Supporting Information

Energy Decomposition Analyses Reveal the Origins of Catalyst and Nucleophile Effects on Regioselectivity in Nucleopalladation of Alkenes

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1. The formation of phthalimide anion through the deprotonation with acetate

In this study, the deprotonation of phthalimide using acetate is considered. As shown in Figure S1, the deprotonation transition state was located (**24-TS**) with an energy barrier of 2.5 kcal/mol. The formation of phthalimide anion is slightly endergonic by 1.6 kcal/mol, which indicates that this deprotonation is a facile process. This is consistent with the experimental pK_a values, which indicate phthalimide is only slightly less acidic than acetic acid in DMSO (13.4 and 12.6, respectively. See *J. Org. Chem.* **1991**, *56*, 7172 and *Aust. J. Chem.* **1991**, *44*, 1077).

This equilibrium suggests that a higher concentration of acetate anion may promote the deprotonation of phthalimide to form the active nucleophile, phthalimide anion.

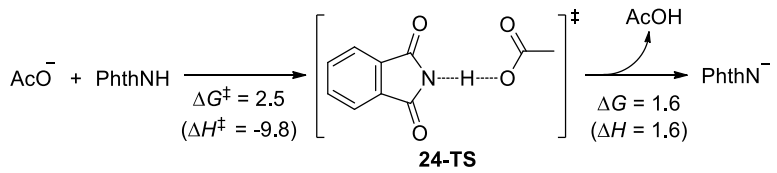

Figure S1. The formation of phthalimide anion through the deprotonation with acetate.

2. Proposed aminopalladation and allylic C–H activation pathways for Pd-catalyzed oxidative amination of terminal alkenes

The proposed mechanisms of the oxidative amination are shown in Figure S2. In the aminopalladation mechanisms (a and b), the coordination of the alkene to the palladium catalyst forms a π-alkene-palladium complex (**I** or **III**). Subsequent aminopalladation of the alkene may occur through either the *trans*- or *cis*-attack of the phthalimide anion towards the C=C double bond. The resulting alkyl palladium species (**II** or **IV**) then undergoes *β*-H elimination and alkene migration to afford the amination products.

In addition to the aminopalladation mechanisms, the allylic C–H activation mechanism is also considered and calculated for the Pd-catalyzed oxidative amination of terminal alkenes. As shown in Figure S2c, the analogous allylic C–H activation pathway from the anionic palladate species **11** is kinetically disfavored because the relative free energy of transition state **12b-TS** is higher than that of aminopalladation transition state **12A-TS** by 3.6 kcal/mol. Meanwhile, from the neutral Pd species **5**, the allylic C–H bond cleavage with acetate via a cyclic transition state **6b-TS** requires 31.8 kcal/mol (Figure S2c), which is 10.8 kcal/mol higher than the aminopalladation transition state **9M-TS**. Based on these results, the C–H activation mechanism could be ruled out. This conclusion is consistent with the experimental deuterium labeling and kinetic isotope effects studies reported by Hull and coworkers (*Nat. Chem.* **2018**, *10*, 333).

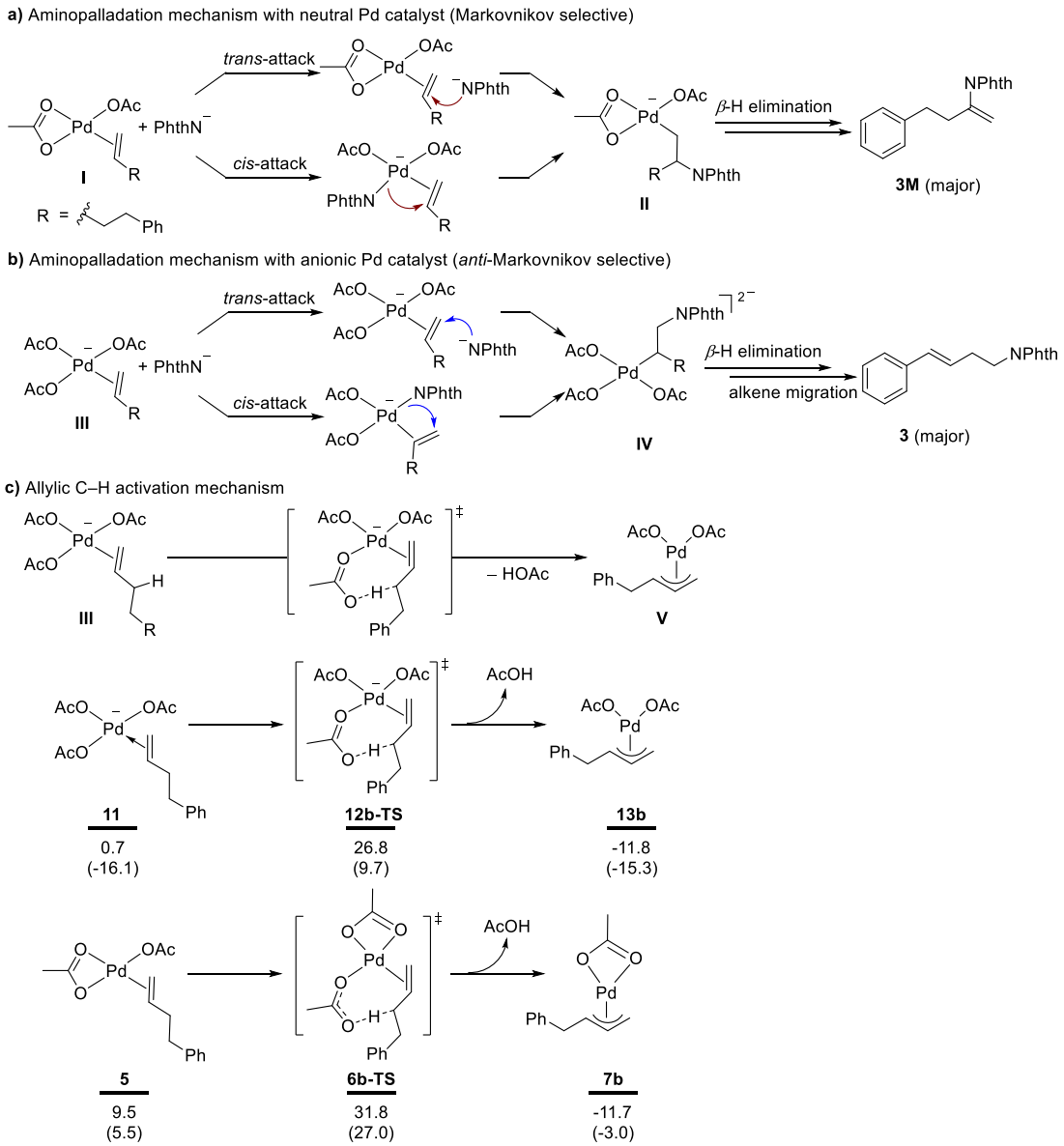

Figure S2. Proposed mechanisms of Pd-catalyzed oxidative amination of terminal alkenes.

3. The computed relative stabilities of monomeric and dimeric palladate complexes

We have considered a few possible monomeric and dimeric neutral palladium and anionic palladate complexes in the pre-reaction equilibrium. The optimized structures, relative Gibbs free energies (ΔG) and enthalpies (ΔH) are shown in Figure S3. The trimer of $Pd(OAc)_2$ (**4**) is the most stable species. The relative free energy of

monomeric $Pd(OAc)_2$ is higher than complex **4** by 13.1 kcal/mol. In addition, the dimeric and monomeric anionic palladate complexes $[Pd_2(OAc)_6]^{2-}$, $[Pd_2(OAc)_5]^-$ and $[Pd(OAc)_4]^{2-}$ are less stable by 8.5, 0.9 and 2.7 kcal/mol, respectively. Monomeric monoanionic palladate species **10** is only 1.7 kcal/mol less stable than **4**. These results suggest a few low-energy complexes, including the neutral $[Pd(OAc)_2]_3$, and the monomeric and dimeric palladate complexes are most likely under rapid equilibrium in experiment due to their similar free energies. The lowest-energy structure, $[Pd(OAc)_2]_3$, was used as the energy zero in the potential energy profiles of the aminopalladation pathways.

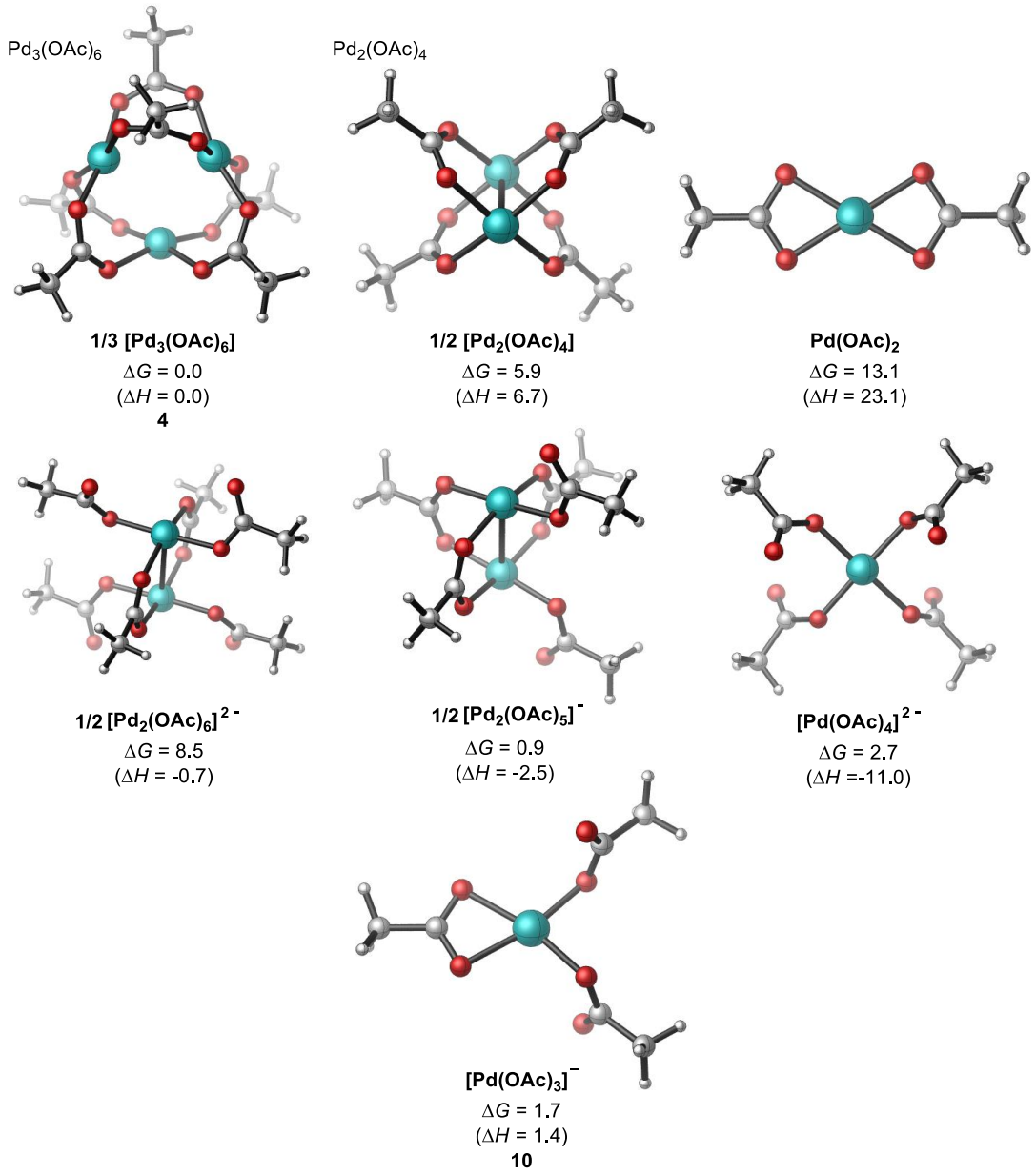

Figure S3. The computed relative stabilities of $Pd(OAc)_2$ trimer, dimer, monomer,

and monomeric and dimeric palladate complexes. The energies are in kcal/mol.

4. Dimeric palladate catalyzed aminopalladation pathway

In the Pd-catalyzed oxidative amination of alkene reported by Hull and coworkers (*Nat. Chem.* **2018**, *10*, 333), there might be an equilibrium between monomeric and dimeric palladate complexes as the kinetic analyses observed the reaction is 1.4 order in [Pd], zero order in nucleophile, and first order in olefin **1**. This result also suggested that the rate-determining step is most likely to be the alkene coordination to palladium rather than the aminopalladation step. Further kinetic analysis experiment on a homoallylic alcohol system revealed a first order in [Pd], which suggests that a monomeric palladate complex is most likely to be the active catalyst for the homoallylic alcohol system.

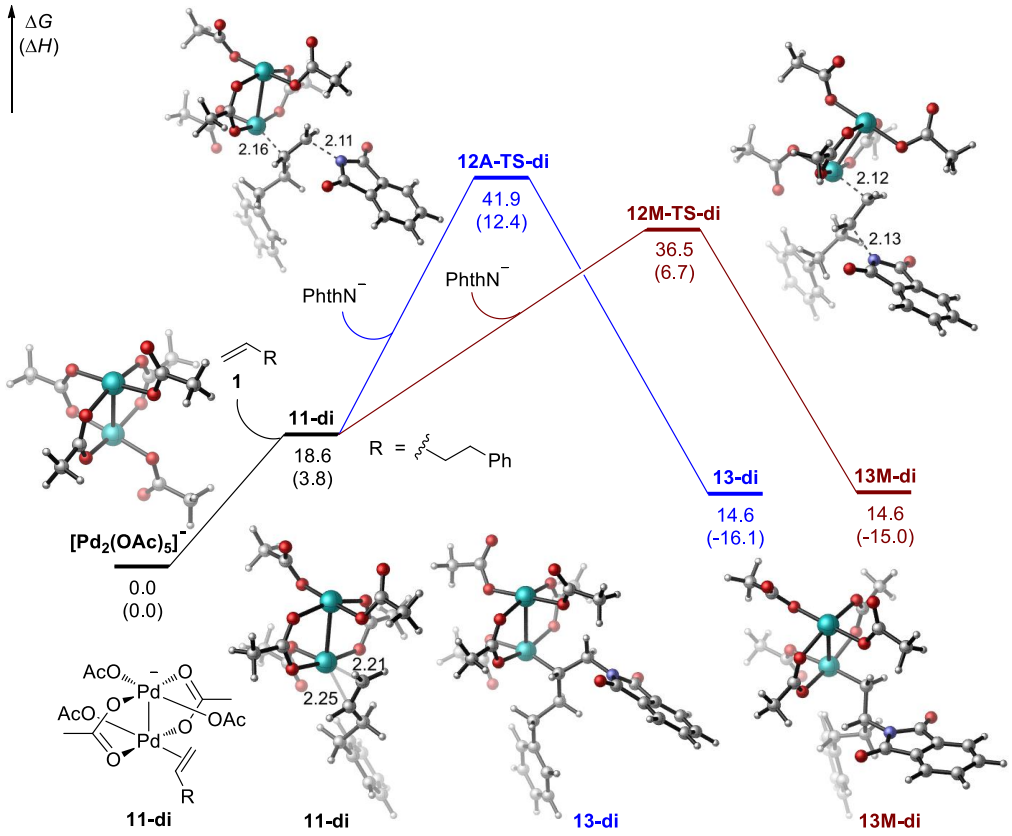

Figure S4. Free energy profile of the dimeric palladate catalyzed aminopalladation with phthalimide anion.

In our theoretical calculation, the dimeric palladate complex $Pd_2(OAc)_5^-$ catalyzed aminopalladation with phthalimide anion is also studied. As shown in Figure S4, the formation of π-alkene-palladium complex **11-di** through alkene coordination to $Pd_2(OAc)_5^-$ is endergonic by 18.6 kcal/mol. The *anti*-Markovnikov and Markovnikov aminopalladation transition states are located as **12A-TS-di** and **12M-TS-di**, respectively. In this case, transition state **12A-TS-di** is higher in energy because of the steric repulsion between [$Pd_2(OAc)_5^-$] part and the internal carbon of the alkene. Compared with monomeric palladate complex catalyzed *anti*-Markovnikov aminopalladation, the free energy barriers of **12A-TS-di** and **12M-TS-di** are higher than that of **12A-TS** (Figure 2). Consequently, the dimeric palladate complex $Pd_2(OAc)_5^-$ is less reactive in the *anti*-Markovnikov aminopalladation.

