.837107000
1	-1.907132000	4.736707000	-1.854670000
7	1.197977000	0.493160000	-1.286750000
6	3.406021000	-0.223536000	-0.784697000
6	4.403019000	-0.411430000	0.184162000
6	3.550171000	-0.824862000	-2.038641000
6	5.520927000	-1.180369000	-0.103546000
6	4.679474000	-1.591771000	-2.312459000
6	5.670257000	-1.778465000	-1.354712000
1	4.291948000	0.057307000	1.156898000
1	2.783359000	-0.687449000	-2.789899000
1	6.281864000	-1.314434000	0.657635000
1	4.779250000	-2.050007000	-3.290610000
1	6.544211000	-2.379069000	-1.576957000
7	2.319615000	0.599549000	-0.468426000
1	2.103541000	0.615190000	0.526750000
1	0.664099000	-0.360303000	-1.130536000



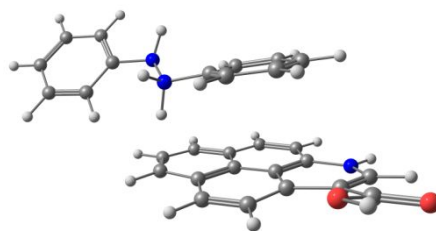
(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1394.919678

6	4.612936000	-1.579765000	-0.959367000
6	3.457702000	-1.945916000	-1.678308000
6	2.193141000	-1.783744000	-1.121520000
6	2.076421000	-1.220674000	0.195532000
6	3.255134000	-0.866180000	0.922593000
6	4.528859000	-1.058886000	0.306728000
6	0.982824000	-2.157170000	-1.810531000
6	0.786571000	-0.992509000	0.758641000
6	-0.434996000	-1.289441000	-0.002683000
6	-0.246229000	-1.968957000	-1.248663000
6	-1.676005000	-1.354728000	0.850141000
6	-1.662990000	-0.733741000	2.057286000
6	0.722165000	-0.419529000	2.030688000
6	3.123057000	-0.323724000	2.217849000
1	4.013986000	-0.062017000	2.778137000
1	1.069270000	-2.601074000	-2.796527000
1	5.586648000	-1.715365000	-1.420166000
1	3.548344000	-2.363274000	-2.675651000
1	5.420919000	-0.775686000	0.855569000
1	-1.120414000	-2.283189000	-1.802866000
1	-2.555417000	-0.684382000	2.668354000
6	-2.984157000	-1.883907000	0.472810000
8	-4.018126000	-1.729635000	1.107003000
8	-2.998203000	-2.582253000	-0.675732000
1	-3.911426000	-2.867052000	-0.834973000
7	-0.561595000	-0.116586000	2.561035000
1	-0.597454000	0.184134000	3.526155000
1	1.761467000	0.319944000	3.751037000
1	-0.759088000	0.054263000	-0.671705000
6	1.870171000	-0.108840000	2.759065000
6	-2.570919000	1.248603000	-0.762420000
6	-3.323623000	0.531041000	-1.686930000

6	-3.164551000	1.904209000	0.307361000
6	-4.701822000	0.462414000	-1.529765000
6	-4.546889000	1.820752000	0.453331000
6	-5.315854000	1.102835000	-0.456368000
1	-2.828917000	0.026377000	-2.510744000
1	-2.576576000	2.470621000	1.017730000
1	-5.293067000	-0.097651000	-2.244656000
1	-5.021425000	2.324803000	1.287024000
1	-6.390018000	1.041051000	-0.329048000
7	-1.129478000	1.187058000	-0.931719000
6	1.004572000	2.115313000	-0.399932000
6	1.820916000	2.755872000	0.537472000
6	1.567451000	1.591205000	-1.562334000
6	3.182870000	2.873022000	0.309638000
6	2.937876000	1.727708000	-1.785530000
6	3.750928000	2.364820000	-0.858867000
1	1.374753000	3.155743000	1.442507000
1	0.981173000	1.052804000	-2.297776000
1	3.804333000	3.365618000	1.048919000
1	3.363713000	1.313427000	-2.692494000
1	4.815514000	2.459490000	-1.037078000
7	-0.391262000	2.089382000	-0.109005000
1	-0.538593000	1.798293000	0.860090000
1	-0.914097000	1.398755000	-1.909700000



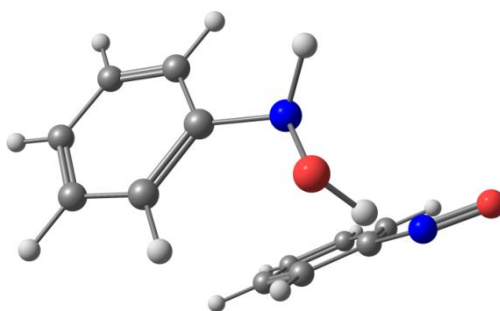
Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1394.926031

6	2.061248000	1.419208000	1.824985000
6	1.400035000	0.226077000	2.163082000
6	0.008724000	0.071067000	1.857863000
6	-0.645322000	1.098453000	1.092436000
6	0.067420000	2.294111000	0.727416000
6	1.440724000	2.429203000	1.126391000
6	-0.744068000	-1.052168000	2.231542000
6	-1.997388000	0.910051000	0.677401000
6	-2.697509000	-0.304100000	0.979462000
6	-2.059914000	-1.229706000	1.792945000
6	-4.052649000	-0.449801000	0.387448000
6	-4.610577000	0.622907000	-0.253834000
6	-2.619374000	1.959340000	-0.051965000
6	-0.598745000	3.273562000	-0.018707000
1	-0.069298000	4.177354000	-0.300298000
1	-0.279669000	-1.815213000	2.848054000
1	3.104922000	1.533704000	2.107951000
1	1.887028000	-0.518968000	2.783547000
1	1.976886000	3.332056000	0.855974000
1	-2.581013000	-2.130580000	2.085764000
1	-5.605591000	0.560051000	-0.676799000
6	-4.845702000	-1.664303000	0.310107000
8	-6.009531000	-1.733435000	-0.066275000
8	-4.189105000	-2.787785000	0.663705000
1	-4.803543000	-3.529859000	0.556087000
7	-3.973039000	1.785548000	-0.423503000
1	-4.427640000	2.527644000	-0.938091000
1	-2.451761000	3.882574000	-0.949954000
6	-1.937409000	3.108133000	-0.388392000
6	0.723194000	-0.720237000	-1.312809000
6	-0.199266000	-1.751775000	-1.240901000
6	0.479391000	0.450404000	-2.018497000
6	-1.420516000	-1.601310000	-1.889303000
6	-0.740576000	0.576595000	-2.675498000
6	-1.689865000	-0.439980000	-2.608672000

1	0.026155000	-2.649012000	-0.674434000
1	1.213560000	1.245710000	-2.045214000
1	-2.158560000	-2.392604000	-1.824511000
1	-0.951405000	1.483066000	-3.230747000
1	-2.641414000	-0.326024000	-3.115587000
7	1.971766000	-0.876518000	-0.548394000
6	4.342904000	-0.474552000	-0.580159000
6	5.464444000	-0.171839000	-1.358160000
6	4.503399000	-0.948860000	0.719816000
6	6.735670000	-0.338648000	-0.832088000
6	5.789242000	-1.111032000	1.234717000
6	6.906905000	-0.807608000	0.470092000
1	5.327934000	0.196494000	-2.369513000
1	3.652889000	-1.191150000	1.345688000
1	7.598273000	-0.099974000	-1.443686000
1	5.904931000	-1.481387000	2.246774000
1	7.901817000	-0.935495000	0.879356000
7	3.075425000	-0.214803000	-1.168090000
1	3.066286000	-0.459217000	-2.157992000
1	1.835098000	-0.454934000	0.430067000
1	2.157605000	-1.883236000	-0.412269000

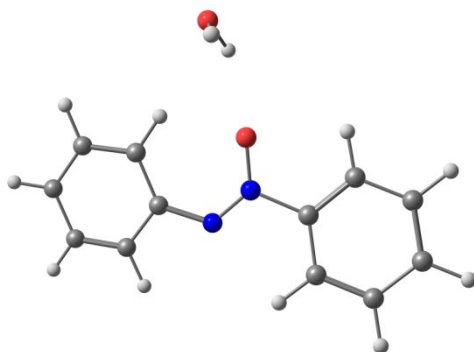
2.3.4. *Thermodynamic assesment of dimerization processes*



Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -724.043376

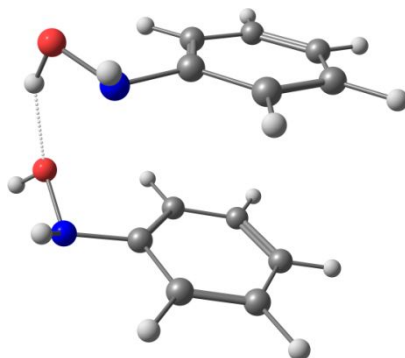
8	-0.540165000	2.520777000	0.735278000
6	-1.767549000	0.791663000	-0.272082000
6	-2.161593000	0.322778000	0.982671000
6	-2.317723000	0.220018000	-1.427219000
6	-3.088675000	-0.713382000	1.072606000
6	-3.239363000	-0.810947000	-1.321734000
6	-3.631691000	-1.288395000	-0.070742000
1	-1.750685000	0.776262000	1.874474000
1	-2.009298000	0.587680000	-2.400646000
1	-3.390099000	-1.066646000	2.052581000
1	-3.656648000	-1.243630000	-2.224175000
1	-4.352681000	-2.093095000	0.008209000
7	-0.777094000	1.776215000	-0.430919000
6	2.134013000	0.126789000	0.161038000
6	2.994955000	-0.593144000	-0.669102000
6	1.198129000	-0.506380000	0.972997000
6	2.904427000	-1.974942000	-0.677727000
6	1.115774000	-1.893302000	0.959538000
6	1.967426000	-2.621560000	0.133517000
1	3.707700000	-0.065826000	-1.290920000
1	0.551312000	0.095309000	1.601635000
1	3.558114000	-2.557191000	-1.316033000
1	0.391297000	-2.401607000	1.584210000
1	1.903075000	-3.703446000	0.116838000
7	2.130979000	1.559195000	0.231180000
1	-1.009638000	2.424349000	-1.178686000
8	2.979792000	2.122281000	-0.405521000
1	0.414563000	2.400322000	0.870066000



Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -724.097352

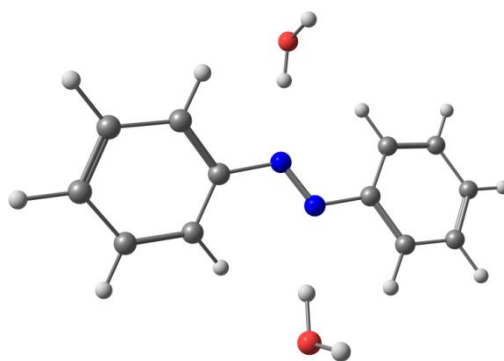
7	0.497953000	0.192350000	0.027318000
7	-0.279720000	-0.790430000	-0.060311000
6	1.930368000	-0.120899000	0.010200000
6	2.816811000	0.931258000	-0.172490000
6	2.362793000	-1.430869000	0.179959000
6	4.179551000	0.657452000	-0.193729000
6	3.727527000	-1.685413000	0.160372000
6	4.635558000	-0.646087000	-0.027614000
1	2.443776000	1.938259000	-0.296917000
1	1.646738000	-2.226867000	0.327841000
1	4.883802000	1.467385000	-0.340363000
1	4.081353000	-2.700374000	0.295444000
1	5.699124000	-0.853563000	-0.042351000
6	-1.677344000	-0.631823000	-0.038112000
6	-2.341872000	-1.869863000	-0.071329000
6	-2.435257000	0.551784000	-0.001282000
6	-3.723613000	-1.937292000	-0.060936000
6	-3.824898000	0.466063000	0.003874000
6	-4.473455000	-0.762469000	-0.023383000
1	-1.741328000	-2.771535000	-0.103057000
1	-1.968064000	1.521768000	0.020085000
1	-4.216858000	-2.901863000	-0.084566000
1	-4.403771000	1.382281000	0.030047000
1	-5.556391000	-0.806907000	-0.016934000
8	0.183812000	1.399860000	0.125286000
8	-1.170515000	3.872226000	0.074013000
1	-0.712565000	3.385611000	-0.620377000
1	-0.846837000	3.444635000	0.874528000



Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -725.257059

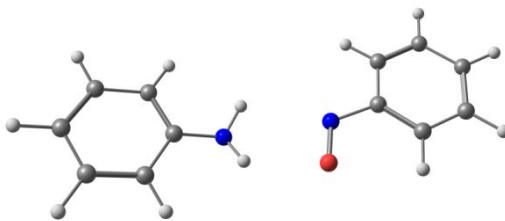
8	0.234400000	3.041247000	-0.418306000
6	-1.076271000	1.088899000	-0.561518000
6	-1.596388000	1.325884000	0.712064000
6	-1.578717000	0.030555000	-1.328665000
6	-2.605878000	0.504747000	1.208180000
6	-2.584140000	-0.779465000	-0.821290000
6	-3.104461000	-0.551700000	0.453298000
1	-1.204807000	2.143326000	1.302224000
1	-1.165617000	-0.152885000	-2.315799000
1	-3.002874000	0.696823000	2.199122000
1	-2.961406000	-1.597818000	-1.424680000
1	-3.886986000	-1.188700000	0.847599000
7	0.015031000	1.816372000	-1.070513000
6	1.832843000	-0.529061000	0.112332000
6	1.098037000	-0.852836000	1.251354000
6	1.804801000	-1.378010000	-0.998169000
6	0.336612000	-2.018945000	1.270938000
6	1.051600000	-2.544101000	-0.961871000
6	0.309796000	-2.872374000	0.172601000
1	1.109723000	-0.187205000	2.104242000
1	2.373455000	-1.115709000	-1.884839000
1	-0.240640000	-2.257909000	2.157583000
1	1.036158000	-3.194016000	-1.829682000
1	-0.286129000	-3.777121000	0.194711000
7	2.665373000	0.612832000	0.053979000
1	-0.085777000	2.012636000	-2.061850000
8	2.216847000	1.633386000	0.922070000
1	1.005642000	2.842782000	0.134455000
1	2.636138000	1.009028000	-0.882635000
1	2.973306000	1.823718000	1.489657000



Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -725.333415

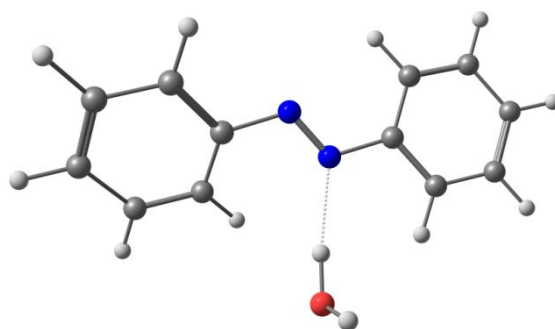
8	0.034584000	3.318129000	0.575084000
6	1.765280000	-0.197600000	-0.087988000
6	2.651124000	-1.160905000	0.394182000
6	2.240753000	1.013891000	-0.598659000
6	4.015195000	-0.895071000	0.408777000
6	3.605474000	1.263234000	-0.593529000
6	4.492939000	0.316079000	-0.082652000
1	2.264382000	-2.104141000	0.762424000
1	1.549586000	1.734591000	-1.017091000
1	4.703653000	-1.635939000	0.797260000
1	3.981036000	2.196763000	-0.995876000
1	5.557426000	0.519320000	-0.081144000
7	0.382000000	-0.539229000	-0.062709000
6	-1.785987000	0.152665000	-0.051897000
6	-2.603665000	1.283474000	-0.027119000
6	-2.347171000	-1.128197000	-0.088211000
6	-3.985913000	1.139852000	-0.040069000
6	-3.727198000	-1.260291000	-0.099380000
6	-4.548354000	-0.131352000	-0.076020000
1	-2.140221000	2.263224000	0.002890000
1	-1.718334000	-2.008436000	-0.108924000
1	-4.619197000	2.018656000	-0.022902000
1	-4.168396000	-2.249561000	-0.128572000
1	-5.625691000	-0.248452000	-0.086699000
7	-0.390801000	0.431246000	-0.041113000
1	-0.259009000	3.426791000	1.484858000
1	0.018024000	2.359823000	0.434066000
8	0.173307000	-3.531907000	-0.006096000
1	0.247713000	-2.576506000	-0.143059000
1	-0.027349000	-3.604693000	0.933010000



Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -648.883699

6	-2.893022000	-0.005087000	-0.296965000
6	-3.469674000	1.268970000	-0.178275000
6	-3.692776000	-1.127964000	-0.034598000
6	-4.802264000	1.408499000	0.188899000
6	-5.024190000	-0.975860000	0.331395000
6	-5.593416000	0.290839000	0.446574000
1	-2.860573000	2.144662000	-0.379098000
1	-3.256936000	-2.118038000	-0.123401000
1	-5.225173000	2.403540000	0.276980000
1	-5.621358000	-1.858940000	0.532026000
1	-6.631633000	0.404598000	0.733685000
7	-1.580432000	-0.153209000	-0.719945000
6	2.796229000	-0.111780000	-0.017698000
6	3.749735000	-1.124134000	0.118042000
6	3.154554000	1.232895000	-0.040547000
6	5.082713000	-0.769305000	0.231982000
6	4.495127000	1.579910000	0.076109000
6	5.452750000	0.579163000	0.211220000
1	3.433842000	-2.160053000	0.130811000
1	2.377605000	1.981548000	-0.148516000
1	5.840834000	-1.535992000	0.337976000
1	4.792147000	2.621384000	0.062018000
1	6.499387000	0.846394000	0.301733000
7	1.392032000	-0.364958000	-0.142782000
1	-1.131535000	-1.020163000	-0.452488000
8	1.068105000	-1.524705000	-0.113362000
1	-0.977235000	0.638995000	-0.542575000



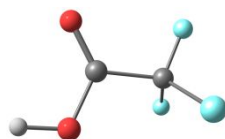
Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -648.926788

8	0.156242000	3.013141000	0.505492000
6	1.756557000	-0.518634000	-0.058728000
6	2.607716000	-1.478876000	0.485934000
6	2.274010000	0.640463000	-0.643748000
6	3.980115000	-1.261468000	0.489721000
6	3.647018000	0.840908000	-0.651595000
6	4.499899000	-0.101728000	-0.077706000
1	2.177890000	-2.378883000	0.910716000
1	1.608740000	1.356257000	-1.110822000
1	4.643287000	-1.999415000	0.925539000
1	4.056291000	1.732622000	-1.111888000
1	5.570994000	0.063987000	-0.086483000
7	0.367913000	-0.820365000	-0.010439000
6	-1.779001000	-0.117771000	-0.051434000
6	-2.616015000	0.994648000	0.015574000
6	-2.312681000	-1.407570000	-0.123763000
6	-3.995417000	0.820909000	0.019966000
6	-3.689258000	-1.570922000	-0.120798000
6	-4.532154000	-0.460252000	-0.047870000
1	-2.173195000	1.983280000	0.065456000
1	-1.648702000	-2.260309000	-0.184484000
1	-4.647461000	1.684720000	0.072319000
1	-4.111355000	-2.567476000	-0.180080000
1	-5.607191000	-0.598747000	-0.048367000
7	-0.382297000	0.166511000	-0.056232000
1	-0.121463000	3.116040000	1.421552000
1	0.058183000	2.061537000	0.335982000

2.3.5. Thermodynamic assessment of protonation steps

Reactants in order to make this evaluation: addition of the Free energies of the products of hydride transfer processes to the free energy of Trifluoroacetica acid molecule .

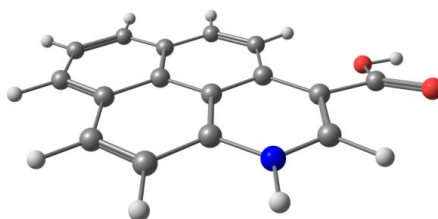


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -526.775920

8	-1.473787000	1.221330000	-0.001979000
6	-0.941748000	0.151928000	-0.004002000
8	-1.509495000	-1.033177000	-0.002052000
6	0.589057000	-0.002565000	-0.001437000
9	0.992615000	-0.630301000	1.104548000
9	0.996086000	-0.718092000	-1.050180000
9	1.173546000	1.186117000	-0.047782000
1	-2.477824000	-0.940924000	0.005597000

Product in order to make this evaluation: addition of the Free energies of the products of protonation (including carboxylate) to the free energy of model organic fragment shown below generated as a result of hydride transfer.

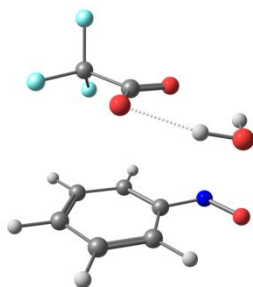


Charge = 1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -820.546340

6	-4.074661000	-1.199152000	-0.009765000
6	-2.976234000	-2.049425000	-0.040520000
6	-1.675928000	-1.530983000	-0.038412000
6	-1.489313000	-0.130361000	-0.004697000
6	-2.611754000	0.733748000	0.021759000
6	-3.896966000	0.179058000	0.020343000
6	-0.519158000	-2.369107000	-0.080233000
6	-0.172333000	0.401524000	-0.001955000
6	0.969835000	-0.452304000	-0.020956000
6	0.744753000	-1.864818000	-0.075446000
6	2.248310000	0.173130000	-0.012191000
6	2.327672000	1.547826000	-0.008865000
6	-0.025434000	1.804027000	0.018846000
6	-2.398990000	2.149211000	0.047157000

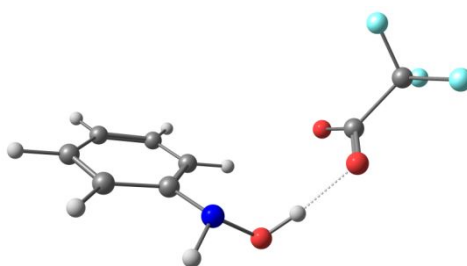
1	-3.264058000	2.802979000	0.066156000
1	-0.667628000	-3.443015000	-0.122023000
1	-5.076146000	-1.611450000	-0.011009000
1	-3.115241000	-3.124647000	-0.067437000
1	-4.755713000	0.841274000	0.042051000
1	1.586190000	-2.537153000	-0.116425000
1	3.275772000	2.067713000	-0.013300000
6	3.583386000	-0.501283000	-0.006624000
8	4.601437000	0.082339000	-0.289529000
8	3.555577000	-1.772610000	0.366428000
1	4.459841000	-2.127741000	0.342349000
7	1.230236000	2.311624000	0.009527000
1	1.344698000	3.324274000	0.022579000
1	-0.974496000	3.745801000	0.059763000
6	-1.146681000	2.676036000	0.044129000