5. The outer-sphere *cis*-aminopalladation pathway with the anionic Pd catalyst

The free energy profile of the outer-sphere *cis*-aminopalladation pathway with the anionic Pd catalyst is shown in Figure S5. Because the palladium center in the anionic palladate complex **11** is already four-coordinated, there is no available coordination site for an additional phthalimide anion. The *cis*-aminopalladation mechanism with the anionic Pd catalyst thus occurs *via* an outer-sphere pathway, *i.e.* the phthalimide attacking from the same face as the Pd without coordinating with the Pd. The corresponding aminopalladation transition states for the formation of *anti*-Markovnikov and Markovnikov addition products are **12A-TS-*cis*** and **12M-TS-*cis***, respectively. Compared with the *trans*-aminopalladation transition states **12A-TS** and **12M-TS**, the activation free energies of **12A-TS-*cis*** and **12M-TS-*cis*** are higher by 19.2 and 13.4 kcal/mol, respectively. Therefore, this outer-sphere *cis*-aminopalladation pathway is highly unfavored.

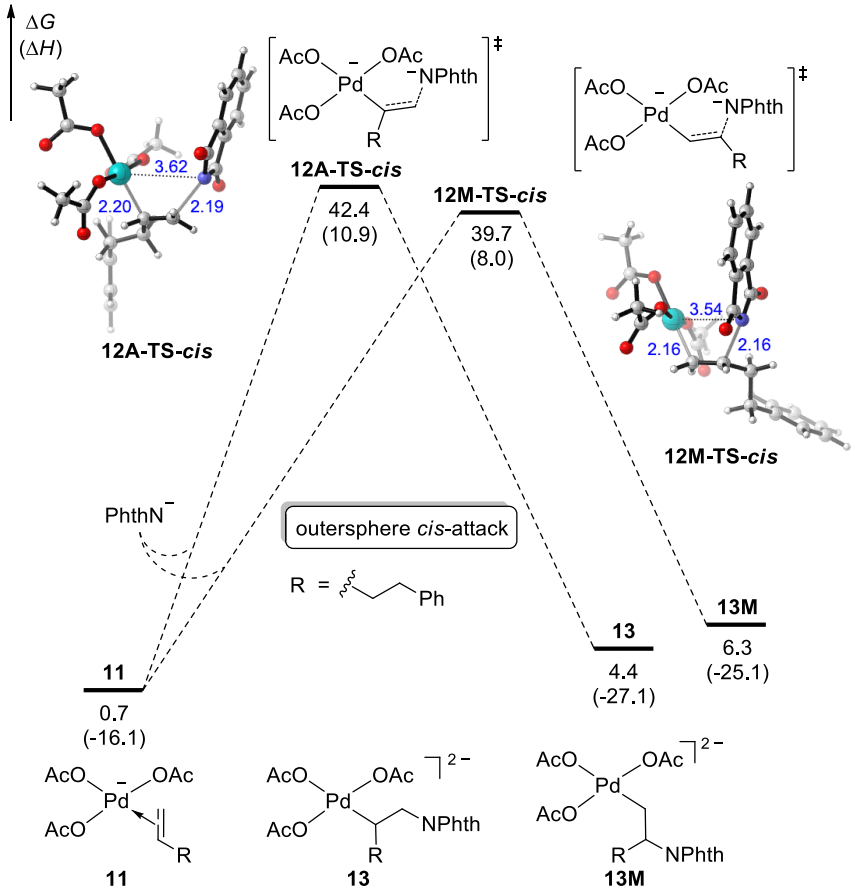

Figure S5. Free energy profiles of the outer-sphere *cis*-aminopalladation pathways with the anionic Pd catalyst.

6. The *trans*-aminopalladation from complex 8 using another phthalimide anion

The free energy profile of *trans*-aminopalladation from complex **8** using another phthalimide anion as the nucleophile is shown in Figure S6. From the anionic palladate complex **8**, the *anti*-Markovnikov aminopalladation could occur through transition state **8A-TS** and the Markovnikov aminopalladation occurs through **8M-TS**. Computational results show that the relative free energy of Markovnikov addition transition state **8M-TS** is higher than that of *anti*-Markovnikov addition transition state **8A-TS** by 0.8 kcal/mol. Consequently, the *trans*-aminopalladation from complex **8** with another phthalimide anion also favors the *anti*-Markovnikov selectivity. This conclusion is consistent with the anionic palladate complex **11** involved

trans-aminopalladation.

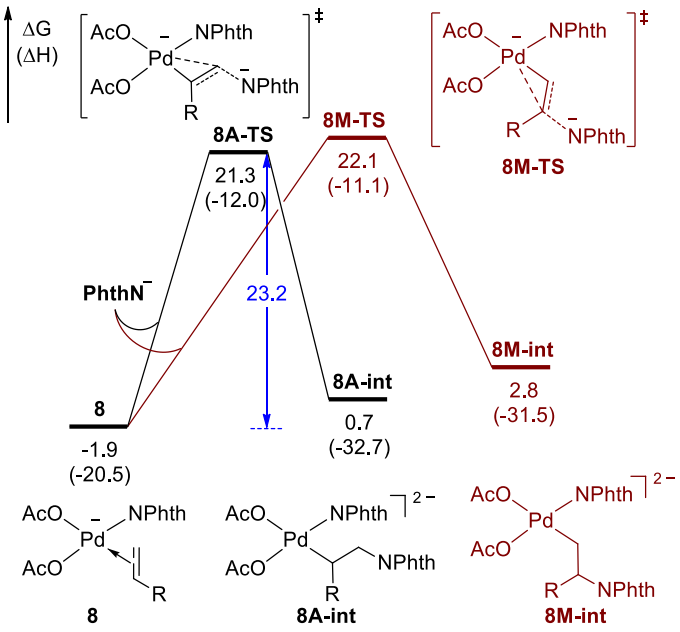

Figure S6. Free energy profile of *trans*-aminopalladation from complex **8** using another phthalimide anion as the nucleophile.

7. Free energy profiles of the *β*-hydride elimination step after aminopalladation

After aminopalladation, the four-coordinated alkyl palladium intermediate **13** dissociates an acetate anion to form **7**, which then undergoes *β*-hydride elimination and alkene isomerization. The corresponding free energy profiles in the *anti*-Markovnikov oxidative amination pathway are given in Figure S7a. The computations indicate the *β*-hydride elimination (**14-TS**), alkene migration (**16-TS** and **18-TS**), and the final HOAc reductive elimination (**21-TS**) steps all require much lower activation energies than the aminopalladation. The similar *β*-hydride elimination in the Markovnikov oxidative amination pathway is summarized in Figure S7b. The dissociation of one acetate from anionic palladate complex **13M** generates the primary alkyl palladium intermediate **7M**. Subsequent *β*-hydride elimination occurs through a four-membered cyclic transition state **14M-TS**. The alkene **3M** is

then released as the Markovnikov adduct. The activation free energy of *β*-hydride elimination is determined to be 15.5 kcal/mol, which is slightly higher than that in *anti*-Markovnikov amination pathway. Nonetheless, because the *β*-hydride elimination still requires a much low barrier than aminopalladation, the aminopalladation is also irreversible in the Markovnikov-selective pathway. Therefore, the aminopalladation is the regioselectivity-determining step in both Markovnikov and *anti*-Markovnikov addition pathways.

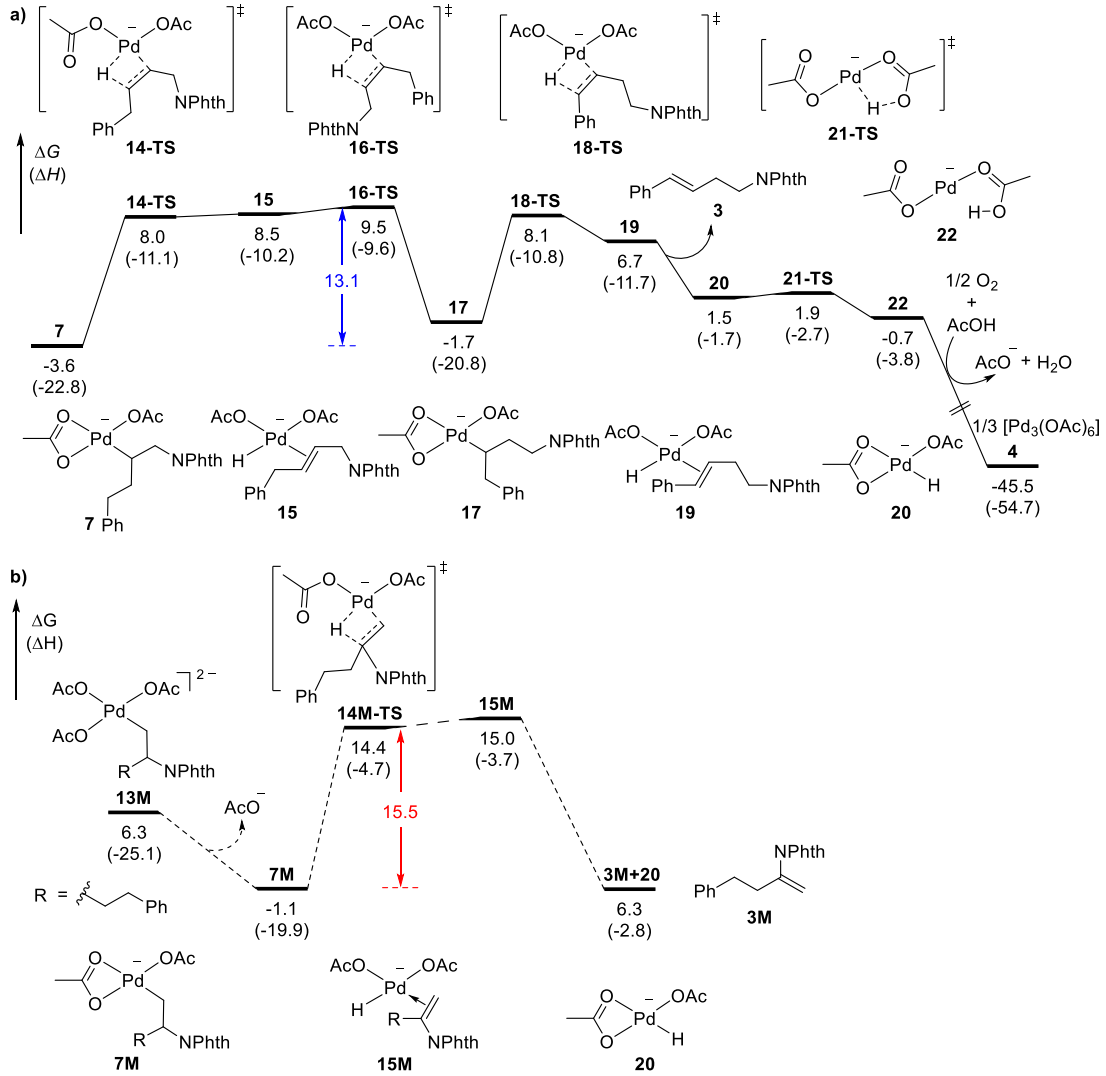

Figure S7. Free energy profile of the *β*-hydride elimination from Pd complex **7** (a) and **7M** (b) in the Markovnikov and *anti*-Markovnikov-selective pathway.

8. Detailed reaction mechanisms of the aminopalladation of the neutral π-alkene/Pd complex with *i*Pr$_2$NH as the nucleophile

To study the steric effects of the nucleophile using our energy decomposition approach, we computed the nucleopalladation with the sterically hindered diisopropylamine (*i*Pr$_2$NH) as the nucleophile. The original experiment was performed with a stoichiometric amount of a palladium-π-alkene complex formed from (PhCN)$_2$PdCl$_2$ plus a terminal aliphatic alkene and an excess of amine (Hegedus, L. S. *et al. Organomet. Chem.* **1974**, *72*, 127). In the main text, we considered the origin of regioselectivity in the aminopalladation of the Pd(OAc)$_2$-π-alkene complex **5** using *i*Pr$_2$NH as the nucleophile (**23A-TS** and **23M-TS**). This allows for the direct comparison with the reaction between the same π-alkene complex and another nucleophile (phthalimide anion). Two additional possible mechanisms for the aminopalladation with *i*Pr$_2$NH are considered below.

Under the experimental conditions in the Hegedus study, an *i*Pr$_2$NH molecule is likely to coordinate with the neutral Pd catalyst due to the strong binding ability of the amine. Therefore, the free energy profiles of these possible aminopalladation mechanisms with *i*Pr$_2$NH were calculated and summarized in Figure S8. Figure S8a shows the nucleophilic addition of *i*Pr$_2$NH to the π-alkene palladium complex **5** via an outer-sphere *trans*-attack pathway. The *anti*-Markovnikov and Markovnikov addition transition states are **23A-TS** and **23M-TS**, respectively. The activation free energy of **23A-TS** is 4.5 kcal/mol lower than that of **23M-TS**. As such, the *trans*-aminopalladation of *i*Pr$_2$NH with the π-alkene palladium complex **5** favors *anti*-Markovnikov addition.

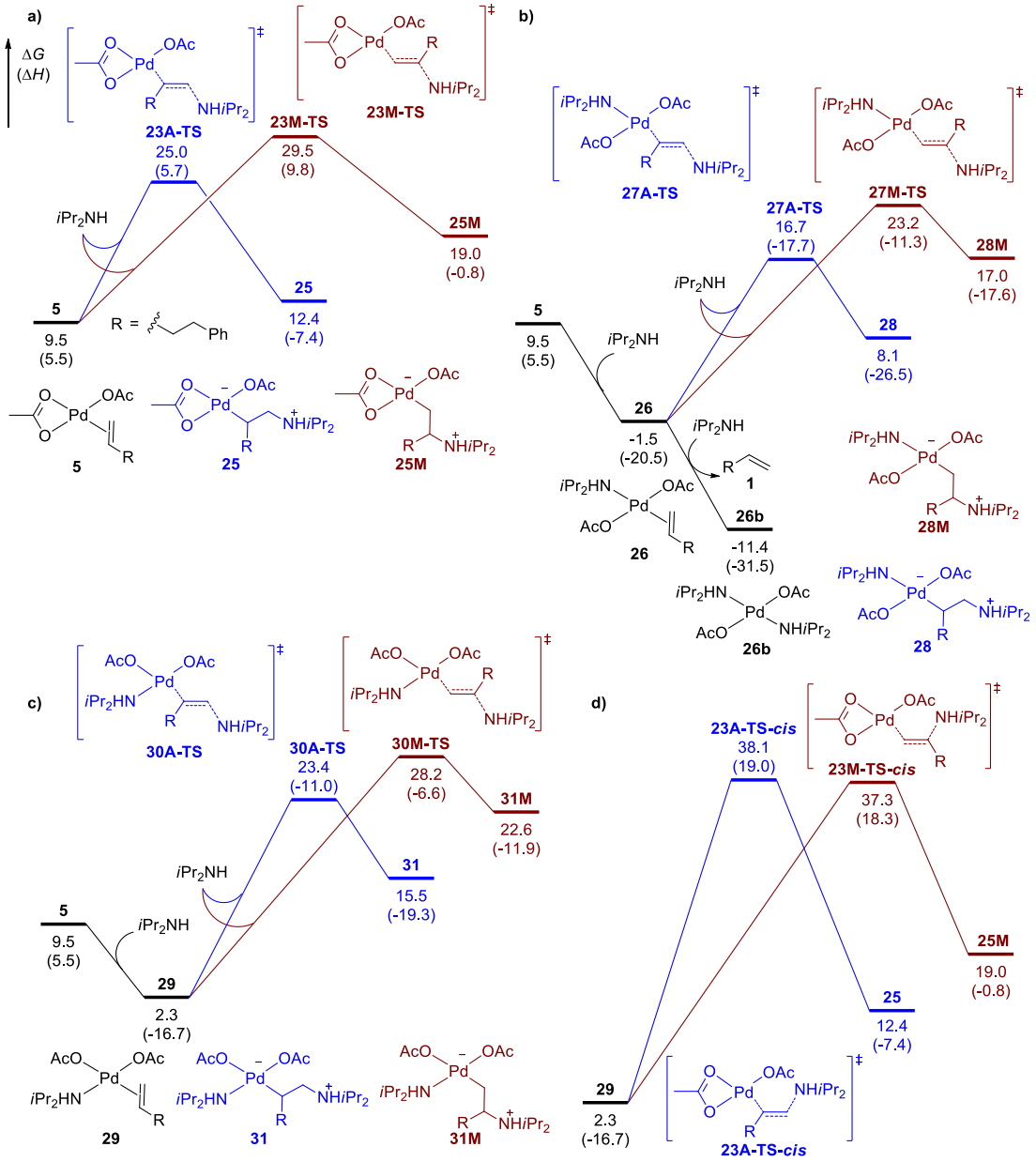

Figure S8. Free energy profiles of aminopalladation through the *trans*-nucleophilic addition of *i*Pr$_2$NH to neutral Pd complexes a) **5**, b) **26**, and c) **29**. d) The outer-sphere *cis*-aminopalladation pathway with *i*Pr$_2$NH.

Aminopalladation pathways in which another molecule of *i*Pr$_2$NH coordinates to the Pd prior to the aminopalladation were also considered. As shown in Figure S8b and S8c, *i*Pr$_2$NH may coordinate with complex **5** at either the *trans*- or *cis*-position to the alkene. The coordination of the amine is exergonic, leading to stable complexes **26** and **29**. Moreover, exchanging the alkene in complex **26** with another *i*Pr$_2$NH forms of an even more stable bis(amine) complex **26b**. This result is consistent with the

experimental hypothesis that the irreversible formation of this stable bi(amine) complex is most likely to be the main cause of low yields of amination products. At lower temperatures, the alkene displacement is slow, and thus the aminopalladation of the C=C double bond can be achieved in higher yields. It is noteworthy that all three *trans*-aminopalladation mechanisms in Figure S8 favor the *anti*-Markovnikov addition, which reproduced the regioselectivity in the experiment. Comparison between **27A-TS** and **30A-TS** suggests that during the aminopalladation process, one *i*Pr$_2$NH should coordinate to the Pd at the *trans*-position (Figure S8b) with respect to alkene rather than the *cis*-position (Figure S8c). The *cis*-aminopalladation pathway (Figure S8d) turns out to be disfavored compared with *trans*-aminopalladation mechanisms (Figure S8a and S8b), which is consistent with anionic palladate complex catalyzed aminopalladation using phthalimide anion and previous studies (Kočovský, P.; Bäckvall, J.-E. *Chem.-Eur. J.* **2015**, *21*, 36).

Since both pathways in Figure S6a and S6b favor the *anti*-Markovnikov addition, the coordination of *i*Pr$_2$NH to the palladium does not affect the regioselectivity of the aminopalladation. This is further confirmed by the EDA analysis of transition states **30A-TS** and **30M-TS** in the amine-coordinated pathway (Figure S9, see the main text for the EDA analysis of **23A-TS** and **23M-TS** in the amino-uncoordinated pathway). Here, the steric effects ($\Delta\Delta E_{steric}$) is also the dominant factor in controlling the *anti*-Markovnikov regioselectivity (Figure S9).

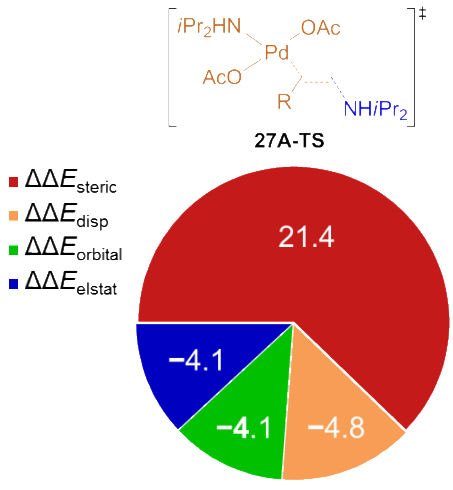

Figure S9. Energy decomposition analysis of the origin of regioselectivity in the

aminopalladation using *i*Pr$_2$NH with another *i*Pr$_2$NH coordinated to the Pd. The $\Delta\Delta E$ values are calculated from the energy difference between Markovnikov and the *anti*-Markovnikov transition states (**27M-TS** versus **27A-TS**). Positive $\Delta\Delta E$ values indicate effects that promote *anti*-Markovnikov addition; negative $\Delta\Delta E$ values indicate effects that promote Markovnikov addition. The energies are in kcal/mol.

9. COVP orbital interactions in the aminopalladation transition states 9A-TS, 9M-TS, 6A-TS, and 6M-TS

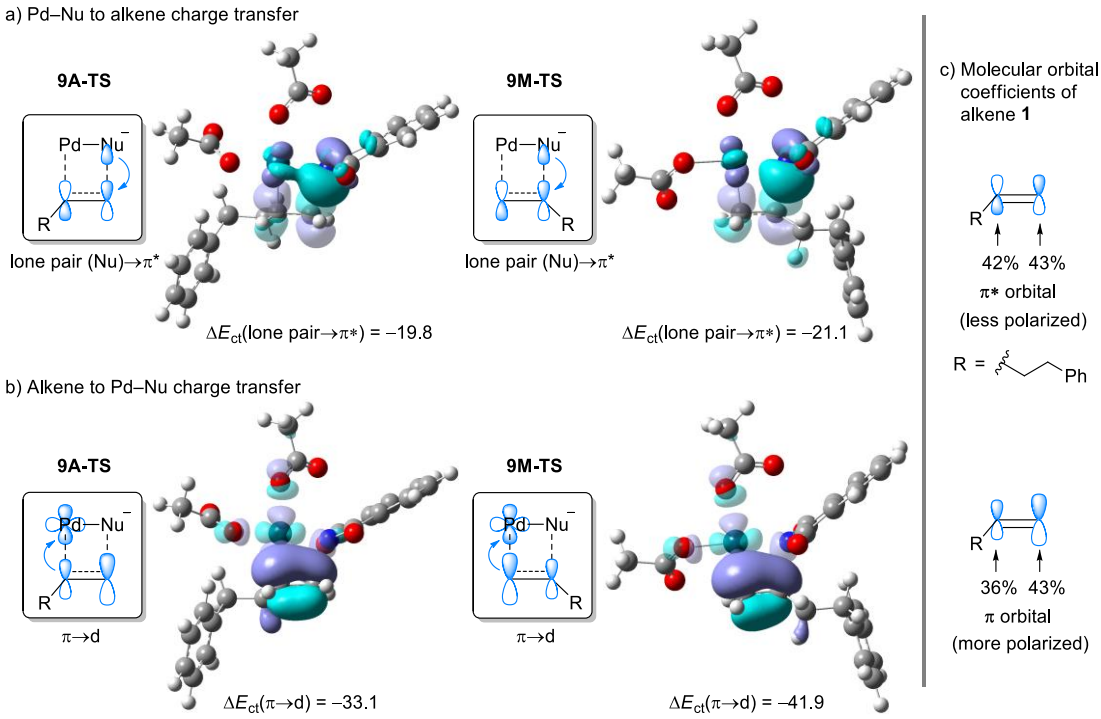

Figure S10. a) Pd–Nu to alkene and b) alkene to Pd–Nu charge transfers in the *cis*-aminopalladation transition states **9A-ts** and **9M-ts**. The computed shapes of the most significant orbital pairs (occupied in solid, vacant in transparent) and the COVP charge transfer energies are provided. The energies are in kcal/mol. c) Molecular orbital coefficients of the π and π* orbitals of alkene **1** calculated using Mulliken population analysis at the B3LYP/6-31G(d) level of theory.

A shown in Figure S10a, the most significant COVP with the Pd–Nu as the donor and the alkene as the acceptor is the lone pair (Nu)→π* interaction. The strength of this COVP interaction is similar between the Markovnikov and *anti*-Markovnikov transition states ($\Delta E_{ct(\text{lone pair}\rightarrow\pi^*)}$ = −19.8 and −21.1 kcal/mol in **9A-TS** and **9M-TS**, respectively). On the other hand, the COVP interaction in which the alkene acting as the donor and Pd–Nu as the acceptor is the π→d donation of the alkene π electrons to the vacant d orbital of the Pd (Figure 10b). This π→d orbital interaction is much more pronounced in the Markovnikov transition state **9M-TS** than in the *anti*-Markovnikov transition state **9A-TS** ($\Delta E_{ct(\pi\rightarrow d)}$ = −41.9 and −33.1 kcal/mol, respectively). This is because the terminal alkenyl carbon of **1** has a greater π orbital coefficient than the internal carbon (Figure S10c). Thus, the π→d orbital interaction is more favorable in **9M-TS** because of the greater lobe of the π orbital on the terminal carbon.

Our EDA analysis also showed that the orbital interactions ($\Delta\Delta E_{orbital}$) played a much less pronounced role in affecting the regioselectivity of neutral Pd-catalyzed *trans*-aminopalladation than in *cis*-aminopalladation. Thus, the COVPs analysis is employed to study the interfragmental orbital interactions in the *trans*-aminopalladation transition states (**6A-ts** and **6M-ts**). Two different fragmentation schemes were used in the COVP analysis of the *trans*-aminopalladation transition states. In Figure S11a, the transition states are dissected into the π-alkene-palladium complex as one fragment and the nucleophile as the other fragment. In this case, the most significant COVP represents the charge transfer from the lone pair of phthalimide anion to the π* of alkene. The ΔE_{ct}(lone parir→π*) of **6A-ts** and **6M-ts** are found to be very close to each other (-14.3 versus -14.2 kcal/mol), which suggests that this interfragmental orbital interactions, i.e. the charge transfer term ($\Delta\Delta E_{ct}$) does not play a significant role in the regioselectivity control.

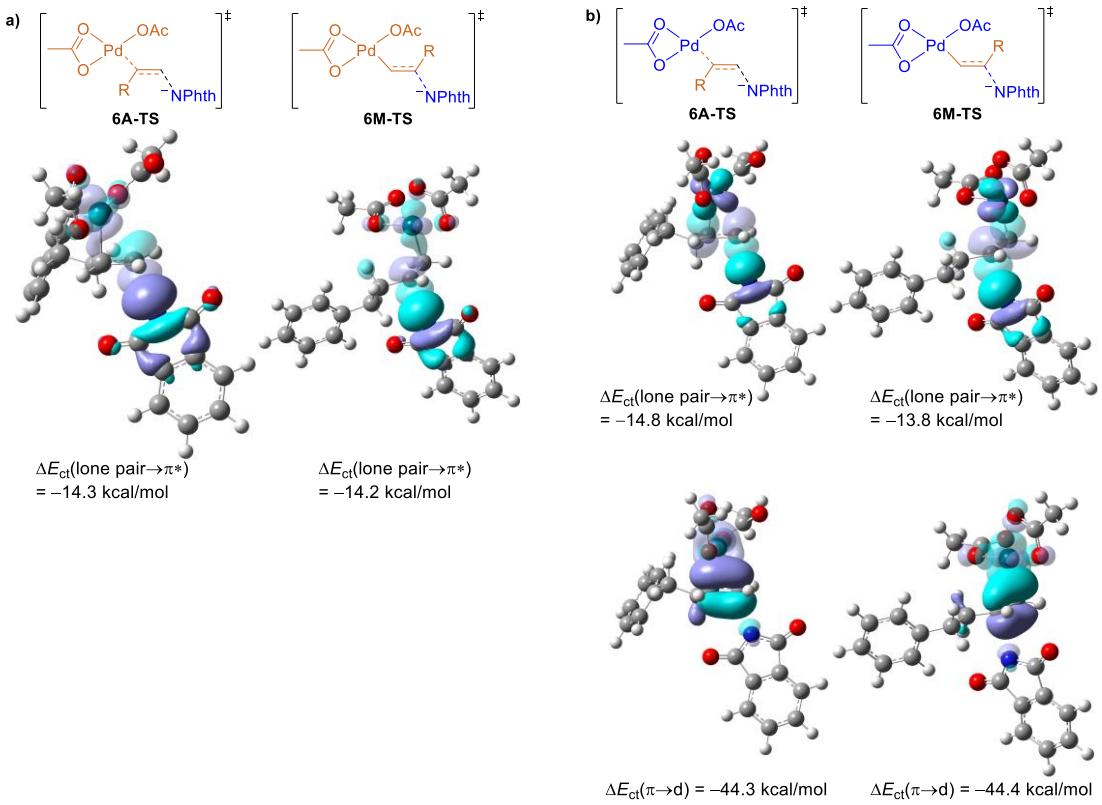

Figure S11. a) The most significant COVP orbital interactions between the π-alkene-palladium fragment and the nucleophile, and b) the most significant COVP orbital interactions between the $Pd(AcO)_2$/Nu fragment and the alkene fragment in the *trans*-aminopalladation transition states **6A-ts** and **6M-ts**.

A different fragmentation scheme was used in Figure S11b. The transition states were dissected into the alkene as one fragment and the $Pd(OAc)_2$ plus the nucleophile as the second fragment. This less counterintuitive fragmentation scheme allows a direct comparison with the *cis*-aminopalladation pathways (**9A-ts** and **9M-ts**), since the same atoms are included in each fragment. According to this scheme, the most significant COVP with the alkene as the acceptor is similar to that in Figure S10a. This involves electron transfer from the lone pair of the phthalimide anion to the π* of the alkene. The ΔE_{ct}(lone parir→π*) of **6A-ts** and **6M-ts** are -14.8 and -13.8 kcal/mol, respectively. The charge transfer energy difference is only 1.0 kcal/mol. The most significant COVP with the alkene as the donor is the π→d donation of the alkene π electrons to the vacant d orbital of the Pd, which is the same COVP in the

cis-aminopalladation transition states (**9A-ts** and **9M-ts**). The $\Delta E_{ct}(\pi \rightarrow d)$ of **6A-ts** and **6M-ts** are -44.3 and -44.4 kcal/mol, respectively. These two charge transfer energies are comparable because the η^2 to η^1 slippage is less prominent in the *trans*-aminopalladation transition states (**6A-ts** and **6M-ts**) than in the *cis*-transition states (as shown in Figure S12) The above COVP results using both fragmentation schemes suggest the orbital interactions in the *anti*-Markovnikov and Markovnikov transition states are similar in the *trans*-aminopalladation.

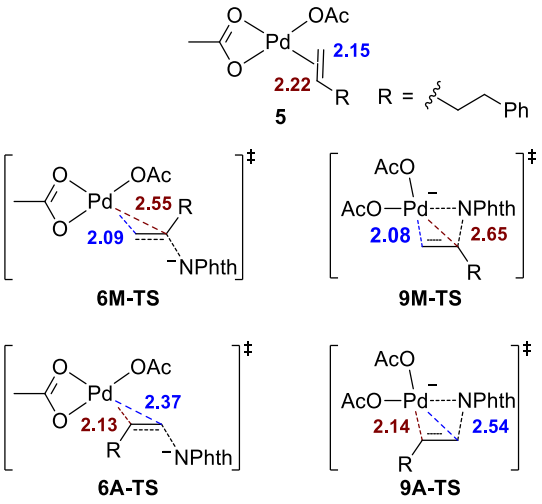

Figure S12. The comparison of η^2 to η^1 slippage between neutral *trans*-aminopalladation transition states (**6M-TS** and **6A-TS**) and neutral *cis*-amiopalladation transition states (**9M-TS** and **9A-TS**). The red numbers represent the distance between Pd and the internal carbon, while the blue numbers represent the distance between Pd and the terminal carbon. These values are in Å.