Charge = -1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -964.165898

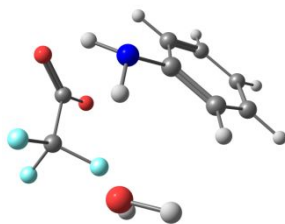
1	-1.193708000	-2.550054000	0.553844000
8	-1.586369000	-2.265276000	1.388768000
8	-3.320831000	-1.240662000	-0.869041000
6	-1.820363000	0.398224000	-0.648754000
6	-0.748088000	1.034607000	-1.266873000
6	-2.284734000	0.798155000	0.605803000
6	-0.118615000	2.089981000	-0.618377000
6	-1.653489000	1.852700000	1.244246000
6	-0.573392000	2.494718000	0.633472000
1	-0.416428000	0.679394000	-2.236011000
1	-3.113879000	0.272754000	1.062325000
1	0.723410000	2.589922000	-1.081478000
1	-1.992381000	2.175447000	2.221374000
1	-0.078664000	3.312578000	1.145060000
7	-2.383335000	-0.689919000	-1.389492000
8	0.670432000	-1.775472000	-0.413958000
1	-0.932100000	-1.602739000	1.668791000
6	1.072474000	-0.902073000	0.368782000
8	0.637364000	-0.540957000	1.474582000
6	2.358484000	-0.177257000	-0.114758000
9	3.418587000	-1.000497000	-0.018601000
9	2.274422000	0.191097000	-1.403142000
9	2.650176000	0.920149000	0.591575000



Charge = -1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -888.967034

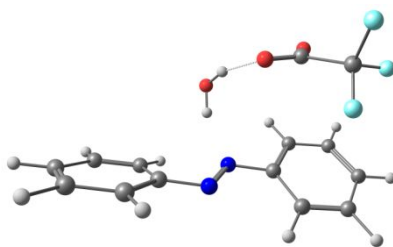
1	0.149739000	-1.705490000	-0.722451000
8	-0.773209000	-1.887240000	-1.022094000
6	-2.427971000	-0.635158000	0.077879000
6	-2.130729000	0.498482000	-0.681886000
6	-3.593600000	-0.660969000	0.853247000
6	-2.994151000	1.589293000	-0.660014000
6	-4.442056000	0.437518000	0.870582000
6	-4.151184000	1.571133000	0.112936000
1	-1.228069000	0.516840000	-1.278142000
1	-3.826164000	-1.545824000	1.437815000
1	-2.753544000	2.463726000	-1.255044000
1	-5.342502000	0.403819000	1.474290000
1	-4.817767000	2.425263000	0.125311000
7	-1.541476000	-1.724237000	0.144817000
8	1.633765000	-1.317783000	-0.054155000
1	-2.038530000	-2.595267000	0.307014000
6	1.960818000	-0.154929000	-0.363469000
8	1.395183000	0.672593000	-1.082867000
6	3.276755000	0.352287000	0.280327000
9	4.025022000	-0.626713000	0.798000000
9	4.038485000	1.010851000	-0.604699000
9	3.004711000	1.213649000	1.277011000



Charge = -1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -890.218175

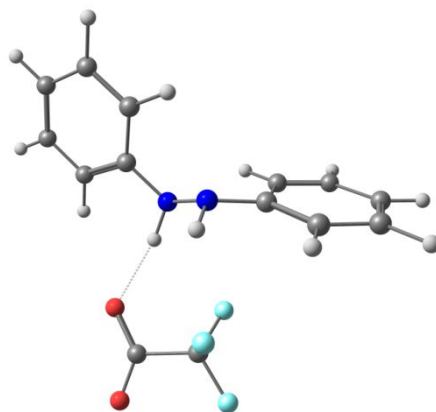
6	-1.381901000	0.362572000	0.795121000
6	-2.007794000	1.220018000	-0.123288000
6	-1.825922000	-0.966200000	0.876976000
6	-3.043021000	0.760982000	-0.927112000
6	-2.859753000	-1.414994000	0.064694000
6	-3.481827000	-0.558905000	-0.841454000
1	-1.660316000	2.244660000	-0.204267000
1	-1.335649000	-1.643933000	1.568565000
1	-3.507497000	1.442532000	-1.632154000
1	-3.179318000	-2.448975000	0.140071000
1	-4.287233000	-0.914407000	-1.472924000
7	-0.380893000	0.836316000	1.632600000
1	0.256213000	0.120608000	1.962553000
1	0.103744000	1.654171000	1.274526000
8	1.422880000	-1.644339000	1.392547000
8	0.823632000	3.221946000	0.149989000
1	0.110473000	3.864768000	0.070836000
1	0.786460000	2.724111000	-0.674324000
6	1.335668000	-1.494670000	0.163575000
8	0.830516000	-2.216034000	-0.705923000
6	1.968182000	-0.194405000	-0.412521000
9	2.482819000	0.615750000	0.519328000
9	2.958765000	-0.485266000	-1.273002000
9	1.063011000	0.527658000	-1.105207000



Charge = -1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1175.262559

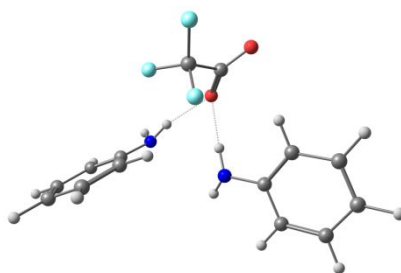
8	0.887934000	-1.650436000	-2.109452000
6	-0.280883000	1.448783000	-0.453526000
6	-1.205521000	0.992621000	-1.390645000
6	-0.635923000	2.423496000	0.481399000
6	-2.507028000	1.479653000	-1.370691000
6	-1.930908000	2.919746000	0.480825000
6	-2.869116000	2.445026000	-0.437256000
1	-0.901663000	0.231536000	-2.100768000
1	0.099173000	2.780140000	1.191847000
1	-3.232926000	1.102087000	-2.081381000
1	-2.215442000	3.679395000	1.199885000
1	-3.882174000	2.830411000	-0.421646000
7	1.011920000	0.859505000	-0.537865000
6	3.041640000	0.456595000	0.328013000
6	3.715120000	0.227890000	1.526372000
6	3.642967000	0.144291000	-0.894291000
6	4.977855000	-0.352025000	1.509664000
6	4.910228000	-0.419775000	-0.903392000
6	5.575214000	-0.676987000	0.295562000
1	3.230078000	0.497285000	2.457629000
1	3.131474000	0.370791000	-1.821724000
1	5.496787000	-0.543540000	2.441501000
1	5.386731000	-0.654580000	-1.848141000
1	6.564882000	-1.118761000	0.279513000
7	1.748591000	1.039559000	0.444111000
8	-0.783239000	-1.910317000	0.119071000
1	0.301789000	-1.937591000	-1.385773000
1	1.138582000	-0.763243000	-1.813719000
6	-1.952171000	-1.708026000	-0.264166000
8	-2.484817000	-1.917579000	-1.357554000
6	-2.864147000	-1.120417000	0.845780000
9	-2.289428000	-0.085189000	1.473295000
9	-4.048085000	-0.698232000	0.387158000
9	-3.118472000	-2.050573000	1.786287000



Charge = -1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1100.044317

6	2.355092000	-0.084085000	-0.036143000
6	3.074543000	0.957873000	-0.639372000
6	3.051245000	-1.084042000	0.651461000
6	4.459718000	0.988903000	-0.559383000
6	4.439712000	-1.038215000	0.724011000
6	5.156506000	-0.008404000	0.121416000
1	2.534426000	1.740890000	-1.162092000
1	2.500294000	-1.887578000	1.124164000
1	4.998184000	1.803689000	-1.031402000
1	4.965137000	-1.822358000	1.258844000
1	6.237925000	0.019151000	0.181973000
7	0.968236000	-0.121186000	-0.202146000
6	-0.698887000	-1.758709000	0.268289000
6	-1.781738000	-2.117201000	1.081585000
6	-0.545291000	-2.376577000	-0.977079000
6	-2.683280000	-3.084518000	0.657844000
6	-1.458448000	-3.340265000	-1.389829000
6	-2.530720000	-3.705747000	-0.580390000
1	-1.909735000	-1.627177000	2.041684000
1	0.286058000	-2.094274000	-1.610769000
1	-3.517805000	-3.348171000	1.298645000
1	-1.326788000	-3.811049000	-2.358377000
1	-3.238480000	-4.456825000	-0.910382000
7	0.236680000	-0.836874000	0.746337000
1	-0.107426000	-0.259628000	1.507229000
8	0.031413000	2.673613000	-0.334767000
1	0.558719000	0.789843000	-0.416440000
6	-1.158191000	3.012207000	-0.184892000
8	-1.684302000	4.127218000	-0.204327000
6	-2.106131000	1.813010000	0.092242000
9	-3.400985000	2.128539000	0.021904000
9	-1.892419000	0.805173000	-0.770571000
9	-1.888439000	1.311607000	1.326644000

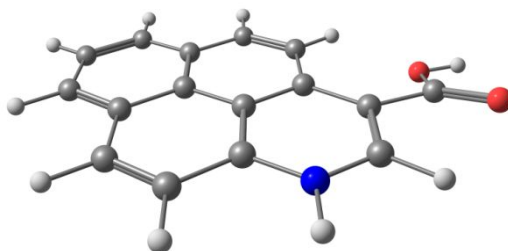


Charge = -1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1101.264872

6	2.816497000	-0.760774000	0.760843000
6	4.099408000	-1.262461000	1.029210000
6	2.349941000	-0.796783000	-0.563975000
6	4.886147000	-1.778552000	0.006236000
6	3.146779000	-1.311744000	-1.577741000
6	4.421085000	-1.808132000	-1.306443000
1	4.471340000	-1.239670000	2.048771000
1	1.353720000	-0.426677000	-0.778142000
1	5.875376000	-2.157584000	0.240003000
1	2.765355000	-1.325565000	-2.593150000
1	5.038529000	-2.208064000	-2.101579000
7	2.002727000	-0.295072000	1.781240000
6	-2.285468000	-1.398046000	0.283754000
6	-3.075038000	-0.272865000	-0.008790000
6	-2.867091000	-2.670039000	0.164459000
6	-4.397495000	-0.425418000	-0.405149000
6	-4.190799000	-2.808589000	-0.234486000
6	-4.970099000	-1.690643000	-0.524033000
1	-2.646219000	0.720386000	0.079510000
1	-2.267704000	-3.546286000	0.390801000
1	-4.987128000	0.458535000	-0.624136000
1	-4.616843000	-3.802798000	-0.317627000
1	-6.001881000	-1.802212000	-0.834447000
7	-0.950500000	-1.251261000	0.625554000
1	-0.707340000	-0.357447000	1.044863000
1	2.492747000	-0.052074000	2.631949000
1	1.305902000	0.403546000	1.526706000
8	-0.331544000	1.482880000	1.596023000
6	0.143571000	2.412929000	-0.505905000
9	0.011879000	3.559166000	-1.183492000
9	1.455159000	2.254026000	-0.255433000
9	-0.205306000	1.419917000	-1.356433000
1	-0.540211000	-2.037019000	1.112554000
6	-0.730539000	2.340019000	0.778925000
8	-1.710733000	3.077855000	0.791871000

+



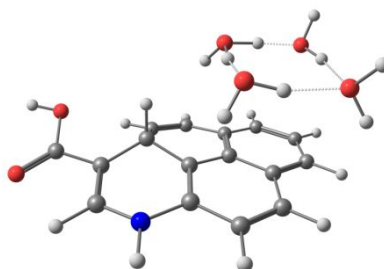
Charge = 1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -820.546340