10. Chloride ion involved aminopalladation with anionic palladate Pd catalyst

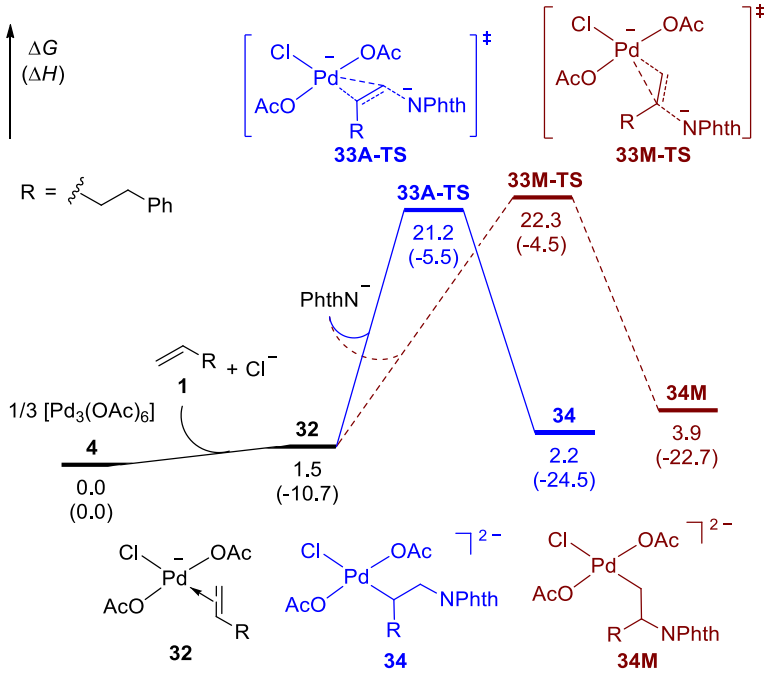

Figure S13. Free energy profile of chloride ion involved aminopalladation with anionic palladate Pd catalyst.

In the theoretical study, the chloride ion involved palladate Pd catalyzed aminopalladation with phthalimide anion is also considered. As shown in Figure S13, anionic Pd complex **32** could be formed through the coordination of alkene **1** and chloride ion to neutral Pd complex **4**. The *anti*-Markovnikov and Markovnikov addition transition states are located as **33A-TS** and **33M-TS**, respectively. The relative free energy of **33M-TS** is higher than that of **33A-TS** by 1.1 kcal/mol, which suggests that the *anti*-Markovnikov selectivity is also favored for chloride ion involved palladate Pd catalyzed aminopalladation. This conclusion is consistent with $Pd(OAc)_3^-$ catalyzed aminopalladation with phthalimide anion. Besides, the activation free energy of **33A-TS** is found to be 2.0 kcal/mol lower than that of **12A-TS** (23.2 kcal/mol in Figure 2), which implies that the utilization of chloride ion might reduce the energy barrier of aminopalladation. The energy decomposition approach was also used to study the nucleophile-substrate interactions on the regioselectivity in

$PdCl(OAc)_2^-$ catalyzed *trans*-aminopalladation with phthalimide anion. The comparison between Figure S14 and Figure 8 suggest that replacing the OAc anionic ligand with a chloride has a minimal impact on the steric, electronic, and dispersion effects on regioselectivity. Therefore, the formal charge of the Pd catalyst plays a much more significant role on regioselectivity than the nature of the ligand.

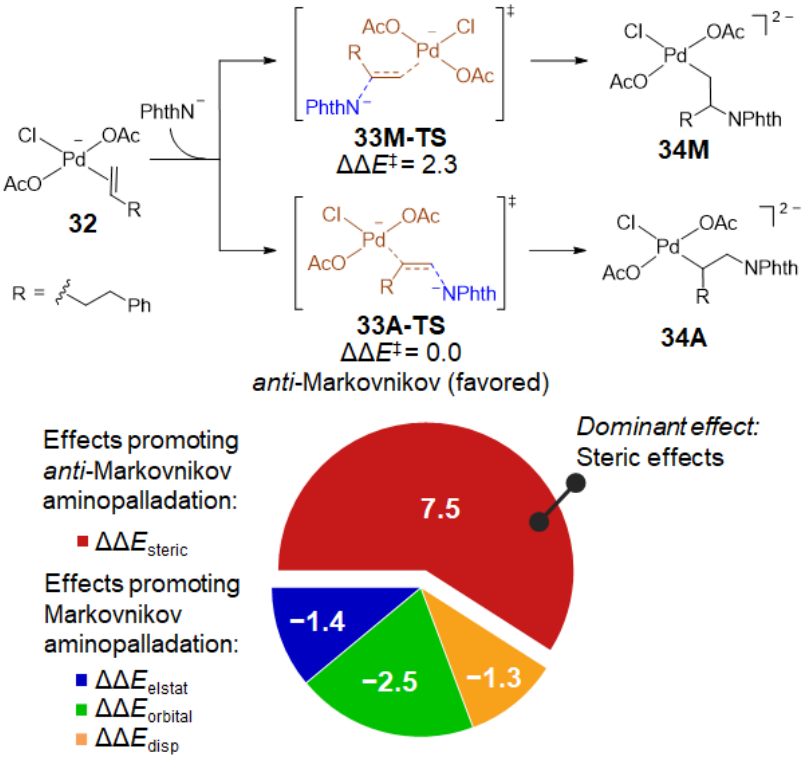

Figure S14. Comparison of different types of nucleophile-substrate interactions on the regioselectivity in $PdCl(OAc)_2^-$ catalyzed *trans*-aminopalladation with phthalimide anion. The computed regioselectivity ($\Delta\Delta E^‡$) is calculated from the energy difference between Markovnikov and *anti*-Markovnikov transition states ($\Delta\Delta E^‡ = \Delta E_M^‡ - \Delta E_A^‡$). Each energy component ($\Delta\Delta E_{steric}$, $\Delta\Delta E_{elstat}$, $\Delta\Delta E_{orbital}$ and $\Delta\Delta E_{disp}$) is calculated in a similar fashion ($\Delta\Delta E = \Delta E_M - \Delta E_A$). All energies are in kcal/mol.

11. Energy decomposition analysis along the reaction coordinates of anionic $Pd(OAc)_3^-$ catalyzed *trans*-aminopalladation with phthalimide anion and $Pd(OAc)_2$ catalyzed *trans*-aminopalladation with *i*Pr$_2$NH.

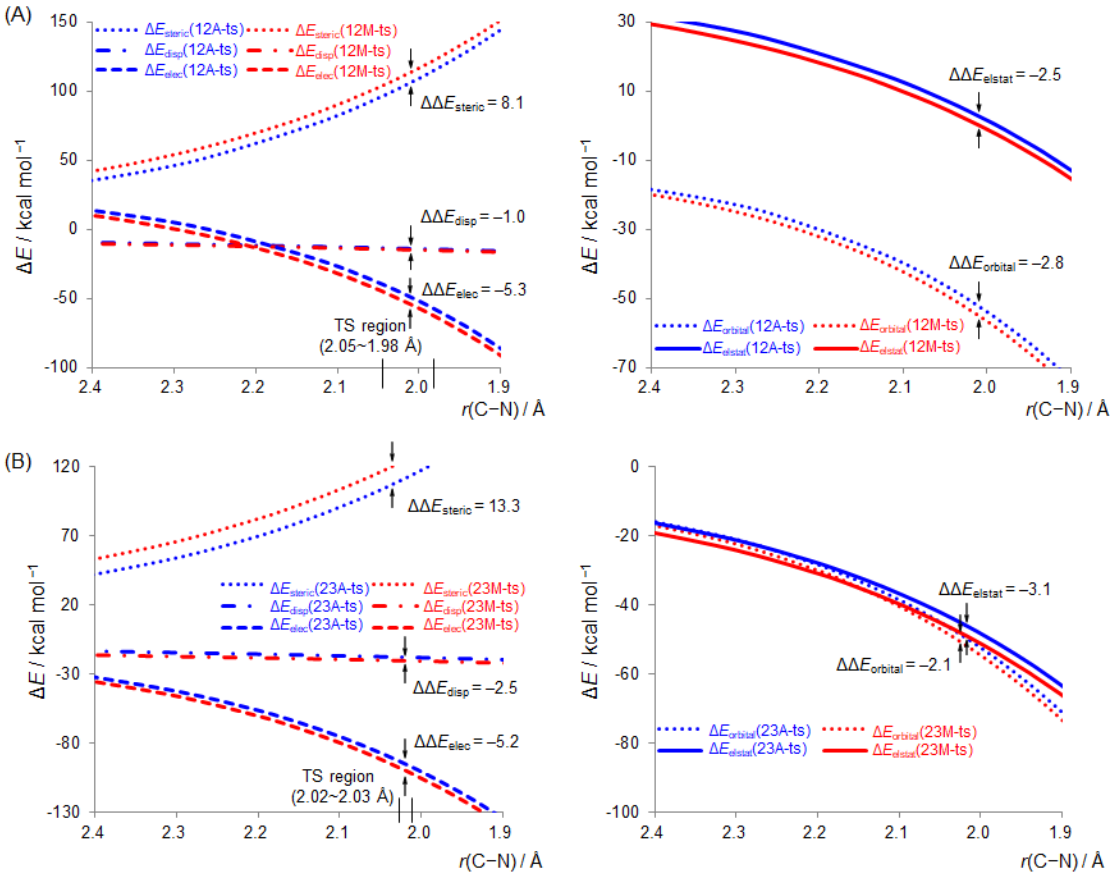

Figure S15. Energy decomposition analysis along the reaction coordinates of anionic $Pd(OAc)_3^-$ catalyzed *trans*-aminopalladation with phthalimide anion (**A**) and neutral $Pd(OAc)_2$ catalyzed *trans*-aminopalladation with *i*Pr$_2$NH (B). The overall electronic effect term (ΔE_{elec}, left column) is further dissected into electrostatics (ΔE_{elstat}) and orbital interactions ($\Delta E_{orbital}$) in the right column. The $\Delta\Delta E$ values are calculated from the energy difference between Markovnikov and *anti*-Markovnikov transition states ($\Delta\Delta E = \Delta E_M - \Delta E_A$).

12. Comparison of Two strategies for Calculating the $\Delta\Delta E$ values

In the main text, the energy terms are calculated using the following equation,

$$\Delta\Delta E_{ave} = 1/2\ [(\Delta E_{M(dis1)} - \Delta E_{A(dis1)}) + (\Delta E_{M(dis2)} - \Delta E_{A(dis2)})] \quad \text{Eq. 1}$$

using the average of energy difference between Markovnikov and anti-Markovnikov transition states (TS-M and TS-A, respectively) computed at two distances, dis1 and dis2, which are the C-N bond distances in TS-M and TS-A, respectively. One of the reviewers recommended the use of one of the distances to evaluate the energy difference ($\Delta\Delta E_{dis1} = \Delta E_{M(dis1)} - \Delta E_{A(dis1)}$, Eq. 2), rather than the average of the two distances. We considered the strategy proposed by the reviewer (Eq. 2) and compared the results with the average $\Delta\Delta E_{ave}$ values computed using Eq. 1. As show in the following Table, the two strategies provided almost identical energy values for each energy term. This is because the $\Delta\Delta E$ values computed at the two different distances ($\Delta\Delta E_{dis1}$ and $\Delta\Delta E_{dis2}$) are very close to each other. Therefore, using either $\Delta\Delta E_{dis1}$ or $\Delta\Delta E_{ave}$ has a minimal impact on the computed energy terms.

Table S1. Comparison of Two strategies for Calculating the $\Delta\Delta E$ values

		$\Delta\Delta E_{steric}$	$\Delta\Delta E_{elstat}$	$\Delta\Delta E_{orbital}$	$\Delta\Delta E_{disp}$
9M-TS	$\Delta\Delta E_{dis1}$ (from Eq. 2)	28.5	-10.4	-17.0	-2.0
vs	$\Delta\Delta E_{dis2}$	28.3	-10.4	-17.1	-1.9
9A-TS	$\Delta\Delta E_{ave}$ (from Eq. 1)	28.4	-10.4	-17.1	-2.0
6M-TS	$\Delta\Delta E_{dis1}$	9.3	-5.3	-3.6	-2.9
vs	$\Delta\Delta E_{dis2}$	9.4	-5.4	-3.6	-2.9
6A-TS	$\Delta\Delta E_{ave}$	9.4	-5.4	-3.6	-2.9
12M-TS	$\Delta\Delta E_{dis1}$	8.1	-2.5	-2.7	-1.0
vs	$\Delta\Delta E_{dis2}$	8.1	-2.6	-2.8	-0.9
12A-TS	$\Delta\Delta E_{ave}$	8.1	-2.5	-2.8	-1.0

13. Decomposition of the activation energies into steric effects ($\Delta\Delta E_{steric}$), electrostatics ($\Delta\Delta E_{elstat}$), polarization ($\Delta\Delta E_{pol}$), charge-transfer ($\Delta\Delta E_{ct}$), and dispersion ($\Delta\Delta E_{disp}$)

As shown in Figure S16, the activation free energies in $Pd(OAc)_2$-catalyzed *cis*- and *trans*-aminopalldation with phthalimide anion (a and b), and anionic $Pd(OAc)_3^-$ catalyzed *trans*-aminopalldation with phthalimide anion (c) are decomposed into

steric effects ($\Delta\Delta E_{steric}$), electrostatics ($\Delta\Delta E_{elstat}$), polarization ($\Delta\Delta E_{pol}$), charge-transfer ($\Delta\Delta E_{ct}$), and dispersion ($\Delta\Delta E_{disp}$). These results show that both charge transfer and polarization are both important components that favors Markovnikov addition. Therefore, these two effects all paly significant roles in determining the regioselectivity of nucleopalladation.

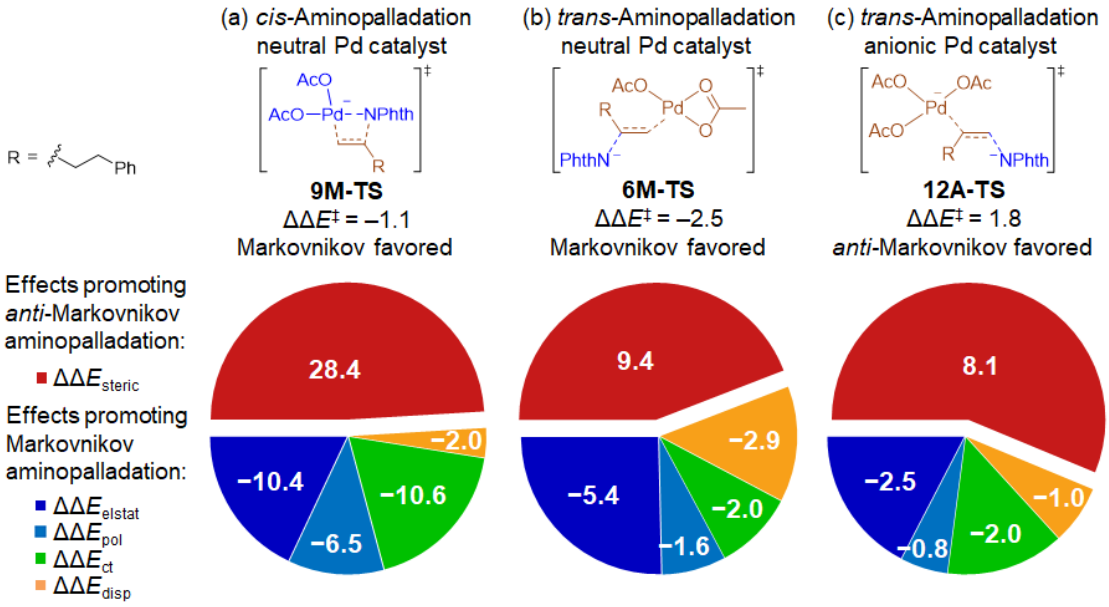

Figure S16. Decomposition of the activation energies into steric effects ($\Delta\Delta E_{steric}$), electrostatics ($\Delta\Delta E_{elstat}$), polarization ($\Delta\Delta E_{pol}$), charge-transfer ($\Delta\Delta E_{ct}$), and dispersion ($\Delta\Delta E_{disp}$).