6	-4.074661000	-1.199152000	-0.009765000
6	-2.976234000	-2.049425000	-0.040520000
6	-1.675928000	-1.530983000	-0.038412000
6	-1.489313000	-0.130361000	-0.004697000
6	-2.611754000	0.733748000	0.021759000
6	-3.896966000	0.179058000	0.020343000
6	-0.519158000	-2.369107000	-0.080233000
6	-0.172333000	0.401524000	-0.001955000
6	0.969835000	-0.452304000	-0.020956000
6	0.744753000	-1.864818000	-0.075446000
6	2.248310000	0.173130000	-0.012191000
6	2.327672000	1.547826000	-0.008865000
6	-0.025434000	1.804027000	0.018846000
6	-2.398990000	2.149211000	0.047157000
1	-3.264058000	2.802979000	0.066156000
1	-0.667628000	-3.443015000	-0.122023000
1	-5.076146000	-1.611450000	-0.011009000
1	-3.115241000	-3.124647000	-0.067437000
1	-4.755713000	0.841274000	0.042051000
1	1.586190000	-2.537153000	-0.116425000
1	3.275772000	2.067713000	-0.013300000
6	3.583386000	-0.501283000	-0.006624000
8	4.601437000	0.082339000	-0.289529000
8	3.555577000	-1.772610000	0.366428000
1	4.459841000	-2.127741000	0.342349000
7	1.230236000	2.311624000	0.009527000
1	1.344698000	3.324274000	0.022579000
1	-0.974496000	3.745801000	0.059763000
6	-1.146681000	2.676036000	0.044129000

2.4. PBE-D2 Optimized geometries associated with the Organic Catalyst: ox-CF

2.4.1. Hydrogen Evolution Reaction

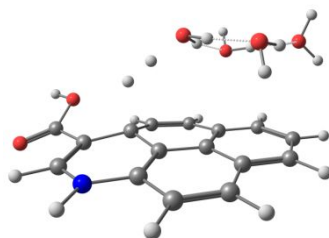


Charge = 1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1126.527429

6	-3.383431	0.655284	-1.625123
6	-2.484535	-0.424027	-1.820431
6	-1.181563	-0.364185	-1.335097
6	-0.739142	0.798789	-0.615229
6	-1.629997	1.918812	-0.479423
6	-2.959988	1.809758	-0.977139
6	-0.199076	-1.405577	-1.618634
6	0.579173	0.857920	-0.089107
6	1.454636	-0.399441	-0.012522
6	1.038956	-1.407633	-1.068942
6	2.935110	-0.002833	-0.006757
6	3.285387	1.245353	0.429053
6	1.033659	2.076681	0.424062
6	-1.146105	3.105363	0.137783
1	-1.822645	3.955543	0.253660
1	-0.484347	-2.187522	-2.328976
1	-4.403307	0.586098	-2.010345
1	-2.805863	-1.309412	-2.374821
1	-3.636509	2.659548	-0.853544
1	1.751471	-2.190801	-1.325788
1	4.333685	1.522626	0.545603
6	4.056278	-0.932498	-0.196895
8	5.239523	-0.617420	-0.296937
8	3.671308	-2.247487	-0.200498
1	4.494949	-2.767632	-0.319977
7	2.376418	2.201962	0.770290
1	2.713691	3.113556	1.076180
1	0.562216	4.119393	0.980860
1	1.253681	-0.888782	0.971423
8	-0.892664	-2.635429	1.105210
1	-0.925372	-1.703485	1.629835
1	-1.930072	-2.847227	0.864736

1	-0.415541	-2.475771	0.248305
8	-1.212237	-0.464900	2.308808
1	-0.657538	0.285093	2.016138
1	-2.142478	-0.236946	2.031498
8	-3.300336	-2.920758	0.585957
1	-3.663619	-2.026021	0.836092
1	-3.769648	-3.575537	1.138439
8	-3.727964	-0.355378	1.323988
1	-3.789509	0.218973	0.526269
1	-4.471447	-0.093858	1.902033
6	0.166011	3.194802	0.552422



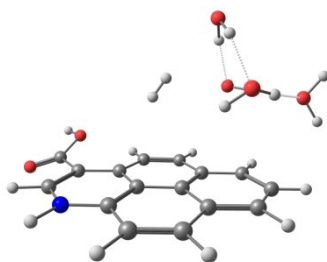
(Transition state)

Charge = 1 Multiplicity =1

Sum of electronic and thermal Free Energies= -1126.496841

6	-3.374540	-0.235356	-1.930788
6	-2.337542	-1.187500	-1.996591
6	-1.059775	-0.892950	-1.506643
6	-0.816024	0.385988	-0.911693
6	-1.865116	1.361049	-0.866552
6	-3.143991	1.024423	-1.380758
6	0.048650	-1.808457	-1.644779
6	0.478160	0.700800	-0.413929
6	1.518994	-0.338731	-0.322123
6	1.277686	-1.542975	-1.130090
6	2.872699	0.175224	-0.087296
6	3.037018	1.484938	0.314611
6	0.716783	2.002314	0.061091
6	-1.586226	2.648777	-0.316049
1	-2.390656	3.386528	-0.267275
1	-0.121296	-2.732524	-2.203622
1	-4.361711	-0.483444	-2.327472
1	-2.517298	-2.164949	-2.451076
1	-3.939292	1.773586	-1.346023
1	2.094615	-2.250546	-1.254184
1	4.022474	1.884147	0.553071
6	4.119440	-0.626681	-0.081955
8	5.245997	-0.150216	-0.118308
8	3.897274	-1.963464	0.026249
1	4.781049	-2.393217	0.034543
7	1.997683	2.336637	0.449973
1	2.176867	3.289792	0.772024
1	-0.092183	3.963181	0.524255
1	1.202432	-0.965343	1.043198
8	-0.373134	-1.346427	2.619239
1	-0.872608	-0.460818	2.630926
1	-1.007907	-1.969890	2.122309
1	0.593058	-1.150322	1.732596
8	-1.861377	0.831919	2.513570

1	-1.542477	1.525775	1.907120
1	-2.662844	0.454294	2.072208
8	-2.119981	-2.763300	1.249096
1	-2.845313	-2.091867	1.187046
1	-2.505047	-3.497850	1.761539
8	-3.862148	-0.629593	1.298922
1	-4.082017	-0.307631	0.400998
1	-4.716250	-0.728664	1.761819
6	-0.321286	2.971130	0.127887

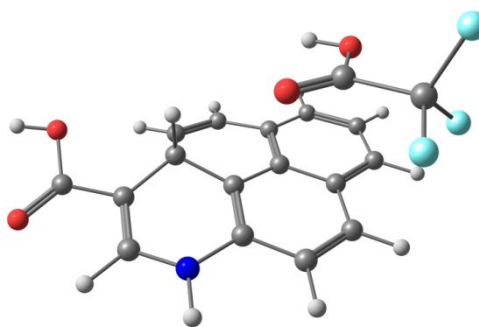


Charge = 1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1126.537031

6	-2.960735	1.388398	-1.326475
6	-2.322706	0.161237	-1.536740
6	-0.974193	-0.018720	-1.162591
6	-0.264192	1.067477	-0.570416
6	-0.923248	2.318512	-0.351285
6	-2.274352	2.454714	-0.735199
6	-0.292167	-1.259464	-1.349278
6	1.094894	0.893829	-0.188557
6	1.768473	-0.363310	-0.386194
6	1.023947	-1.427948	-0.983924
6	3.141525	-0.442452	0.025226
6	3.746643	0.680055	0.578669
6	1.764481	1.997873	0.407125
6	-0.199455	3.390639	0.260071
1	-0.713655	4.339786	0.427863
1	-0.856560	-2.093840	-1.770286
1	-4.004582	1.518368	-1.621775
1	-2.855820	-0.681002	-1.981906
1	-2.777929	3.408618	-0.560836
1	1.505762	-2.389028	-1.143120
1	4.788586	0.673795	0.895051
6	4.063611	-1.619883	-0.077619
8	5.276741	-1.524013	0.020778
8	3.434673	-2.801486	-0.258708
1	4.134301	-3.490219	-0.313725
7	3.073734	1.830145	0.761546
1	3.565683	2.621418	1.188863
1	1.677688	4.052043	1.098622
1	-0.106430	-0.667223	1.790832
8	-2.499388	-2.512529	2.335547
1	-2.789292	-1.571413	2.379683
1	-2.575308	-2.697743	1.370985
1	-0.663814	-1.158200	1.934791
8	-3.239824	0.202266	1.990962
1	-2.446002	0.427965	1.471937
1	-3.899690	-0.039875	1.300462

8	-3.014322	-2.773784	-0.457083
1	-3.767547	-2.143816	-0.352172
1	-3.442969	-3.631618	-0.626769
8	-4.986371	-0.895091	0.101498
1	-5.331050	-0.345543	-0.628188
1	-5.775728	-1.274450	0.533537
6	1.115165	3.240386	0.632417

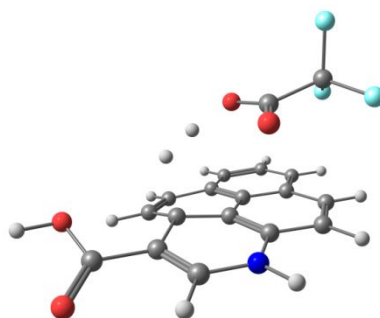


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1347.061464

6	-2.271086	3.048663	0.651999
6	-1.056668	3.312902	-0.027929
6	-0.010994	2.391043	-0.016498
6	-0.179085	1.145093	0.683638
6	-1.383160	0.916080	1.434951
6	-2.426704	1.881913	1.381832
6	1.302483	2.684096	-0.579916
6	0.849453	0.170255	0.654756
6	1.987157	0.288527	-0.361333
6	2.268201	1.746083	-0.678265
6	3.185760	-0.553010	0.086079
6	2.999246	-1.570418	0.984035
6	0.732642	-0.944764	1.485793
6	-1.493541	-0.284143	2.191056
1	-2.415366	-0.479068	2.744652
1	1.497552	3.714775	-0.892879
1	-3.078877	3.783698	0.614543
1	-0.918615	4.264376	-0.549612
1	-3.350823	1.683181	1.931140
1	3.250400	2.000953	-1.075936
1	3.819251	-2.240654	1.245057
6	4.503645	-0.526025	-0.554483
8	5.506180	-1.132190	-0.177514
8	4.528287	0.227289	-1.700792
1	5.445774	0.160403	-2.041631
7	1.803134	-1.837017	1.574557
1	1.738348	-2.607805	2.236957
1	-0.504912	-2.086035	2.852479
1	1.592277	-0.150641	-1.307104
6	-0.444597	-1.180108	2.243002
6	-3.120441	-1.483106	-0.839687
9	-2.666706	-2.555551	-0.160353
9	-3.941962	-0.780374	-0.025320
9	-3.859361	-1.929851	-1.890323
6	-1.928311	-0.640090	-1.368493

8	-0.826134	-1.113599	-1.524215
8	-2.335414	0.600238	-1.648063
1	-1.552027	1.136058	-1.914136