14. Decomposition of the activation energies into distortion energy ($\Delta\Delta E_{dist}$), Pauli repulsion ($\Delta\Delta E_{Pauli}$), electrostatics ($\Delta\Delta E_{elstat}$), orbital interactions ($\Delta\Delta E_{orbital}$), and dispersion ($\Delta\Delta E_{disp}$)

As shown in Figure S17, the overall activation free energies are decomposed into distortion energy ($\Delta\Delta E_{dist}$), Pauli repulsion ($\Delta\Delta E_{Pauli}$), electrostatics ($\Delta\Delta E_{elstat}$), orbital interactions ($\Delta\Delta E_{orbital}$), and dispersion ($\Delta\Delta E_{disp}$). In neutral $Pd(OAc)_2$-catalyzed *cis*-aminopalladation with phthalimide anion (Figure S17a), $\Delta\Delta E_{dist}$ is much smaller than that of $\Delta\Delta E_{Pauli}$. While in $Pd(OAc)_2$- and $Pd(OAc)_3^-$-catalyzed

trans-aminopalladation (Figure S17b and c), $\Delta\Delta E_{dist}$ and $\Delta\Delta E_{Pauli}$ are comparable. For these three cases, distortion energy ($\Delta\Delta E_{dist}$) always favor the *anti*-Markovnikov nucleopalladation, which is analogous to Pauli repulsion ($\Delta\Delta E_{Pauli}$). Therefore, distortion ($\Delta\Delta E_{dist}$) and Pauli repulsion ($\Delta\Delta E_{Pauli}$) can be combined and discussed as a whole.

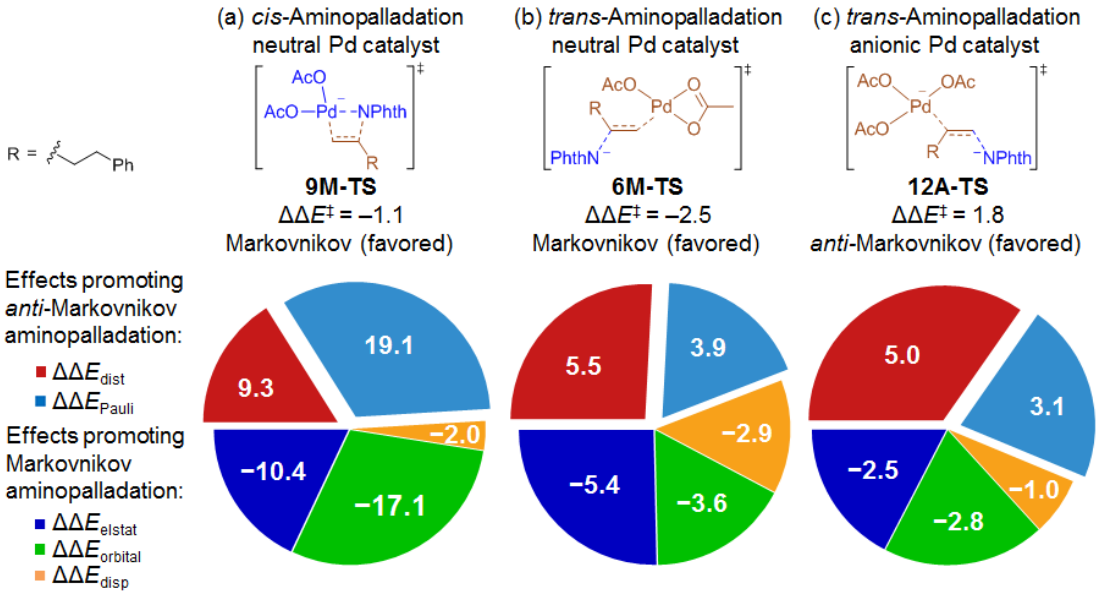

Figure S17. Decomposition of the activation energies into distortion energy ($\Delta\Delta E_{dist}$), Pauli repulsion ($\Delta\Delta E_{Pauli}$), electrostatics ($\Delta\Delta E_{elstat}$), orbital interactions ($\Delta\Delta E_{orbital}$), and dispersion ($\Delta\Delta E_{disp}$). The computed regioselectivity ($\Delta\Delta E^{‡}$) is calculated from the energy difference between Markovnikov and *anti*-Markovnikov transition states ($\Delta\Delta E^{‡} = \Delta E_{M}^{‡} - \Delta E_{A}^{‡}$). All energies are in kcal/mol.

15. Summary of Other EDA Results Regarding the Catalyst Effects and Nucleophile Effects on Regioselectivity

To reveal the quantitative effects of different O- and N-nucleophiles on the regioselectivity, the energy decomposition approach was employed to study $Pd(OAc)_2$-catalyzed *trans*-nucleopalladation with different nucleophiles. These EDA results are shown in Figure 7 (Figure S18) and the detailed discussions are provided in

the main text. Based on these results, we drew the conclusion that the variation of O-nucleophile from neutral to anionic could intensify the electrostatic interaction and promote the Markovnikov addition. We also uncovered that the regioselectivity of nucleopalladation is not sensitive to the steric effects of primary amines and alcohols, only the extremely bulky amines have the potential to reverse the Markovnikov nucleophilic addition to *anti*-Markovnikov selectivity.

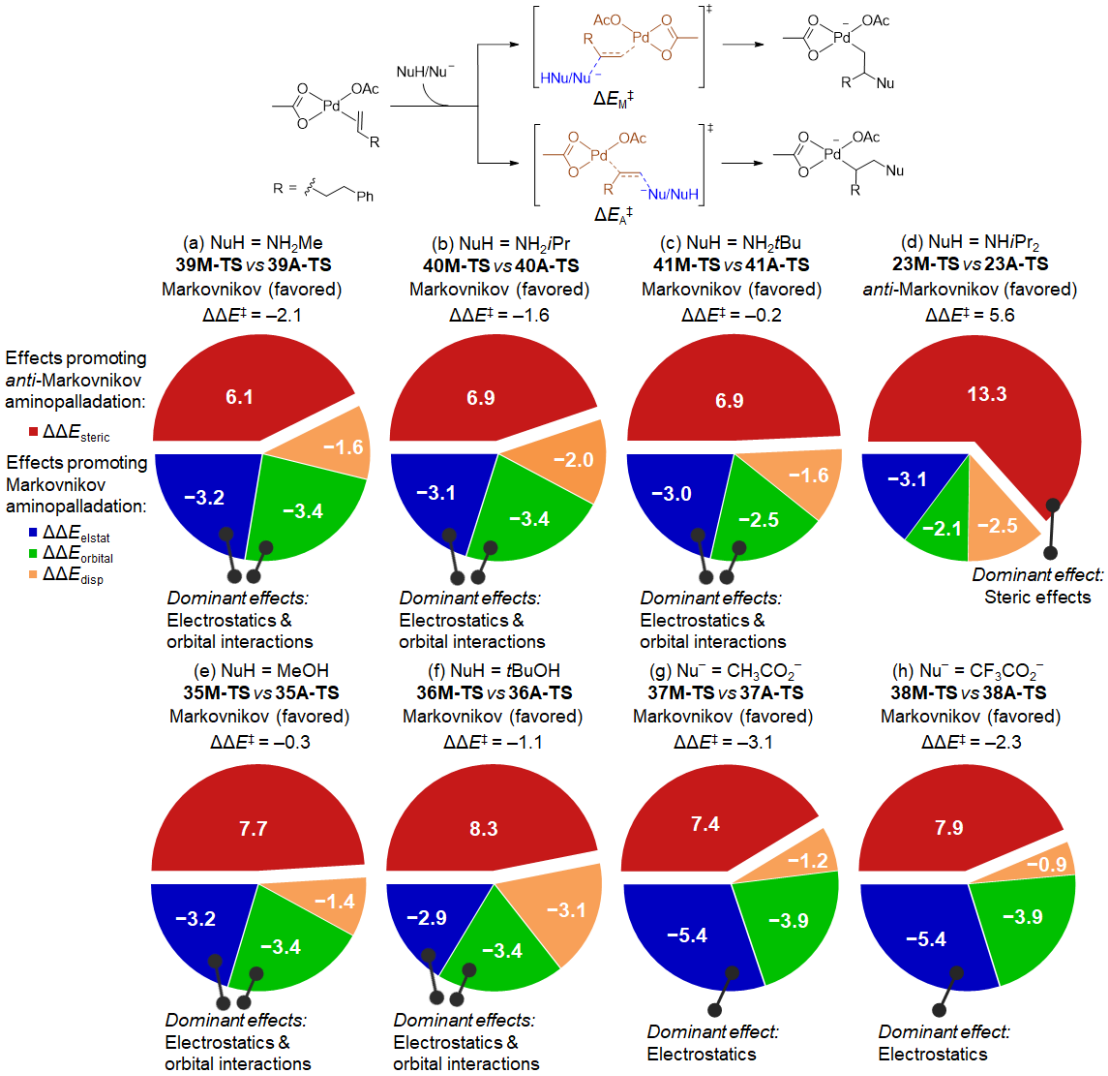

Figure S18. Comparison of the effects of different O- and N-nucleophiles on the regioselectivity of $Pd(OAc)_2$-catalyzed *trans*-nucleopalladation. The computed regioselectivity ($\Delta\Delta E^{\ddagger}$) is calculated from the energy difference between Markovnikov and *anti*-Markovnikov transition states ($\Delta\Delta E^{\ddagger} = \Delta E_M^{\ddagger} - \Delta E_A^{\ddagger}$). Each energy component ($\Delta\Delta E_{steric}$, $\Delta\Delta E_{elstat}$, $\Delta\Delta E_{orbital}$ and $\Delta\Delta E_{disp}$) is calculated in a similar

fashion ($\Delta\Delta E$ = ΔE_M – ΔE_A). Positive $\Delta\Delta E$ values indicate effects that promote *anti*-Markovnikov addition; negative $\Delta\Delta E$ values indicate effects that promote Markovnikov addition. All energies are in kcal/mol.

In addition to the nucleophile effects, the catalyst effects on regioselectivity of nucleopalladation of aliphatic alkenes are also studied in this work. The energy decomposition approach was employed to study several anionic palladate catalyzed *trans*-aminopalladation with phthalimide anion. For example, $Pd(OAc)_3^-$ (Figure 8), $PdCl(OAc)_2^-$ (Figure S14), $Pd(OPiv)_3^-$ (Figure S19a), and $Pd(CF_3CO_2)_3^-$ (Figure S19b), are all considered in our calculation. Moreover, the other two nucleophiles employed in Hull's experiments are used in EDA calculation (Figure S19c and S19d). Computational results show that all these aminopalladation reactions prefer the *anti*-Markovnikov selectivity. The proportion of each nucleophile-substrate interactions in these EDA results also show the same trend, which lead to the same conclusion that steric effects is the dominant factor favoring the *anti*-Markovnikov addition due to the diminished electrostatic effect.

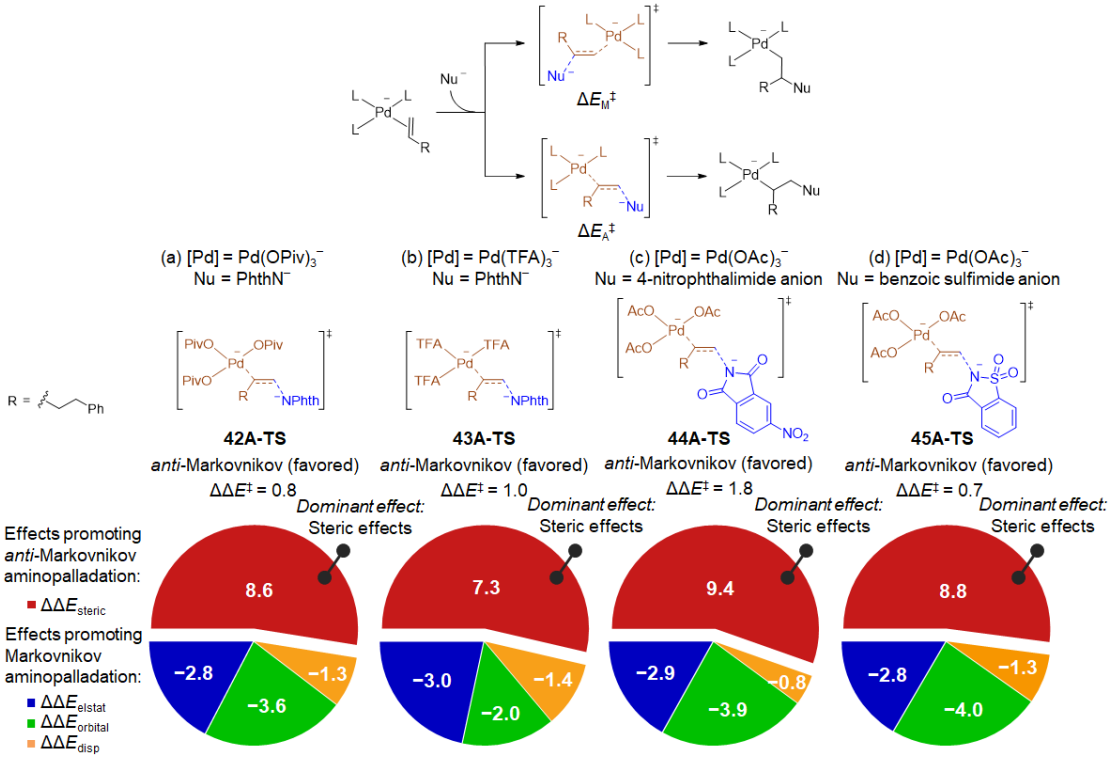

Figure S19. Comparison of different types of nucleophile-substrate interactions on

the regioselectivity in anionic palladate-catalyzed *trans*-aminopalladation with anionic nucleophiles. The computed regioselectivity ($\Delta\Delta E^{\ddagger}$) is calculated from the energy difference between Markovnikov and *anti*-Markovnikov transition states ($\Delta\Delta E^{\ddagger} = \Delta E_M^{\ddagger} - \Delta E_A^{\ddagger}$). Each energy component ($\Delta\Delta E_{steric}$, $\Delta\Delta E_{elstat}$, $\Delta\Delta E_{orbital}$ and $\Delta\Delta E_{disp}$) is calculated in a similar fashion ($\Delta\Delta E = \Delta E_M - \Delta E_A$). Positive $\Delta\Delta E$ values indicate effects that promote *anti*-Markovnikov addition; negative $\Delta\Delta E$ values indicate effects that promote Markovnikov addition. All energies are in kcal/mol.

The neutral $Pd(H_2O)Cl_2$-catalyzed *trans*-nucleopalladation with different nucleophiles is also studied to reveal the catalyst and nucleophile effects on regioselectivity. The corresponding EDA results are shown in Figure S20. Neutral nucleophiles, MeOH, *t*BuOH, NH_2Me, and anionic nucleophile, phthalimide anion, are all employed to enable a comprehensive understanding on catalyst effects. The comparison among Figure S20, Figure 7 (Figure S18) and Figure 6b suggest that replacing the $Pd(OAc)_2$ catalyst by $Pd(H_2O)Cl_2$ doesn't change the EDA results. These conclusions shown here are consistent with the summary of catalyst effects and nucleophile effects in the main manuscript (Figure 9).

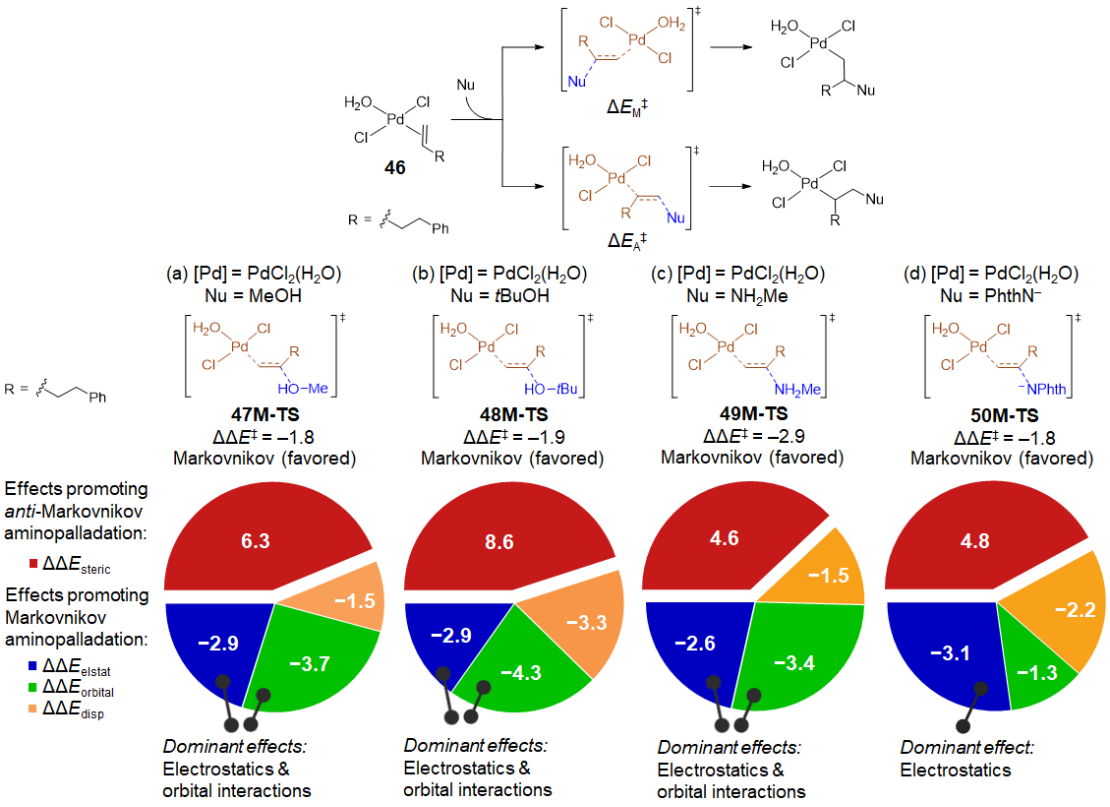

Figure S20. Comparison of different types of nucleophile-substrate interactions on the regioselectivity in neutral $Pd(H_2O)Cl_2$-catalyzed *trans*-nucleopalladation with different nucleophiles. The computed regioselectivity ($\Delta\Delta E^{\ddagger}$) is calculated from the energy difference between Markovnikov and *anti*-Markovnikov transition states ($\Delta\Delta E^{\ddagger} = \Delta E_M^{\ddagger} - \Delta E_A^{\ddagger}$). Each energy component ($\Delta\Delta E_{steric}$, $\Delta\Delta E_{elstat}$, $\Delta\Delta E_{orbital}$ and $\Delta\Delta E_{disp}$) is calculated in a similar fashion ($\Delta\Delta E = \Delta E_M - \Delta E_A$). Positive $\Delta\Delta E$ values indicate effects that promote *anti*-Markovnikov addition; negative $\Delta\Delta E$ values indicate effects that promote Markovnikov addition. All energies are in kcal/mol.

16. $Pd(OAc)_2$-catalyzed nucleopalladation of alkene using neutral phthalimide with interacting AcO anion

The $Pd(OAc)_2$-catalyzed nucleopalladation of alkene using neutral phthalimide with interacting AcO anion are also considered in calculation. As shown below, the corresponding transition states are located as **6M′-TS** and **6A′-TS** (Figure S21). With the interaction of AcO anion with phthalimide, the activation free energy of **6M′-TS** is

2.3 kcal/mol higher than that of **6M-TS** (Figure 1) and the activation free energy of **6A′-TS** is 1.5 kcal/mol higher than that of **6M-TS**, which suggest that this nucleopalladation mechanism is kinetically disfavored. More importantly, this pathway favors *anti*-Markovnikov addition, which is inconsistent with the experimentally reported Markovnikov selectivity. Energy decomposition analyses further reveal that the electrostatics ($\Delta\Delta E_{elstat}$) is –3.8 kcal/mol, which is lower than that in Figure 5b (–5.4 kcal/mol). Because of the diminished $\Delta\Delta E_{elstat}$, the steric effects override the electronic effects and dispersion and thus leads to the *anti*-Markovnikov selectivity. Therefore, the nucleopalladation mechanism using neutral phthalimide with interacting AcO anion is unlikely for this reaction.

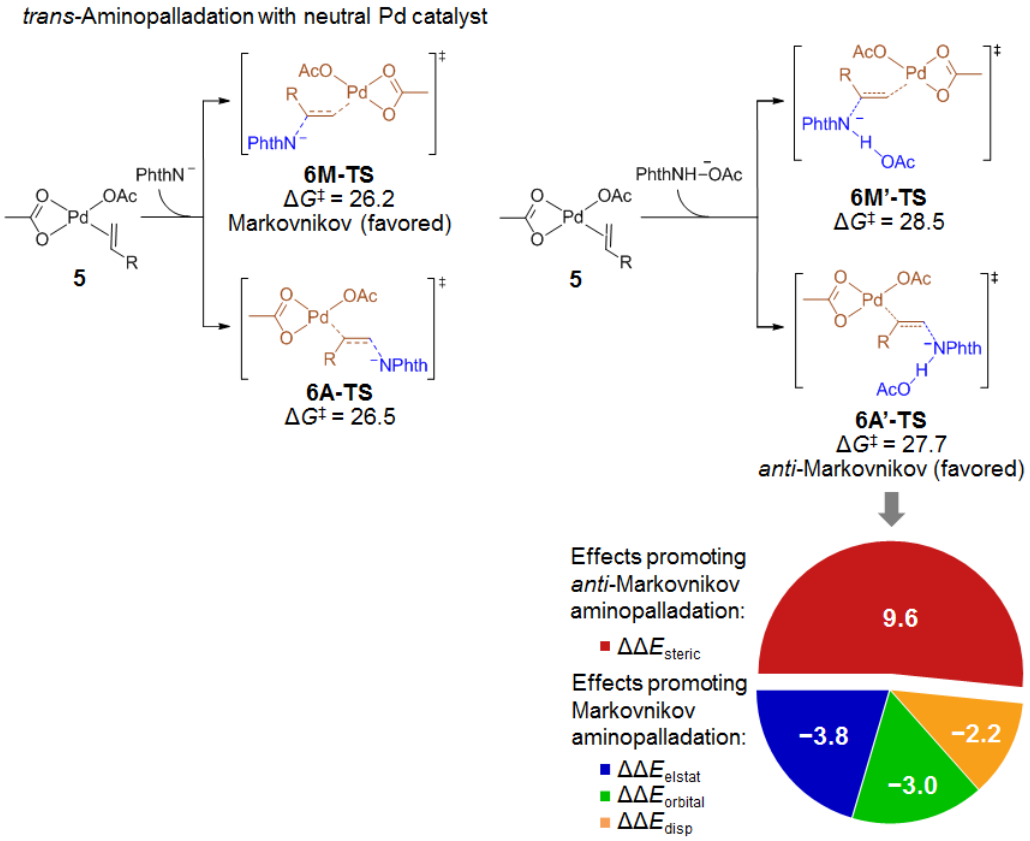

Figure S21. $Pd(OAc)_2$-catalyzed nucleopalladation of alkene using neutral phthalimide with interacting AcO anion. The computed regioselectivity ($\Delta\Delta E^{‡}$) is calculated from the energy difference between Markovnikov and *anti*-Markovnikov transition states ($\Delta\Delta E^{‡} = \Delta E_M^{‡} - \Delta E_A^{‡}$). All energies are in kcal/mol. The activation free energies are with respect to 1/3[$Pd_3(OAc)_6$] **4**.

17. Cartesian coordinates and energies of optimized structures

1

B3LYP SCF energy: -388.27940389 a.u.
B3LYP enthalpy: -388.078523 a.u.
B3LYP free energy: -388.124900 a.u.
B3LYP free energy after quasi-harmonic correction: -388.123518 a.u.
M06 SCF energy in solution: -388.05605756 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.658729	-1.095442	-0.273867
C	-1.319831	-1.214542	0.109196
C	-0.548278	-0.080150	0.405410
C	-1.158345	1.180058	0.310929
C	-2.496865	1.305872	-0.071949
C	-3.252325	0.167112	-0.366854
H	-3.238939	-1.988213	-0.494666
H	-0.868641	-2.202429	0.185083
H	-0.579960	2.072128	0.544835
H	-2.950097	2.292288	-0.135009
H	-4.294321	0.262063	-0.661665
C	0.912842	-0.209180	0.781684
H	1.201814	0.612682	1.448776
H	1.070111	-1.139847	1.343497
C	1.854589	-0.202401	-0.450047
H	1.549291	-1.017503	-1.122917
H	1.719890	0.733073	-1.008011
C	3.301140	-0.374280	-0.072388
H	3.549202	-1.298806	0.454065
C	4.275503	0.507424	-0.321032
H	4.079925	1.443217	-0.842701
H	5.303510	0.324521	-0.017786

2

B3LYP SCF energy: -513.10648883 a.u.
B3LYP enthalpy: -512.981568 a.u.
B3LYP free energy: -513.023209 a.u.
B3LYP free energy after quasi-harmonic correction: -513.023209 a.u.
M06 SCF energy in solution: -512.91665726 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.176269	-0.699786	0.000184
C	0.176239	0.699781	0.000048
C	1.360292	1.425717	-0.000386
C	2.561650	0.701356	-0.000306
C	2.561679	-0.701269	0.000185
C	1.360350	-1.425677	0.000496
C	-1.243300	-1.172128	-0.000654
C	-1.243352	1.172074	0.000690
H	1.350447	2.511606	-0.000439
H	3.508532	1.234359	-0.000492
H	3.508581	-1.234234	0.000208

H	1.350547	-2.511567	0.000627
N	-2.012937	-0.000052	0.000282
H	-3.025664	-0.000081	0.000029
O	-1.678866	2.306737	-0.000100
O	-1.678740	-2.306752	-0.000331

3

B3LYP SCF energy: -900.19372384 a.u.
B3LYP enthalpy: -899.887471 a.u.
B3LYP free energy: -899.955266 a.u.
B3LYP free energy after quasi-harmonic correction: -899.949487 a.u.
M06 SCF energy in solution: -899.78382752 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	3.799127	0.742946	-0.132405
C	3.926668	-0.639517	0.029796
C	5.151633	-1.227563	0.315463
C	6.262445	-0.378610	0.436640
C	6.134465	1.008427	0.273955
C	4.891470	1.592026	-0.015258
C	2.366509	1.046766	-0.429618
C	2.579173	-1.256385	-0.159851
H	5.241113	-2.302809	0.438927
H	7.238232	-0.801354	0.660033
H	7.012988	1.640130	0.373623
H	4.782612	2.664886	-0.143729
N	1.704423	-0.191895	-0.432197
O	2.259833	-2.430227	-0.104675
O	1.839928	2.124731	-0.637223
C	0.276255	-0.354689	-0.683035
H	-0.021869	0.415894	-1.399039
H	0.142883	-1.337125	-1.145511
C	-0.570575	-0.242772	0.602725
H	-0.446120	0.759744	1.028879
H	-0.179778	-0.965374	1.333264
C	-2.024334	-0.521841	0.338260
H	-2.259064	-1.537327	0.016695
C	-3.005074	0.388161	0.467758
H	-2.724245	1.394123	0.784778
C	-4.447574	0.199845	0.236124
C	-5.305601	1.306251	0.379981
C	-5.022378	-1.036633	-0.119904
C	-6.681931	1.189505	0.173554
H	-4.883603	2.270448	0.656043
C	-6.395577	-1.155680	-0.326175
H	-4.393357	-1.915160	-0.233273
C	-7.234319	-0.043443	-0.181335
H	-7.320737	2.061387	0.290664
H	-6.815463	-2.120813	-0.598958
H	-8.304933	-0.140170	-0.341876

3M

B3LYP SCF energy: -900.18289695 a.u.
B3LYP enthalpy: -899.877533 a.u.
B3LYP free energy: -899.944855 a.u.
B3LYP free energy after quasi-harmonic correction: -899.939115 a.u.
M06 SCF energy in solution: -899.77563297 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	3.038174	0.138696	0.532695
C	2.650344	-0.792978	-0.430374
C	3.362133	-1.968169	-0.635116
C	4.489743	-2.186362	0.169967
C	4.879006	-1.250192	1.139894
C	4.153505	-0.065816	1.335410
C	2.079695	1.280757	0.498805
C	1.431310	-0.279272	-1.118180
H	3.052287	-2.685666	-1.389050
H	5.072604	-3.094409	0.041731
H	5.757791	-1.446958	1.747967
H	4.447163	0.665926	2.082089
N	1.133285	0.963709	-0.513997
O	0.806790	-0.797349	-2.024583
O	2.082436	2.282147	1.184237
C	0.190542	3.089288	-1.090090
H	1.169799	3.553222	-1.052996
H	-0.660333	3.729991	-1.300363
C	0.006551	1.784353	-0.862759
C	-1.341777	1.102285	-0.880317
H	-2.088906	1.840016	-1.193483
C	-1.749494	0.511168	0.493258
H	-1.003785	-0.232425	0.802432
C	-3.120043	-0.132477	0.456238
C	-4.257406	0.571109	0.879286
C	-3.287653	-1.438872	-0.029762
C	-5.527656	-0.010109	0.818262
H	-4.146618	1.582619	1.265923
C	-4.554648	-2.024444	-0.093173
H	-2.417051	-2.002462	-0.360263
C	-5.680468	-1.311127	0.330962
H	-6.395423	0.551910	1.155120
H	-4.662199	-3.038695	-0.470087
H	-6.666455	-1.766609	0.285115
H	-1.731387	1.308705	1.246226
H	-1.345436	0.303470	-1.629654

4

B3LYP SCF energy: -1754.90694680 a.u.
B3LYP enthalpy: -1754.556011 a.u.
B3LYP free energy: -1754.663146 a.u.
B3LYP free energy after quasi-harmonic correction: -1754.652439 a.u.
M06 SCF energy in solution: -1754.46302152 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.282312	1.304581	-1.870556

O	1.270466	2.024433	-1.610156
O	2.637647	0.235174	-1.288758
C	3.156593	1.758898	-3.022386
H	4.206780	1.553808	-2.798991
H	2.885217	1.182120	-3.914701
H	3.004627	2.820417	-3.226992
Pd	-1.638074	-0.906829	0.000707
C	0.002193	-2.613133	-1.881497
O	1.130388	-2.094924	-1.620001
O	-1.100544	-2.390700	-1.296465
C	-0.042810	-3.596553	-3.033996
H	-0.668064	-4.453074	-2.766661
H	-0.505469	-3.105004	-3.897808
H	0.963083	-3.924503	-3.302204
C	2.309635	1.233736	1.885494
O	1.574528	2.096968	1.318564
O	2.386356	-0.006058	1.624625
C	3.221623	1.747129	2.982004
H	3.503337	0.934676	3.655165
H	4.132669	2.145347	2.519014
H	2.736412	2.557526	3.531055
Pd	1.610768	-0.965313	0.005286
C	-0.089529	-2.612343	1.886257
O	1.023343	-2.423692	1.309635
O	-1.195684	-2.044761	1.630390
C	-0.106576	-3.653127	2.987999
H	-0.941784	-3.473905	3.668370
H	-0.237602	-4.641767	2.531569
H	0.843292	-3.650090	3.527784
C	-2.236686	1.387001	1.870711
O	-2.627590	0.329150	1.290585
O	-1.200513	2.070984	1.609566
C	-3.094861	1.873575	3.021367
H	-2.824555	1.307559	3.920913
H	-4.149933	1.682211	2.809693
C	-2.265836	1.309123	-1.884494
O	-1.503886	2.149320	-1.318325
O	-2.380096	0.072146	-1.623321
C	-3.162603	1.849977	-2.980305
H	-3.467230	1.046897	-3.654749
H	-2.654766	2.647302	-3.528054
Pd	0.031734	1.873980	-0.000319
H	-4.062176	2.272887	-2.516762
H	-2.923552	2.935539	3.208041