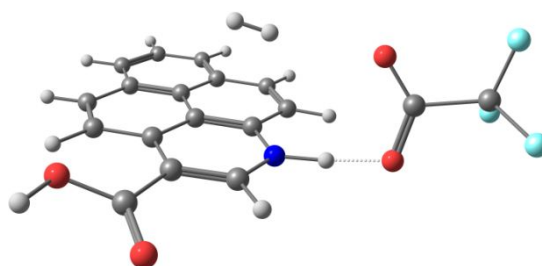
(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1347.030890

6	-2.258325	3.640170	-0.082933
6	-0.976887	3.714611	-0.660489
6	-0.023634	2.714169	-0.425052
6	-0.366031	1.610794	0.419400
6	-1.653152	1.563448	1.044623
6	-2.592443	2.585558	0.762016
6	1.322702	2.786311	-0.944928
6	0.583527	0.580571	0.657058
6	1.818340	0.513606	-0.140197
6	2.213055	1.770013	-0.790018
6	2.806872	-0.452937	0.344590
6	2.443970	-1.367187	1.313669
6	0.264674	-0.425830	1.585243
6	-1.948859	0.483184	1.930151
1	-2.939351	0.435904	2.388725
1	1.620946	3.698367	-1.469391
1	-2.989610	4.424788	-0.289915
1	-0.709071	4.561903	-1.297564
1	-3.581045	2.533993	1.225415
1	3.219334	1.847452	-1.196708
1	3.141698	-2.129671	1.658650
6	4.159107	-0.659849	-0.220925
8	5.052221	-1.294259	0.326220
8	4.310544	-0.112240	-1.457518
1	5.230697	-0.310865	-1.738011
7	1.218607	-1.377711	1.876066
1	0.988988	-2.108361	2.551593
1	-1.220754	-1.299423	2.903974
1	1.290859	-0.201608	-1.449137
6	-1.007222	-0.478521	2.215884
6	-2.639974	-1.896066	-0.758387
9	-2.893132	-2.539241	0.410383
9	-3.292076	-0.703671	-0.712015

9	-3.217344	-2.631112	-1.755729
6	-1.104243	-1.756767	-1.020018
8	-0.348554	-2.579444	-0.509622
8	-0.844404	-0.763040	-1.804829
1	0.432698	-0.502082	-1.715975



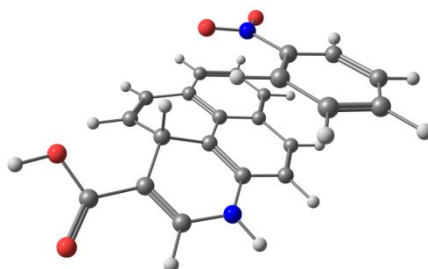
Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1347.090569

6	3.969944	-3.657528	0.177401
6	4.571342	-2.398773	0.279382
6	3.799296	-1.223908	0.166070
6	2.393274	-1.331768	-0.057089
6	1.783957	-2.622042	-0.164401
6	2.592928	-3.771426	-0.042235
6	4.372605	0.082664	0.258968
6	1.604281	-0.153037	-0.172365
6	2.195866	1.153195	-0.056311
6	3.612160	1.223291	0.153367
6	1.319775	2.278572	-0.186811
6	-0.034927	2.050541	-0.435051
6	0.207560	-0.295776	-0.410489
6	0.373176	-2.708576	-0.396600
1	-0.081220	-3.698993	-0.478517
1	5.451144	0.163909	0.418051
1	4.579511	-4.558946	0.269348
1	5.647278	-2.309535	0.449674
1	2.124544	-4.755622	-0.122488
1	4.090730	2.196223	0.230151
1	-0.730971	2.882958	-0.544005
6	1.676552	3.728136	-0.093509
8	0.943213	4.624668	-0.482652
8	2.872309	3.969341	0.492884
1	2.995018	4.944757	0.493869
7	-0.557867	0.823507	-0.537192
1	-1.672942	0.694778	-0.664482
1	-1.474509	-1.637878	-0.709566
1	-0.414671	1.277456	2.632998
6	-0.400567	-1.580513	-0.520071
6	-5.033438	-0.491974	0.109472

9	-5.832586	0.245680	-0.715122
9	-4.918007	-1.733649	-0.457337
9	-5.707062	-0.652433	1.277252
6	-3.624358	0.157729	0.299352
8	-3.063595	0.397794	-0.826694
8	-3.215361	0.333284	1.452403
1	-1.059035	1.066423	2.300160

2.4.2. Hydride transfer processes

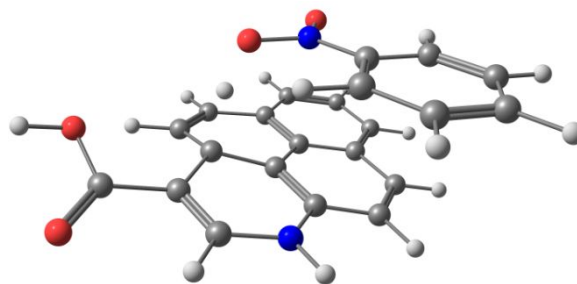


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1256.946231

6	-2.945481	3.210722	0.459362
6	-1.685358	3.560679	-0.084360
6	-0.596760	2.695928	0.007878
6	-0.762595	1.422931	0.655720
6	-2.019798	1.107033	1.277116
6	-3.107098	2.015269	1.141083
6	0.748951	3.084374	-0.397754
6	0.327132	0.518097	0.736186
6	1.574060	0.739698	-0.121879
6	1.784424	2.217930	-0.387263
6	2.764470	-0.026736	0.456616
6	2.545010	-1.072988	1.312653
6	0.198656	-0.606453	1.554863
6	-2.124447	-0.098280	2.025418
1	-3.080860	-0.352028	2.489982
1	0.907381	4.130641	-0.678029
1	-3.784345	3.904711	0.363643
1	-1.548962	4.535389	-0.561747
1	-4.066002	1.755717	1.598490
1	2.784825	2.545731	-0.669478
1	3.371939	-1.694926	1.657769
6	4.144080	0.103928	-0.021316
8	5.136723	-0.423599	0.479225
8	4.247857	0.860833	-1.160508
1	5.202266	0.866716	-1.388262
7	1.309190	-1.427034	1.756622
1	1.217693	-2.218745	2.390418
1	-1.087449	-1.826023	2.801349
1	1.342823	0.300447	-1.122280
6	-1.028198	-0.920189	2.192178
8	-0.239971	0.034156	-2.672777
8	-2.324484	0.397857	-2.121721
6	-1.315723	-1.558656	-1.352616
6	-0.134723	-2.303579	-1.250136

6	-2.517200	-1.978017	-0.771016
6	-0.162596	-3.500299	-0.531337
6	-2.531150	-3.185787	-0.068190
6	-1.358188	-3.943470	0.055279
1	0.781203	-1.936376	-1.713538
1	-3.411469	-1.363895	-0.873520
1	0.752233	-4.087171	-0.427429
1	-3.459814	-3.531521	0.390523
1	-1.373962	-4.883293	0.612036
7	-1.293950	-0.286130	-2.098705



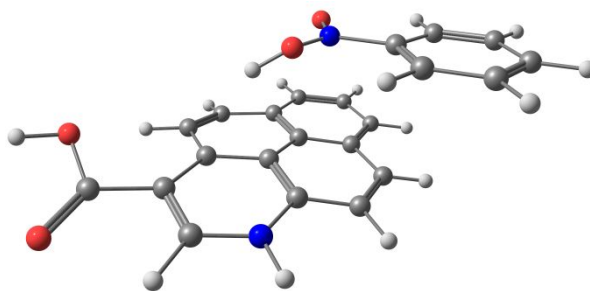
(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1256.935085

6	2.589867	3.639215	-0.191058
6	1.278887	3.822023	0.291767
6	0.290301	2.847729	0.086278
6	0.640166	1.639816	-0.602245
6	1.972639	1.464889	-1.105526
6	2.933498	2.487239	-0.888744
6	-1.078539	3.032411	0.503871
6	-0.330651	0.614087	-0.772465
6	-1.646277	0.705376	-0.091359
6	-2.008394	2.040197	0.381633
6	-2.646423	-0.301422	-0.547737
6	-2.213414	-1.379307	-1.282688
6	0.030521	-0.533441	-1.499796
6	2.289178	0.266257	-1.810566
1	3.304515	0.133409	-2.192209
1	-1.360248	3.998378	0.931578
1	3.338809	4.416882	-0.021666
1	1.012503	4.741113	0.820977
1	3.947368	2.345777	-1.272441
1	-3.030373	2.207607	0.717347
1	-2.896741	-2.178315	-1.568328
6	-4.066095	-0.371262	-0.149921
8	-4.898018	-1.133294	-0.634893
8	-4.390991	0.482431	0.864047
1	-5.346428	0.342351	1.041127
7	-0.919757	-1.531957	-1.669870
1	-0.656555	-2.365773	-2.194389
1	1.562693	-1.617806	-2.578456
1	-1.209345	0.170341	1.113943
6	1.330871	-0.702154	-2.028926
8	-0.682435	-0.420541	2.029599
8	1.306801	0.593379	2.222844
6	1.226334	-1.543699	1.258581

6	0.443391	-2.655611	0.883717
6	2.621391	-1.536842	1.052281
6	1.066903	-3.747407	0.279253
6	3.223916	-2.644367	0.452971
6	2.454538	-3.748881	0.056204
1	-0.631087	-2.644612	1.063534
1	3.197951	-0.664923	1.360192
1	0.463029	-4.607840	-0.019546
1	4.303935	-2.640919	0.286232
1	2.932526	-4.609550	-0.417191
7	0.629604	-0.406756	1.873210

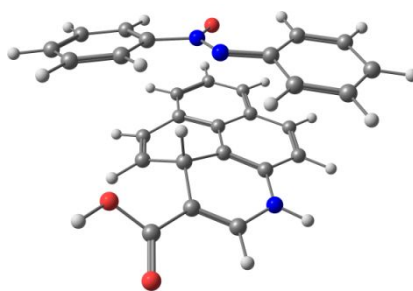


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1256.944633

6	-2.891221	-1.676066	1.502614
6	-2.209577	-0.484100	1.789413
6	-0.866897	-0.307239	1.392984
6	-0.202667	-1.368915	0.698574
6	-0.902568	-2.590559	0.419868
6	-2.255671	-2.717406	0.827673
6	-0.150047	0.904228	1.633689
6	1.153052	-1.203530	0.282878
6	1.864042	0.034390	0.544326
6	1.203670	1.028453	1.289165
6	3.216353	0.128451	0.012434
6	3.784988	-0.979065	-0.592169
6	1.784398	-2.283637	-0.378436
6	-0.216439	-3.637027	-0.264695
1	-0.753478	-4.564067	-0.480348
1	-0.633987	1.691167	2.214043
1	-3.933496	-1.788108	1.811571
1	-2.710102	0.323231	2.328326
1	-2.787420	-3.646269	0.605533
1	1.735610	1.938192	1.564264
1	4.801739	-0.953222	-0.982923
6	4.064882	1.341993	-0.035942
8	5.264071	1.349016	-0.285962
8	3.369275	2.497570	0.170726
1	4.014598	3.231500	0.073949
7	3.107205	-2.132261	-0.762733
1	3.569012	-2.913478	-1.231520
1	1.633780	-4.292768	-1.170693
1	0.851711	2.239735	-0.399047
6	1.101153	-3.492187	-0.651258
8	0.116900	2.399862	-1.038390
8	-1.226478	3.527631	0.477459
6	-2.095430	1.656050	-0.652625
6	-1.851644	0.547190	-1.494688
6	-3.402470	1.907831	-0.182421
6	-2.914213	-0.265586	-1.884513

6	-4.455988	1.083389	-0.590490
6	-4.224347	-0.005928	-1.441911
1	-0.834850	0.346797	-1.828966
1	-3.564558	2.760060	0.478656
1	-2.717907	-1.118807	-2.539056
1	-5.467435	1.295735	-0.234128
1	-5.049992	-0.649412	-1.754101
7	-1.041995	2.444077	-0.150560

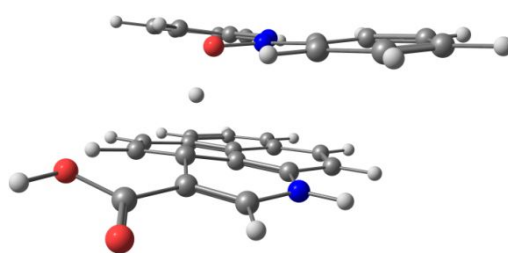


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1467.828706

6	-0.021320	-3.395865	2.492009
6	-1.144968	-2.557438	2.289795
6	-0.990048	-1.232930	1.886297
6	0.333015	-0.715976	1.662749
6	1.472044	-1.542296	1.956159
6	1.262958	-2.895723	2.345121
6	-2.111226	-0.304699	1.799953
6	0.508158	0.621540	1.223118
6	-0.681934	1.400996	0.662295
6	-1.975021	0.946063	1.309868
6	-0.396617	2.903446	0.681718
6	0.896029	3.347052	0.777960
6	1.794512	1.161065	1.229036
6	2.770382	-0.968523	1.860538
1	3.643020	-1.593317	2.068051
1	-3.078994	-0.647627	2.178957
1	-0.172643	-4.435350	2.793928
1	-2.152766	-2.942612	2.469667
1	2.135480	-3.525800	2.539514
1	-2.827205	1.624922	1.276154
1	1.128123	4.409964	0.698343
6	-1.384932	3.930419	0.345733
8	-1.228174	5.148179	0.432748
8	-2.553072	3.406250	-0.151658
1	-3.124443	4.178094	-0.351662
7	1.961800	2.517128	0.935690
1	2.896107	2.916299	0.999085
1	3.919624	0.823461	1.502392
1	-0.765748	1.088781	-0.404168
6	2.927916	0.364772	1.538960
8	0.078554	-2.717022	-1.370508
6	-1.829537	-1.375140	-1.516744
6	-2.583012	-2.402151	-0.939161
6	-2.429532	-0.198198	-1.983126
6	-3.964952	-2.235824	-0.806146
6	-3.812280	-0.047606	-1.846237

6	-4.581478	-1.059383	-1.253357
1	-2.078866	-3.301239	-0.586310
1	-1.819552	0.581845	-2.437465
1	-4.558960	-3.027222	-0.343662
1	-4.288065	0.868346	-2.203435
1	-5.660809	-0.931154	-1.142885
7	-0.372258	-1.558395	-1.582306
6	1.686566	-0.457477	-1.854160
6	2.201707	0.851665	-2.038380
6	2.598904	-1.535181	-1.705996
6	3.573940	1.086125	-2.062794
6	3.974405	-1.283019	-1.738754
6	4.470388	0.016106	-1.911044
1	1.490973	1.674408	-2.144686
1	2.227216	-2.545850	-1.566496
1	3.947438	2.104363	-2.195269
1	4.668673	-2.119066	-1.621946
1	5.548205	0.195115	-1.927900
7	0.290502	-0.476812	-1.827288



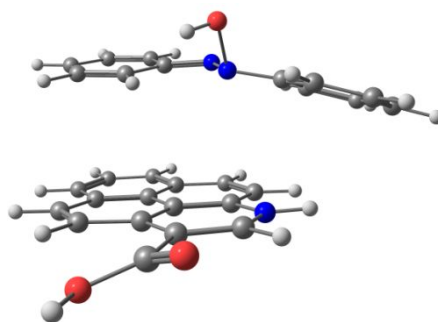
(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1467.818093

6	-3.781163	0.115700	2.044601
6	-3.351849	1.282318	1.386600
6	-1.998058	1.459739	1.060172
6	-1.043779	0.464166	1.457239
6	-1.489106	-0.719006	2.137259
6	-2.875691	-0.879265	2.399733
6	-1.525060	2.613169	0.337125
6	0.341169	0.653392	1.181642
6	0.789226	1.748404	0.285606
6	-0.207340	2.776080	0.009908
6	2.260002	2.033933	0.355358
6	3.083409	1.096874	0.933878
6	1.259037	-0.293872	1.668336
6	-0.521205	-1.692021	2.521500
1	-0.861205	-2.607468	3.012191
1	-2.254562	3.378142	0.057413
1	-4.843212	-0.015779	2.267535
1	-4.071561	2.052465	1.098146
1	-3.214421	-1.789691	2.901294
1	0.107810	3.660510	-0.541222
1	4.164769	1.231948	0.944535
6	2.973292	3.157056	-0.272900
8	4.161236	3.425686	-0.103488
8	2.200365	3.893794	-1.126438
1	2.787306	4.597714	-1.477827
7	2.620010	-0.051484	1.485858
1	3.286538	-0.729139	1.853242
1	1.576285	-2.196335	2.649694
1	0.665342	1.009130	-0.849409
6	0.828203	-1.469680	2.322643
8	0.584006	0.178373	-1.784603
6	1.410070	-1.903739	-1.065796

6	2.716678	-1.408996	-1.209424
6	1.191685	-3.241345	-0.680520
6	3.803502	-2.252635	-0.956641
6	2.288855	-4.067176	-0.429623
6	3.599550	-3.580858	-0.562463
1	2.871966	-0.374455	-1.513186
1	0.172287	-3.610970	-0.580780
1	4.817167	-1.859971	-1.066812
1	2.116498	-5.103511	-0.128936
1	4.452046	-4.234053	-0.362819
7	0.299009	-1.033085	-1.324462
6	-2.055167	-0.823577	-1.402903
6	-3.231909	-1.514165	-0.979118
6	-2.219935	0.425377	-2.078077
6	-4.497203	-0.980761	-1.190037
6	-3.501146	0.940438	-2.282395
6	-4.643905	0.262654	-1.831012
1	-3.105572	-2.473979	-0.473029
1	-1.352375	0.972323	-2.433835
1	-5.378237	-1.526712	-0.842681
1	-3.607020	1.899885	-2.796378
1	-5.637325	0.689186	-1.989608
7	-0.900498	-1.510473	-1.100744



Charge = 0 Multiplicity = 1

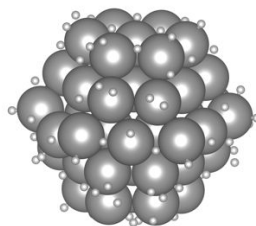
Sum of electronic and thermal Free Energies= -1467.827425

6	3.882558	-0.546183	1.773427
6	3.415421	-1.659540	1.080365
6	2.029307	-1.795712	0.797546
6	1.114911	-0.805335	1.283408
6	1.614199	0.354529	1.965368
6	3.006981	0.470236	2.182866
6	1.505355	-2.864529	0.021426
6	-0.288592	-0.964812	1.063316
6	-0.802381	-2.091333	0.321533
6	0.144944	-3.008264	-0.208924
6	-2.260616	-2.202662	0.202192
6	-3.043630	-1.187630	0.722451
6	-1.159583	0.061477	1.537416
6	0.692873	1.369667	2.359263
1	1.080723	2.270785	2.840432
1	2.201563	-3.599343	-0.391791
1	4.952550	-0.442826	1.971452
1	4.103714	-2.432140	0.729332
1	3.387969	1.355646	2.697721
1	-0.208462	-3.849723	-0.799835
1	-4.129501	-1.216835	0.639359
6	-3.045507	-3.287026	-0.428238
8	-4.270670	-3.294037	-0.519499
8	-2.298262	-4.317327	-0.912759
1	-2.938437	-4.957378	-1.293298
7	-2.522750	-0.110708	1.341666
1	-3.153272	0.626923	1.658748
1	-1.378092	1.980121	2.498710
1	-0.542811	-0.581037	-1.127528
6	-0.670447	1.211067	2.181042
8	-0.663198	0.177222	-1.756323
6	-1.455550	2.183892	-0.768980

6	-2.772709	1.732787	-1.006176
6	-1.243111	3.488093	-0.260520
6	-3.853983	2.571154	-0.718623
6	-2.338781	4.305226	0.020091
6	-3.652183	3.857152	-0.198283
1	-2.937405	0.738030	-1.417351
1	-0.224237	3.833839	-0.091515
1	-4.867405	2.207762	-0.907677
1	-2.161591	5.309952	0.412844
1	-4.503006	4.504221	0.026255
7	-0.357954	1.333027	-0.992051
6	2.008404	1.146691	-1.182426
6	3.201166	1.756379	-0.667665
6	2.176663	0.012191	-2.047055
6	4.463557	1.273425	-0.990795
6	3.452957	-0.455493	-2.350403
6	4.607407	0.147903	-1.820227
1	3.087987	2.626734	-0.017616
1	1.312501	-0.472714	-2.491752
1	5.347302	1.764240	-0.573727
1	3.549667	-1.320266	-3.013399
1	5.598858	-0.239220	-2.066528
7	0.866512	1.767148	-0.771697

2.5. PBE-D2 Optimized geometries associated with the Inorganic Catalyst: Ru-CF

2.5.1. Adsorption energies of the different reagents



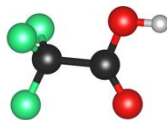
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H 88 Ru 57		
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0.0000000000000000	25.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000
H Ru		
88 57		
Direct		
0.5528452298544688	0.7193158900720705	0.4988039763595636
0.4919664668746489	0.7545516563876662	0.4566448364547648
0.4143621078283493	0.7231358065397163	0.4823303392420863
0.3246353776829808	0.6701712400729040	0.4891105686804098
0.2441059146986728	0.6377349637674176	0.4758018934299579
0.2457786447590602	0.6376122308788509	0.5124561855028500
0.2852054799296551	0.5555978206904952	0.6273199146349889
0.2714116135462563	0.5311261759530692	0.6072668232337851
0.3467085081582549	0.5487416960610435	0.6947918739120036
0.3673193529612535	0.5953677054027696	0.6215306603657682
0.4306479864747679	0.5882195676536573	0.7046225320186136
0.5456987885156213	0.5809278623801658	0.7075031763690313
0.5578110202109094	0.7014900313596033	0.6103247951757949
0.5299153120330555	0.6979890191404751	0.6284505765518785
0.4549698752100614	0.6661188702407609	0.5941087182910110
0.3038075020570391	0.6084937177356041	0.5612863960451336
0.5925226784541747	0.4943888176536463	0.7007448129099990
0.6272471891808843	0.5671575219658919	0.7022919670332651
0.5969416610424192	0.6154144759747256	0.6397316378122125
0.6657020529412495	0.6292159316388605	0.6018489645446148
0.6794021415983816	0.6111772098883507	0.5394227216003814
0.7273118054347369	0.6281381809906857	0.4745567684438792
0.6126919993949246	0.6703778648767607	0.5495671282233264
0.6541896142592133	0.6620589951131720	0.4730956064439860
0.6822832208472496	0.6027121938172858	0.4035251103860747
0.6208181817720243	0.5968207816208061	0.3273918463464978