5

B3LYP SCF energy: -973.22871689 a.u.
B3LYP enthalpy: -972.910491 a.u.
B3LYP free energy: -972.990518 a.u.
B3LYP free energy after quasi-harmonic correction: -972.981273 a.u.
M06 SCF energy in solution: -972.86864527 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-3.124924	-1.612642	-0.947839

O	-2.720318	-0.575328	-1.554421
O	-2.682123	-1.825736	0.247979
C	-4.069233	-2.588509	-1.585285
H	-4.579812	-3.183350	-0.823988
H	-4.793496	-2.054539	-2.206479
H	-3.499545	-3.264355	-2.234937
Pd	-1.573305	-0.083285	0.248269
C	-1.377569	2.652824	-0.111624
O	-2.564124	2.579040	0.204230
O	-0.559381	1.616521	-0.103602
C	-0.720239	3.942882	-0.569424
H	-1.344409	4.793384	-0.286347
H	0.283018	4.049179	-0.145457
H	-0.619523	3.925466	-1.661336
C	4.382514	-1.495517	0.248322
C	3.332763	-0.676012	-0.192025
C	3.651288	0.507691	-0.875714
C	4.982027	0.864095	-1.109959
C	6.019626	0.039648	-0.663234
C	5.715622	-1.143026	0.016926
H	4.155291	-2.423145	0.771138
H	2.848183	1.150401	-1.231032
H	5.208241	1.782653	-1.645951
H	7.055098	0.313994	-0.848050
H	6.514493	-1.794593	0.362670
C	1.888799	-1.040311	0.084205
H	1.260040	-0.736299	-0.761127
H	1.792895	-2.130502	0.177925
C	1.345433	-0.370405	1.366176
H	1.409192	0.718491	1.278731
H	1.982900	-0.663320	2.216333
C	-0.060277	-0.779404	1.715306
H	-0.257455	-1.852801	1.716241
C	-1.001188	0.051977	2.319883
H	-0.763931	1.091179	2.532588
H	-1.859425	-0.366445	2.840938

6A-TS

B3LYP SCF energy: -1485.80301127 a.u.
B3LYP enthalpy: -1485.372510 a.u.
B3LYP free energy: -1485.478284 a.u.
B3LYP free energy after quasi-harmonic correction: -1485.461650 a.u.
M06 SCF energy in solution: -1485.30045059 a.u.
Imaginary frequency: -171.0416 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-3.044283	-3.007579	-1.798740
O	-3.830116	-2.660175	-0.880748
O	-1.859099	-2.499101	-1.868355
C	-3.435362	-4.045673	-2.826021
H	-2.921295	-3.864943	-3.774531
H	-3.138293	-5.036614	-2.460322
H	-4.519387	-4.044154	-2.969531
Pd	-2.024386	-1.335384	-0.162495

C	-2.758639	-0.874057	2.545518
O	-2.784950	-2.101833	2.637417
O	-2.411850	-0.201082	1.475492
C	-3.132289	0.030542	3.718389
H	-2.262130	0.623646	4.023962
H	-3.919953	0.732813	3.421966
H	-3.473603	-0.575371	4.561325
C	-0.666230	4.472023	-1.384867
C	-1.435189	3.552161	-0.654750
C	-2.191425	4.033323	0.426387
C	-2.181874	5.388994	0.766554
C	-1.411995	6.294392	0.028700
C	-0.652407	5.829315	-1.049390
H	-0.069366	4.117275	-2.223075
H	-2.790502	3.332350	1.004175
H	-2.776959	5.738519	1.607765
H	-1.404075	7.350040	0.291193
H	-0.047908	6.522688	-1.630470
C	-1.430823	2.078464	-0.999366
H	-2.416466	1.647068	-0.787902
H	-1.247838	1.953116	-2.075262
C	-0.366293	1.282544	-0.214995
H	-0.549007	1.377363	0.859986
H	0.629291	1.702441	-0.422869
C	-0.300006	-0.172971	-0.607294
H	-0.185951	-0.348100	-1.677913
C	0.305989	-1.127811	0.237771
H	0.355883	-0.982609	1.308846
H	0.585440	-2.103575	-0.137054
C	4.709254	-0.159244	-0.488280
C	4.816092	-0.876274	0.701728
C	6.051759	-1.178045	1.258748
C	7.198562	-0.733608	0.579002
C	7.091018	-0.011260	-0.618649
C	5.833502	0.286935	-1.170377
C	3.225747	-0.023622	-0.778080
C	3.398512	-1.187273	1.144613
H	6.122593	-1.738524	2.187602
H	8.184626	-0.951071	0.984794
H	7.995141	0.321201	-1.124896
H	5.737375	0.846390	-2.097585
N	2.528142	-0.645105	0.227918
O	3.103651	-1.821064	2.159265
O	2.756790	0.560230	-1.759381

6b-TS

B3LYP SCF energy: -973.18991908 a.u.
B3LYP enthalpy: -972.877942 a.u.
B3LYP free energy: -972.955063 a.u.
B3LYP free energy after quasi-harmonic correction: -972.947547 a.u.
M06 SCF energy in solution: -972.82811077 a.u.
Imaginary frequency: -1473.6849 cm-1

Cartesian coordinates

ATOM	X	Y	Z

C	3.994828	-0.644846	0.985071
O	3.629087	0.551232	1.148132
O	3.343111	-1.386047	0.144943
C	5.176036	-1.231602	1.707533
H	6.066296	-1.134239	1.073954
H	5.354125	-0.689429	2.639418
H	5.016754	-2.295229	1.905469
Pd	2.052981	0.102189	-0.414447
C	-0.068726	2.205316	-0.244760
O	-0.926495	1.415029	0.281614
O	1.031184	1.857246	-0.770619
C	-0.402773	3.679015	-0.228602
H	0.371354	4.257105	-0.736528
H	-1.375631	3.844083	-0.703095
H	-0.485597	4.012960	0.812108
C	-4.618213	-1.377924	-0.509953
C	-3.564338	-1.054149	0.357675
C	-3.785555	-0.077700	1.340047
C	-5.024747	0.558343	1.451708
C	-6.066553	0.228689	0.579158
C	-5.859235	-0.742482	-0.404537
H	-4.468234	-2.140850	-1.272098
H	-2.979056	0.193012	2.017191
H	-5.176513	1.310562	2.222041
H	-7.031688	0.721139	0.667683
H	-6.663598	-1.011081	-1.085122
C	-2.218030	-1.739527	0.218364
H	-1.755265	-1.849382	1.208075
H	-2.382895	-2.758333	-0.160888
C	-1.246729	-0.998608	-0.712249
H	-0.947422	0.216307	-0.128187
H	-1.708741	-0.551568	-1.600231
C	0.054754	-1.486578	-0.897393
H	0.414084	-2.258635	-0.212864
C	1.011201	-0.990015	-1.843303
H	0.631910	-0.340215	-2.633693
H	1.776377	-1.694159	-2.173802

6M-TS

B3LYP SCF energy: -1485.80420734 a.u.
B3LYP enthalpy: -1485.373690 a.u.
B3LYP free energy: -1485.475991 a.u.
B3LYP free energy after quasi-harmonic correction: -1485.462302 a.u.
M06 SCF energy in solution: -1485.30154268 a.u.
Imaginary frequency: -147.2649 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-3.791333	-2.218161	-1.637940
O	-4.472860	-1.345963	-1.029464
O	-2.541898	-2.360584	-1.365980
C	-4.419067	-3.130233	-2.665781
H	-4.862310	-3.992854	-2.152570
H	-5.217473	-2.605180	-3.198199
H	-3.664799	-3.496690	-3.367462

Pd	-2.535981	-0.901811	0.114316
C	-3.292367	0.343636	2.591657
O	-3.540615	-0.787288	3.014695
O	-2.798399	0.627961	1.413723
C	-3.548007	1.591900	3.435842
H	-2.624693	2.172622	3.542948
H	-4.281325	2.235930	2.936187
H	-3.922664	1.305763	4.421815
C	1.756173	3.885201	-0.326340
C	0.698800	3.432970	-1.136139
C	-0.128899	4.388801	-1.742852
C	0.088836	5.758582	-1.555794
C	1.144779	6.195812	-0.751915
C	1.975964	5.251680	-0.137026
H	2.400485	3.155642	0.160711
H	-0.955528	4.055804	-2.368106
H	-0.567753	6.480801	-2.036981
H	1.317945	7.259666	-0.603505
H	2.799710	5.580209	0.493411
C	0.470024	1.949158	-1.336806
H	-0.274194	1.797337	-2.130234
H	1.400347	1.474536	-1.672059
C	0.007939	1.230383	-0.056118
H	-0.968191	1.612414	0.268189
H	0.707541	1.435999	0.760455
C	-0.093511	-0.264653	-0.219613
H	-0.023837	-0.680500	-1.219576
C	-0.571752	-1.124298	0.802551
H	-0.520287	-0.769468	1.830698
H	-0.386115	-2.189806	0.671861
C	4.308980	-1.090548	0.597388
C	3.974526	-2.136014	-0.260561
C	4.846336	-3.191598	-0.492792
C	6.084365	-3.171078	0.171487
C	6.420959	-2.118358	1.035408
C	5.529142	-1.055914	1.259382
C	3.130387	-0.137321	0.593679
C	2.588049	-1.828726	-0.790719
H	4.574434	-4.002002	-1.164397
H	6.793382	-3.981754	0.016082
H	7.386072	-2.127757	1.537908
H	5.778810	-0.234567	1.926336
N	2.165556	-0.634241	-0.248784
O	1.962657	-2.539653	-1.578157
O	3.081707	0.914216	1.241116

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B3LYP SCF energy: -1485.84133075 a.u.
B3LYP enthalpy: -1485.407552 a.u.
B3LYP free energy: -1485.506926 a.u.
B3LYP free energy after quasi-harmonic correction: -1485.495298 a.u.
M06 SCF energy in solution: -1485.35313454 a.u.

Cartesian coordinates

ATOM	X	Y	Z

C	2.004312	0.952123	2.740152
O	2.163731	2.002085	2.101251
O	2.032754	-0.257311	2.271100
C	1.704747	1.002311	4.242175
H	0.626205	0.863535	4.390872
H	2.220208	0.194608	4.772776
H	1.995080	1.973180	4.654138
Pd	2.431960	-0.653700	0.301497
C	4.324060	-1.459646	-1.287816
O	4.732232	-1.281500	-0.113241
O	3.094486	-1.262784	-1.611129
C	5.279316	-1.886443	-2.389879
H	6.150861	-2.391291	-1.963575
H	4.774003	-2.538561	-3.109360
H	5.625170	-0.995224	-2.929349
C	0.278270	3.168888	-0.402782
C	0.014260	2.522969	-1.623256
C	-1.025636	3.020815	-2.426909
C	-1.784475	4.126951	-2.032079
C	-1.513421	4.760012	-0.814421
C	-0.481345	4.274321	-0.004707
H	1.069229	2.801090	0.248652
H	-1.239543	2.534767	-3.378346
H	-2.582348	4.494738	-2.675188
H	-2.099954	5.621752	-0.501263
H	-0.261311	4.752080	0.947472
C	0.810571	1.310970	-2.064937
H	0.847340	1.294327	-3.163024
H	1.844989	1.393269	-1.712466
C	0.236068	-0.044856	-1.583576
H	0.688970	-0.843824	-2.182789
H	-0.843535	-0.057710	-1.814213
C	0.455529	-0.340074	-0.100473
H	0.170508	0.513099	0.523637
C	-0.279060	-1.589046	0.398080
H	-0.019672	-2.471708	-0.191970
H	-0.036649	-1.768009	1.447883
C	-3.961464	-1.660575	-0.389675
C	-3.960581	-0.903607	0.781209
C	-5.134980	-0.395390	1.319611
C	-6.330297	-0.668538	0.636959
C	-6.331613	-1.430432	-0.540878
C	-5.137498	-1.941732	-1.072222
C	-2.545379	-2.053188	-0.686671
C	-2.544394	-0.800389	1.262307
H	-5.120064	0.194382	2.231701
H	-7.270372	-0.283242	1.024306
H	-7.272870	-1.625459	-1.049133
H	-5.125599	-2.533400	-1.983213
N	-1.761347	-1.482586	0.320360
O	-2.143110	-0.260706	2.276655
O	-2.148010	-2.748129	-1.607164

7b

B3LYP SCF energy: -744.13414347 a.u.

B3LYP enthalpy: -743.885364 a.u.
B3LYP free energy: -743.948367 a.u.
B3LYP free energy after quasi-harmonic correction: -743.944016 a.u.
M06 SCF energy in solution: -743.83901955 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Pd	1.401758	-0.530158	-0.083557
C	2.420917	1.781521	0.074795
O	1.180636	1.609638	0.325276
O	3.131831	0.781413	-0.272617
C	3.047377	3.147732	0.193886
H	3.806367	3.132564	0.984363
H	3.555574	3.403647	-0.741887
H	2.292293	3.901521	0.426841
C	-3.871828	-0.709481	0.086741
C	-2.560812	-0.335439	0.414207
C	-2.190123	1.012260	0.277817
C	-3.113452	1.956860	-0.178307
C	-4.419283	1.573629	-0.502345
C	-4.797321	0.235513	-0.368219
H	-4.175134	-1.749773	0.191144
H	-1.177849	1.325777	0.518641
H	-2.809497	2.995841	-0.278906
H	-5.135277	2.311887	-0.854852
H	-5.809767	-0.074981	-0.614810
C	-1.568189	-1.374936	0.903456
H	-1.141666	-1.071674	1.868599
H	-2.109231	-2.315117	1.090806
C	-0.444918	-1.672392	-0.076001
H	-0.714954	-1.593618	-1.130977
C	0.654696	-2.496593	0.264701
H	0.776090	-2.843457	1.290747
C	1.744836	-2.553678	-0.639123
H	1.570076	-2.547017	-1.714662
H	2.680995	-3.006713	-0.322373

7M

B3LYP SCF energy: -1485.83744409 a.u.
B3LYP enthalpy: -1485.404141 a.u.
B3LYP free energy: -1485.504417 a.u.
B3LYP free energy after quasi-harmonic correction: -1485.492626 a.u.
M06 SCF energy in solution: -1485.34802108 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.619286	-2.936601	-1.978631
O	-0.855472	-1.878258	-2.576014
O	-0.757323	-3.161147	-0.706942
C	-0.066853	-4.140041	-2.751353
H	1.016590	-4.010048	-2.871173
H	-0.247247	-5.079508	-2.220077
H	-0.512212	-4.175902	-3.750850
Pd	-1.545508	-1.756079	0.559149
C	-3.725345	-1.072832	1.793311

O	-3.903345	-2.050698	1.024867
O	-2.573182	-0.512595	1.918347
C	-4.884046	-0.490497	2.585579
H	-5.567830	-1.287876	2.892766
H	-4.524384	0.060906	3.459308
H	-5.443480	0.202410	1.943939
C	-2.000714	3.477926	-2.147513
C	-2.030990	2.551238	-1.094074
C	-2.809348	2.860979	0.035739
C	-3.528085	4.056539	0.108633
C	-3.485973	4.972551	-0.949428
C	-2.718976	4.677137	-2.080014
H	-1.411500	3.251517	-3.034581
H	-2.848753	2.147668	0.856836
H	-4.126427	4.272440	0.991716
H	-4.048208	5.902531	-0.894124
H	-2.681555	5.377426	-2.912503
C	-1.240375	1.262710	-1.148963
H	-1.860702	0.429569	-0.797996
H	-0.972562	1.021696	-2.183861
C	0.038240	1.333237	-0.287815
H	-0.211701	1.662041	0.726662
H	0.701203	2.099718	-0.713658
C	0.802289	-0.008697	-0.216168
H	0.784505	-0.488318	-1.198335
C	0.300777	-0.993568	0.847998
H	0.260967	-0.512671	1.832661
H	0.965834	-1.865214	0.882118
C	4.283053	0.895965	0.970914
C	4.573382	0.182450	-0.189681
C	5.881330	-0.036496	-0.601638
C	6.907319	0.488761	0.198910
C	6.615059	1.207387	1.367963
C	5.288212	1.421981	1.771673
C	2.791618	0.948133	1.121927
C	3.274212	-0.235640	-0.808778
H	6.093787	-0.595243	-1.508732
H	7.944862	0.337492	-0.089169
H	7.430415	1.602722	1.969065
H	5.048550	1.976355	2.674688
N	2.259507	0.262507	0.022639
O	3.121989	-0.875532	-1.833828
O	2.169041	1.487806	2.020373