0.6331604990370491 0.5454120735360117 0.2661926234966875
0.6047078990330146 0.5556813694261264 0.2463769105373642
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0.5206976410438913 0.6582263625278633 0.3353138162348857
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0.4910198464374878 0.3184187028337117 0.3332698923009137
0.3420475604840563 0.3384871706959780 0.4407133773474754
0.6152923280615310 0.4057781184362034 0.2623907460019271
0.6362454912750771 0.4291167901656925 0.2776097211974199
0.4522671986122600 0.4373400657992462 0.2725860661741470
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0.5965680024591500 0.3717889168650163 0.6367608990676430
0.5382640400703091 0.4049100301424892 0.7035032568899715
0.6661713896573919 0.3472278959042137 0.5934499326637339
0.6467029242406954 0.3243337828083507 0.5755727796495081
0.6419410356696018 0.5458076408826267 0.6168832559062277
0.6443659902969984 0.4408557191368394 0.6123008717414370
0.7226124423760829 0.5457276813988339 0.4717208155668821

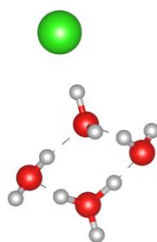
0.7182617771362751 0.5050474329527105 0.5486541672253822
0.7243593655929728 0.4470962491020537 0.4902215891558919
0.7057922678495301 0.3677208266841435 0.5177009778548201
0.6116019603971853 0.2827986673047481 0.4432025922657100
0.6556711476563899 0.3306036413504502 0.4702632303753556
0.5622444980631350 0.2766867129873671 0.5872213909177716
0.5339198423455360 0.2732041405889814 0.6053519998988129
0.2787231944718289 0.4094753369970193 0.6037914997623224
0.2653478301230215 0.4380687555357127 0.5858165240229458
0.4620518570755392 0.3306006358705401 0.6107479043713490
0.3649392019528252 0.3834061472475416 0.6105544807716142
0.6293562300357056 0.3329418914133029 0.3575348602513587
0.6500446755155442 0.3603844318922066 0.3487481211588283
0.6601145906948288 0.4360125170791753 0.3998060312377487
0.6274855716404407 0.4923447622830400 0.3297132403636501
0.4241494237606716 0.4949684009319366 0.4033256240381024
0.4856261254842379 0.4922112171830769 0.3147829179144060
0.5188294472653271 0.4417199197536970 0.4004651242155092
0.5745089867113805 0.4352880887977146 0.3114633019586001
0.4235454283940441 0.6022692291562487 0.4073190638159837
0.4842731359446429 0.5970378819339065 0.3178903133043010
0.5172471727069251 0.5468551305554440 0.3995859036733314
0.5795846037441946 0.5449100448171661 0.3091848177319621
0.6119183461438445 0.4938171941711095 0.4009458519878123
0.5131950302622150 0.6580464724546221 0.4040426513534097
0.6039957148429459 0.6027562648763588 0.3979658119692590
0.4257431263061832 0.4919060881863814 0.5721534194528471
0.4890545272573271 0.4932334709213689 0.4877043447439321
0.5231107659314338 0.4355863584791411 0.5720206979395248
0.5788097671767348 0.4402344993361639 0.4835427913393750
0.4271509107084662 0.6010157640894691 0.5734583597073064
0.4890914443894241 0.5997055951160712 0.4886922118936043
0.5199619090320683 0.5480776078582139 0.5697921286951245
0.5778363109820187 0.5472180762998734 0.4841259036142738
0.6113667197248943 0.4938983658547701 0.5732074797503468
0.6760383431437336 0.4980602398196708 0.5008775908748145
0.4804639169553660 0.7039348110317051 0.4942215179024974
0.5201376924978061 0.6507117982903023 0.5734146400343382
0.5827878954659244 0.6572759037910978 0.4857884926759630
0.6165848702879354 0.6026924851126227 0.5706932564713830
0.6732600539979464 0.5941600908527420 0.4702649380121950
0.4916999784916741 0.4901964866872693 0.6574739595211548
0.5842491944471780 0.4363816200328258 0.6546975907365282
0.4885069601236747 0.5926533582595293 0.6582813513256467
0.5832467354862076 0.5493923794455671 0.6592576675310520
0.3342112091647244 0.4443803350935462 0.4035858418903364
0.3881741115694397 0.4392212789840704 0.3157339246716748

0.3343121969321828 0.5457829085783129 0.4069447887927198
0.3919109002696113 0.5449815619232667 0.3206824106650341
0.2986971057098973 0.4929037592706621 0.4918280284465255
0.3332294834139795 0.4388031082148705 0.5732595875770586
0.3962318777020799 0.4402797077385619 0.4877007925255878
0.3017561792386241 0.6046581195831664 0.4913234398753651
0.3340572700514442 0.5451175436217772 0.5767094210179181
0.3926475688924014 0.5457042311280148 0.4914864745337917
0.3944354926770676 0.6533876591690102 0.4861577768211073
0.4008387300977347 0.4355397597684436 0.6576961568031777
0.4009014029854843 0.5424699089120052 0.6606376107017891
0.4249794770748004 0.3872697727005329 0.4029582340164720
0.4794184835751416 0.3845738645448876 0.3138290853330069
0.5170549825832870 0.3308392444030502 0.3985529081835835
0.6059170948537770 0.3864641148743353 0.3958034134462969
0.4823203867411400 0.2823235712685128 0.4811513821168125
0.4279776213637102 0.3849856302372628 0.5711967896471325
0.4896907810408396 0.3868589367731674 0.4845612774043214
0.5218334205194434 0.3321416114912757 0.5649438874493179
0.5867891568311653 0.3277534059967582 0.4813112822728065
0.6142772674429705 0.3859772129171165 0.5640383694677654
0.6733859448635641 0.4016194773424500 0.4742172852486556
0.4929013338703559 0.3834142388765088 0.6550895450817197
0.3060563373945449 0.3841898895050570 0.4821893836864835
0.3986040166488615 0.3330535536054058 0.4873742346156350



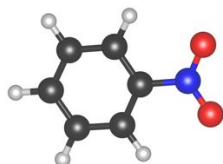
energy(sigma->0) = -48.00691281

H 1 C 2 O 2 F 3		
1.0000000000000000		
25.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	25.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000
H C O F		
1 2 2 3		
Direct		
0.5917318129753645	0.6454038775313128	0.2849535427366042
0.6412560196093282	0.7621857248694578	0.3122700095831328
0.6276842060866759	0.7020959774938634	0.3214630571504984
0.6391393559477195	0.6791019043705844	0.3627110150834899
0.6019569370789227	0.6829767510555350	0.2791610136900871
0.6752557189292859	0.7802252921097891	0.3502312599670994
0.5956447490775238	0.7920669660276860	0.3148489076400013
0.6640492002951872	0.7708719065417790	0.2636279941490897



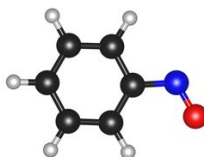
energy(sigma->0) = -65.56576519

H 9 O 4 Cl 1		
1.0000000000000000		
25.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	25.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000
H O Cl		
9 4 1		
Direct		
0.9465747995529601	0.2792783683698929	0.1335062309989899
0.0100887688715582	0.3001698092476405	0.1498434773059441
0.9979316599933332	0.2356808309448935	0.1316618564474368
0.8720900175536600	0.2702896097940845	0.1636200468679650
0.9040829208840409	0.3230483336390697	0.1804084584770714
0.9964054090908305	0.3522472489041278	0.2028422514220474
0.0490511618980120	0.3662901994045042	0.1690920541077832
0.9305449351674787	0.3521972889501619	0.2608573361721861
0.9219829758793624	0.4023197524434374	0.2218266746187950
0.9880477974190167	0.2726825616314151	0.1236353477573833
0.8954642133822632	0.2982714366237035	0.1497659554046769
0.0297507989507820	0.3368527467168773	0.1859161416786206
0.9348479003032785	0.3633967533995514	0.2237756650052054
0.8969496710534167	0.4748335083306427	0.2174018717359116



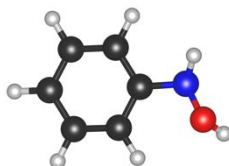
energy(sigma->0) = -91.77426776

	H 5	C 6	N 1	O 2
	1.0000000000000000			
25.0000000000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	25.0000000000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000	0.0000000000000000	0.0000000000000000
	H	C	N	O
	5	6	1	2
	Direct			
0.6776623837429930	0.7517324370619604	0.3970249818170600		
0.6979631255100849	0.8497244700412915	0.3975253307716620		
0.6683660606279220	0.9069400578059907	0.3216896763403396		
0.6169141907264790	0.8671482292930025	0.2462418149508693		
0.5965984399435774	0.7691587600129858	0.2459587309815022		
0.6368453610943338	0.7558299309230083	0.3211063814870356		
0.6190030047148243	0.7872918770023614	0.2785580653387039		
0.6649438817250560	0.7773796142550153	0.3642680646393538		
0.6305577188649231	0.8420366054057788	0.2791120025138468		
0.6760953378003510	0.8322071729860104	0.3641690640753480		
0.6592216752064920	0.8643329508312738	0.3216201185418595		
0.6261831993006763	0.6980716310858276	0.3202081401373779		
0.6411051956149946	0.6707845913256265	0.3590388531407674		
0.6030464251272906	0.6790048719698615	0.2804823752642808		



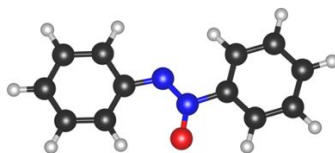
energy(sigma->0) = **-85.13661027**

H C N O		
	1.0000000000000000	
25.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	25.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000
H C N O		
	5	6 1 1
Direct		
0.6859509430565729	0.7491629966983924	0.3930548545461731
0.7152032864021154	0.8450885273853311	0.3854662776829054
0.6799794122477156	0.9016658271756098	0.3117702655758433
0.6160163568571222	0.8644818708632993	0.2453177350555803
0.5864557745708397	0.7685181955786424	0.2535636655906663
0.6347353354264764	0.7543735117668631	0.3236316277324949
0.6146028710565894	0.7862089139395365	0.2818427304631109
0.6711550402369355	0.7751386017085120	0.3613003940779769
0.6310769446454745	0.8393107592463502	0.2775273375464279
0.6871350856540800	0.8281218901039250	0.3567469066420066
0.6671539497073121	0.8601201283756486	0.3149694936317762
0.6155006007536683	0.7007595084191480	0.3241857374681412
0.6331746676526651	0.6716896035639635	0.3604755019978993



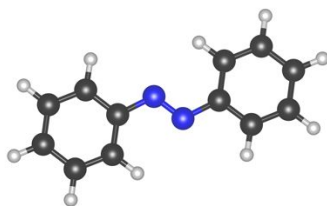
energy(sigma->0) = -93.59992676

H C N O		
	1.0000000000000000	
25.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	25.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000
H C N O		
	7	6 1 1
Direct		
0.6931244721046462	0.7705854355634433	0.3907450585146455
0.7251498840070350	0.8621029438561580	0.3684098872323381
0.6852299451861068	0.9122044388285085	0.2917422550991000
0.6132104110268803	0.8691942887296430	0.2373427263370217
0.5814537427778649	0.7778362820323910	0.2594741631867801
0.5974934423462521	0.6993284990296469	0.3084554780158371
0.6365592370103061	0.6768071672351065	0.4005669606477431
0.6347660443955042	0.7687089482821756	0.3271645396046787
0.6126178845483952	0.7966779511379429	0.2835450336019012
0.6755622860095364	0.7926297430362620	0.3575632049160601
0.6306245317651044	0.8480403519235920	0.2712862788327346
0.6933827813120529	0.8440000403408754	0.3445821332892628
0.6710819172741267	0.8721805871529626	0.3016586546440541
0.6129456179728342	0.7187999303699525	0.3408628767559433
0.6509236825715856	0.6830469523820564	0.3648404879664151



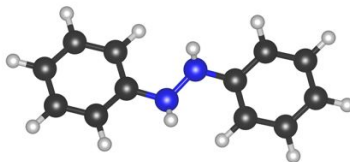
energy(sigma->0) = -166.10430360

H 10 C 12 N 2 O 1		
1.0000000000000000		
25.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	25.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000
H C N O		
10 12 2 1		
Direct		
0.6436560480528377	0.7215427113509019	0.4218852558968747
0.6832843944706208	0.7774718736474382	0.4945875308202047
0.7635419225780589	0.8337486052923931	0.4758675891816762
0.8037342598681386	0.8339173613337996	0.3845992686734279
0.7642543914447223	0.7775890136340065	0.3125494752359346
0.7246649981458070	0.6779297018425687	0.1024344944753429
0.7459800033536876	0.7230892519955751	0.1885470532343517
0.6121233753134269	0.6440549601676347	0.2636669078772755
0.6465648500612504	0.6156607681152964	0.0970838739575803
0.5907199184571077	0.5996229360029844	0.1779593606157325
0.7018855416230533	0.7466788654670764	0.3636470677012239
0.7469088507528000	0.7780091777731539	0.3524077234126962
0.6787277412477295	0.7461928098331252	0.4145211745490416
0.7687647640942352	0.8093293590372993	0.3930880512500851
0.7011782369897486	0.7776507789596525	0.4548461565705476
0.7461412179601191	0.8092260428332941	0.4443171125406015
0.6809553608422246	0.6867836745909471	0.2320930519984600
0.7121111363482272	0.6957599355783206	0.1856088214966055
0.6366408546194281	0.6515501167452453	0.2287191114036623
0.6999758298853045	0.6704804890576582	0.1376093782179499
0.6248972430598103	0.6266382457822111	0.1801315422403117
0.6561514506435729	0.6356592691914790	0.1346127072144086
0.6773953618248334	0.7131290072300798	0.3221344099385945
0.6996537835021586	0.7159193352136309	0.2758811645617008
0.6371384648610992	0.6850937093242208	0.3356225169357272



energy(sigma->0) = -160.23343243

H C N		
1.0000000000000000		
25.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	25.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000
H C N		
10	12	2
Direct		
0.6802690848242406	0.6855832843312117	0.3909015247230087
0.7420457887571908	0.7232095994873828	0.4603453780320934
0.7625214732076676	0.8208069276902665	0.4603872945771327
0.7216352455432903	0.8804046876737240	0.3919043394321101
0.6597439961849993	0.8425960201778744	0.3232215221648275
0.4973286527137933	0.7811734018968286	0.1409252705167948
0.5587718983200685	0.8183108798993490	0.2109113603159835
0.5888005384574081	0.6593498559453994	0.2698688525736230
0.4820932898752604	0.6827729623733749	0.1359768739020218
0.5277106450932907	0.6218912112762000	0.2001993963299161
0.6664529944617394	0.7617987963921613	0.3532476736636142
0.6780429477486259	0.8169842611838225	0.3533396071895632
0.6897309717367652	0.7281678154977116	0.3918572923036272
0.7125018570694520	0.8377473316716040	0.3917868884018117
0.7241635586338300	0.7493523596587207	0.4303768949997878
0.7356313629802155	0.8041267033717888	0.4303955916448948
0.5770472988299008	0.7411265056791975	0.2444133865434548
0.5513702327906599	0.7754095451624955	0.2079647747030352
0.5684850861237795	0.6854636524578870	0.2415337039237249
0.5172069287848595	0.7544772748252769	0.1690959685840959
0.5344308713741360	0.6649240209690387	0.2026025217651995
0.5086802941062382	0.6992537961841371	0.1663477958690077
0.6322507143751871	0.7360856847222895	0.3161771983345983
0.6107929408073881	0.7667438072554005	0.2819315104736905

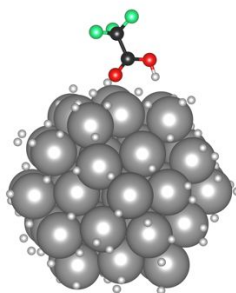


energy(sigma->0) = -168.39802528

H C N		
	1.0000000000000000	
25.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	25.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

H C N		
12	12	2
Direct		
0.6713470093796606	0.6960810046552116	0.4220756381806623
0.6971208993098761	0.7621772595729268	0.4912002131859609
0.7466365522094095	0.8453753852542051	0.4657590500470565
0.7683302234157335	0.8616134295419328	0.3696138870000571
0.7421818114499931	0.7956583607324111	0.3001482373703671
0.7169591902645012	0.6437504042693627	0.0973584841516038
0.7602011907691777	0.6835198525769119	0.1771284800058146
0.6108149510709165	0.6739989488794270	0.2631896119850107
0.6202093776056254	0.6180614345012864	0.0997524116779951
0.5677341253533534	0.6338282859862537	0.1832485999287926
0.6856605282747137	0.6653253359885779	0.3342807320539370
0.7548663132645982	0.6971790398356988	0.2703505312429931
0.7052887221540400	0.7413018538499482	0.3564089906187177
0.7324320494247253	0.7884777394690292	0.3419990429180730
0.6926447017259395	0.7324816301097757	0.4107040670405659
0.7469020141190983	0.8254670397863845	0.3814066956942914
0.7072089177407090	0.7698009500007258	0.4494284330778495
0.7347695118074014	0.8165476642726573	0.4352597925865859
0.6884531579096822	0.6813225754029284	0.2256511033172689
0.7179501427860778	0.6724719163183837	0.1783083528892584
0.6339202683621674	0.6673229799847077	0.2268593734607000
0.6934420910375412	0.6501389741129956	0.1335616111254006
0.6099455630726237	0.6448142857290303	0.1815579849692144
0.6391860781733858	0.6359097779309515	0.1347327061463647
0.6895959861868832	0.7029818493279735	0.3188958151842691
0.7147075830627245	0.7045196676611887	0.2690093499722001

2.5.2. Hydrogen Evolution Reaction



energy(sigma->0) = -851.32336537

```

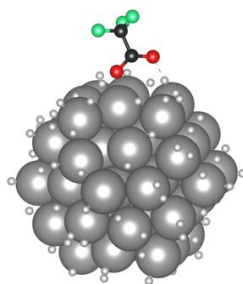
H 89 C 2 O 2 F 3 Ru 57
1.0000000000000000
25.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 25.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
  H C O F Ru
  89 2 2 3 57
  Direct
0.5484514803628082 0.7190774488604716 0.5045685726359552
0.4877837565156712 0.7544854658043685 0.4591293401799550
0.4099830793258649 0.7216525083574640 0.4834619698421254
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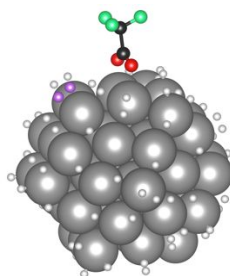
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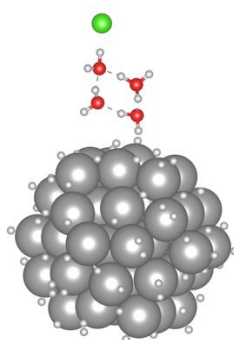
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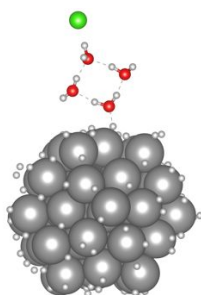
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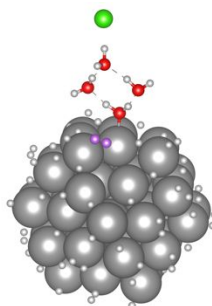
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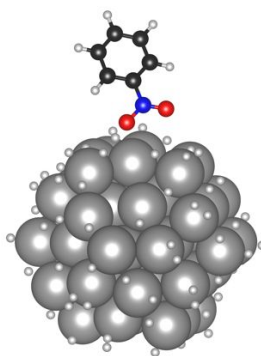
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2.5.3. *Hydride transfer processes*



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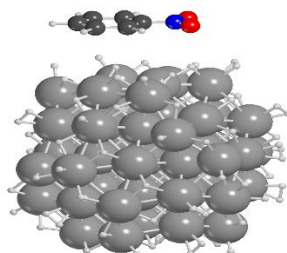
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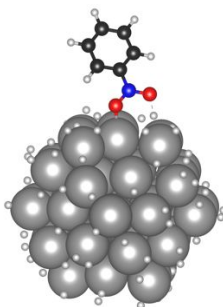
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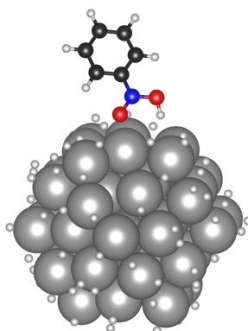
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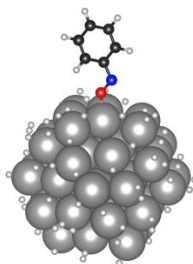
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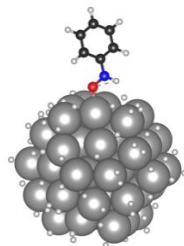
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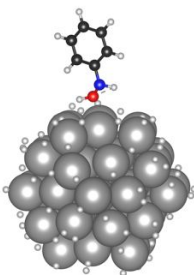
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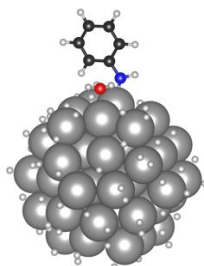
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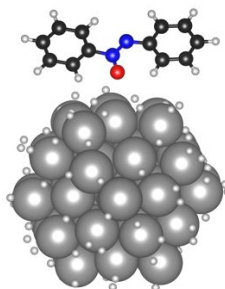
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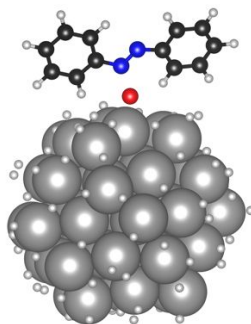
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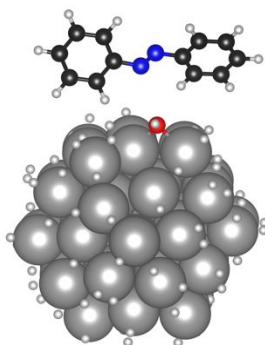
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H	C	N	O	Ru
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Direct

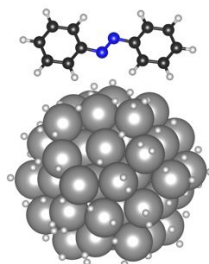
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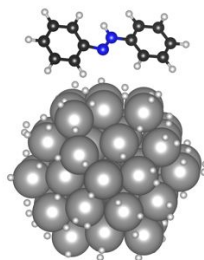
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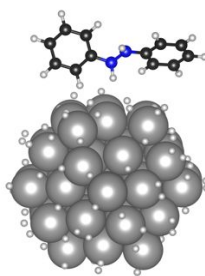
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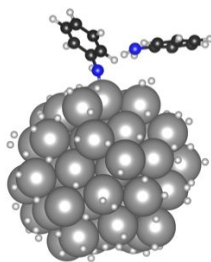
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