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B3LYP SCF energy: -1485.83761541 a.u.
B3LYP enthalpy: -1485.405612 a.u.
B3LYP free energy: -1485.506309 a.u.
B3LYP free energy after quasi-harmonic correction: -1485.494250 a.u.
M06 SCF energy in solution: -1485.34770720 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.301810	2.835990	0.003558
O	-2.795810	2.006339	-0.768898

O	-1.251901	2.669809	0.751969
C	-2.919332	4.229073	0.146493
H	-2.823689	4.603086	1.170805
H	-2.376838	4.919231	-0.512036
H	-3.969599	4.209558	-0.158342
Pd	0.030492	1.093775	0.484544
C	2.061775	2.623145	-1.041990
O	0.850451	2.150522	-1.073961
O	2.878760	2.516056	-0.122677
C	2.417462	3.375593	-2.330436
H	2.337241	2.699498	-3.189677
H	1.707934	4.195155	-2.494088
H	3.433997	3.773014	-2.265126
C	-4.014755	-1.024298	-0.819051
C	-3.308382	-2.157603	-0.382822
C	-4.037321	-3.320270	-0.078880
C	-5.429454	-3.356751	-0.199845
C	-6.122382	-2.220463	-0.631142
C	-5.408623	-1.057859	-0.938226
H	-3.478699	-0.106829	-1.051378
H	-3.504145	-4.211842	0.249698
H	-5.970460	-4.271153	0.036830
H	-7.205944	-2.243218	-0.729016
H	-5.933113	-0.166189	-1.274401
C	-1.800330	-2.137168	-0.226560
H	-1.410332	-3.142131	-0.434788
H	-1.340608	-1.468954	-0.961900
C	-1.317586	-1.735564	1.190596
H	-0.275313	-2.043735	1.321460
H	-1.909537	-2.296768	1.932918
C	-1.450293	-0.271392	1.535925
H	-2.382368	0.207988	1.241611
C	-0.633412	0.379924	2.444211
H	0.217775	-0.115784	2.903436
H	-0.947444	1.321406	2.887163
C	3.128695	-1.647439	-0.713567
C	3.579737	-1.344477	0.567943
C	4.803860	-1.803414	1.035433
C	5.579928	-2.582880	0.162759
C	5.124482	-2.890229	-1.128296
C	3.880669	-2.425028	-1.584394
C	1.778396	-0.998994	-0.875120
C	2.514592	-0.511658	1.230377
H	5.145110	-1.557287	2.037326
H	6.549580	-2.953078	0.488877
H	5.746891	-3.495414	-1.784058
H	3.515706	-2.656118	-2.581643
N	1.489220	-0.334772	0.309862
O	2.541914	-0.122835	2.393264
O	1.062981	-1.084906	-1.866385

9A-TS

B3LYP SCF energy: -1485.78728577 a.u.
B3LYP enthalpy: -1485.357010 a.u.
B3LYP free energy: -1485.455413 a.u.

B3LYP free energy after quasi-harmonic correction: -1485.444774 a.u.
M06 SCF energy in solution: -1485.30608868 a.u.
Imaginary frequency: -359.9638 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.011772	2.594924	-0.403455
O	-1.739314	2.511841	-1.605431
O	-1.665713	1.757818	0.531282
C	-2.840419	3.770192	0.126548
H	-2.154521	4.510634	0.557659
H	-3.399423	4.239737	-0.688060
H	-3.522922	3.451665	0.921983
Pd	-0.043900	0.514307	0.277301
C	2.254895	2.435085	-0.209358
O	1.119116	2.263007	0.377013
O	2.932040	1.579774	-0.807102
C	2.758012	3.883118	-0.133417
H	2.182383	4.495234	-0.839414
H	2.597692	4.297337	0.868079
H	3.817680	3.934467	-0.401014
C	-4.536936	-0.232768	0.530051
C	-4.305357	-1.007622	-0.619807
C	-5.214166	-2.038201	-0.913578
C	-6.314935	-2.294893	-0.090661
C	-6.530596	-1.517768	1.052124
C	-5.636052	-0.486581	1.357000
H	-3.841823	0.567609	0.773286
H	-5.057453	-2.644043	-1.805132
H	-7.005656	-3.097034	-0.344253
H	-7.386883	-1.711515	1.694866
H	-5.793212	0.126635	2.242074
C	-3.104113	-0.759611	-1.510554
H	-3.374084	-1.016847	-2.544009
H	-2.830883	0.299432	-1.510495
C	-1.858835	-1.593873	-1.133800
H	-1.103384	-1.461233	-1.917287
H	-2.142638	-2.661748	-1.150220
C	-1.232257	-1.269990	0.218896
H	-1.920666	-1.035185	1.032727
C	-0.077629	-1.999253	0.612943
H	0.301792	-2.783357	-0.040796
H	0.134877	-2.125440	1.670963
C	3.650962	-1.307669	-0.607045
C	3.799940	-1.149451	0.768539
C	5.046628	-1.222040	1.378765
C	6.156598	-1.454033	0.554718
C	6.005193	-1.613345	-0.832150
C	4.740819	-1.546999	-1.433525
C	2.194565	-1.198170	-0.923882
C	2.444376	-0.912053	1.352896
H	5.150178	-1.093815	2.452668
H	7.150948	-1.506971	0.992387
H	6.885324	-1.784662	-1.447875
H	4.611644	-1.660058	-2.505991
N	1.525354	-0.893730	0.286148
O	2.164181	-0.817425	2.538516

O	1.653370	-1.447118	-1.986591

9M-TS

B3LYP SCF energy: -1485.78999987 a.u.
B3LYP enthalpy: -1485.360038 a.u.
B3LYP free energy: -1485.458760 a.u.
B3LYP free energy after quasi-harmonic correction: -1485.447592 a.u.
M06 SCF energy in solution: -1485.31028598 a.u.
Imaginary frequency: -323.9283 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-3.550210	-3.055914	-0.285165
O	-2.718962	-3.605610	-1.022454
O	-3.420740	-1.941597	0.362500
C	-4.932717	-3.693460	-0.084520
H	-4.888752	-4.765439	-0.299608
H	-5.305057	-3.520492	0.930428
H	-5.640369	-3.226914	-0.782057
Pd	-1.789436	-0.706963	0.237666
C	-2.995030	1.920946	-0.807083
O	-3.200582	0.820925	-0.177756
O	-1.906181	2.361510	-1.227051
C	-4.275449	2.732090	-1.057104
H	-4.907275	2.740857	-0.162116
H	-4.030231	3.754608	-1.359841
H	-4.850744	2.252393	-1.859523
C	3.916291	-0.923074	-1.063214
C	3.999202	-1.105404	0.326827
C	4.998226	-1.958625	0.824377
C	5.884555	-2.614554	-0.034029
C	5.787507	-2.427217	-1.416637
C	4.799689	-1.579787	-1.926140
H	3.151657	-0.271275	-1.478643
H	5.084122	-2.106842	1.899923
H	6.650893	-3.268742	0.376510
H	6.474331	-2.936569	-2.088782
H	4.710508	-1.427199	-2.999138
C	3.035240	-0.421842	1.278514
H	3.555658	-0.216960	2.223005
H	2.743852	0.553296	0.873980
C	1.772169	-1.250672	1.610492
H	1.278609	-0.847756	2.501234
H	2.082424	-2.275498	1.867205
C	0.751401	-1.410299	0.508135
H	1.135784	-1.385206	-0.508914
C	-0.422995	-2.204818	0.706333
H	-0.609248	-2.553933	1.724935
H	-0.669466	-2.921985	-0.078918
C	0.838942	2.478165	-0.522819
C	0.625513	2.638475	0.842893
C	0.883586	3.845034	1.484270
C	1.369485	4.900858	0.701695
C	1.588415	4.736085	-0.676152
C	1.328648	3.513316	-1.308696

C	0.488457	1.069397	-0.877529
C	0.105835	1.344864	1.382601
H	0.706496	3.958746	2.550265
H	1.576755	5.863592	1.163537
H	1.958944	5.575623	-1.260124
H	1.480658	3.377538	-2.375417
N	0.006780	0.438331	0.303612
O	-0.144054	1.097169	2.553412
O	0.715078	0.504951	-1.933418

8A-TS

B3LYP SCF energy: -1998.31579273 a.u.
B3LYP enthalpy: -1997.772381 a.u.
B3LYP free energy: -1997.898217 a.u.
B3LYP free energy after quasi-harmonic correction: -1997.879081 a.u.
M06 SCF energy in solution: -1997.76916696 a.u.
Imaginary frequency: -293.4818 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.460956	-3.501469	2.269669
O	0.514718	-2.695668	3.210262
O	0.625053	-3.264158	1.010686
C	0.161209	-4.986103	2.546251
H	1.018342	-5.596798	2.235436
H	-0.034588	-5.144169	3.611578
H	-0.704133	-5.311935	1.956314
Pd	1.258424	-1.464131	0.224833
C	4.355168	-2.019710	-0.160480
O	4.654689	-1.081497	-0.919398
O	3.207197	-2.334717	0.323172
C	5.471915	-2.977341	0.314707
H	5.621617	-2.853548	1.395303
H	5.174823	-4.019683	0.145577
H	6.410522	-2.764680	-0.208245
C	-1.764264	2.496547	3.756264
C	-0.598387	2.181042	3.038214
C	0.356788	3.197773	2.855083
C	0.147907	4.480784	3.369561
C	-1.019586	4.780263	4.082033
C	-1.977516	3.778952	4.273362
H	-2.512730	1.721044	3.912837
H	1.266406	2.963004	2.306334
H	0.902982	5.250152	3.214903
H	-1.180258	5.780010	4.482939
H	-2.890538	3.994752	4.826949
C	-0.375443	0.799696	2.463932
H	0.690507	0.554152	2.484043
H	-0.880936	0.051083	3.087229
C	-0.879648	0.660904	1.009644
H	-0.349790	1.367215	0.360434
H	-1.945102	0.949084	0.973060
C	-0.745773	-0.759791	0.484749
H	-1.148915	-1.497825	1.180089

C	-1.045076	-1.041417	-0.882764
H	-0.732143	-0.352952	-1.657347
H	-1.131025	-2.077720	-1.185795
C	-5.007714	0.435781	-1.721691
C	-5.333207	-0.829583	-1.241158
C	-6.654318	-1.232860	-1.095703
C	-7.658710	-0.315617	-1.448154
C	-7.330375	0.960369	-1.931090
C	-5.988982	1.353009	-2.074844
C	-3.492387	0.512938	-1.754799
C	-4.021378	-1.545215	-0.974090
H	-6.894283	-2.224652	-0.720030
H	-8.705985	-0.595147	-1.345659
H	-8.127452	1.653211	-2.195651
H	-5.719872	2.338624	-2.446774
N	-2.994087	-0.687738	-1.298373
O	-3.933486	-2.698250	-0.555446
O	-2.855559	1.490576	-2.141493
C	3.229741	2.063818	-1.314872
C	2.914362	1.423917	-2.508111
C	3.350516	1.912369	-3.731498
C	4.130371	3.081008	-3.725479
C	4.448503	3.727133	-2.521433
C	3.995329	3.221236	-1.291541
C	2.593383	1.264359	-0.205947
C	2.076426	0.222366	-2.152293
H	3.097285	1.399746	-4.656127
H	4.495662	3.491776	-4.665615
H	5.056575	4.630357	-2.543249
H	4.236839	3.709072	-0.350365
N	1.912146	0.210252	-0.776017
O	1.605149	-0.567840	-2.964836
O	2.666418	1.552465	0.988941

8A-int

B3LYP SCF energy: -1998.33358582 a.u.
B3LYP enthalpy: -1997.787918 a.u.
B3LYP free energy: -1997.911814 a.u.
B3LYP free energy after quasi-harmonic correction: -1997.894454 a.u.
M06 SCF energy in solution: -1997.80443254 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.048762	-3.746535	1.799432
O	-0.294445	-3.065446	2.782285
O	0.588441	-3.355155	0.701592
C	-0.194641	-5.271283	1.822098
H	-0.962133	-5.529210	1.080234
H	0.722393	-5.804529	1.543458
H	-0.529258	-5.593052	2.814153
Pd	1.231941	-1.450035	0.140566
C	4.404521	-1.949187	-0.096409
O	4.726256	-0.995120	-0.834326
O	3.246679	-2.286831	0.326335
C	5.529547	-2.880518	0.423328

H	5.671969	-2.708734	1.499125
H	5.242714	-3.932082	0.297546
H	6.472688	-2.681582	-0.098401
C	-2.144203	1.721672	3.881560
C	-0.933788	1.607299	3.176156
C	-0.048367	2.701312	3.211492
C	-0.367472	3.862930	3.920786
C	-1.579410	3.962546	4.615878
C	-2.468235	2.882313	4.593184
H	-2.837119	0.881373	3.875289
H	0.896348	2.619635	2.677622
H	0.336339	4.694155	3.933557
H	-1.825600	4.867599	5.169752
H	-3.412848	2.940817	5.133250
C	-0.590662	0.364312	2.387153
H	0.487939	0.183545	2.427931
H	-1.069937	-0.517204	2.828511
C	-0.998167	0.472064	0.899861
H	-0.467604	1.314714	0.437586
H	-2.074650	0.732597	0.862843
C	-0.737841	-0.819213	0.114937
H	-1.275289	-1.644336	0.596773
C	-1.177921	-0.734850	-1.347414
C	-4.641035	0.727607	-1.795639
C	-4.953331	-0.610924	-1.571565
C	-6.268599	-1.054170	-1.534421
C	-7.280032	-0.099518	-1.726511
C	-6.965379	1.249039	-1.951744
C	-5.630373	1.681866	-1.991609
C	-3.143525	0.855804	-1.791106
C	-3.660737	-1.363009	-1.418230
H	-6.496925	-2.101885	-1.358513
H	-8.323260	-0.407270	-1.699022
H	-7.768994	1.968327	-2.095108
H	-5.371488	2.722966	-2.164066
N	-2.637784	-0.419928	-1.530867
O	-3.536864	-2.565547	-1.258830
O	-2.503370	1.871349	-2.004671
C	3.054092	1.714261	-2.171449
C	3.272188	2.233311	-0.900554
C	4.031136	3.378677	-0.704524
C	4.581325	3.998755	-1.839480
C	4.361385	3.474409	-3.122015
C	3.584940	2.317038	-3.302905
C	2.186699	0.492014	-1.999465
C	2.549141	1.331054	0.069901
H	4.195402	3.771374	0.296109
H	5.189231	4.895345	-1.724773
H	4.802038	3.970707	-3.985801
H	3.407814	1.896771	-4.289948
N	1.929997	0.332008	-0.648691
O	2.517648	1.514989	1.288621
O	1.757851	-0.189400	-2.928714
H	-0.645422	0.041116	-1.897663
H	-1.016781	-1.689252	-1.852222

8M-TS

B3LYP SCF energy: -1998.31396613 a.u.
B3LYP enthalpy: -1997.770585 a.u.
B3LYP free energy: -1997.895731 a.u.
B3LYP free energy after quasi-harmonic correction: -1997.877298 a.u.
M06 SCF energy in solution: -1997.76781156 a.u.
Imaginary frequency: -232.2185 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.499204	-0.648857	-3.691975
O	0.391367	0.586550	-3.697853
O	0.141669	-1.470580	-2.762270
C	1.181973	-1.353148	-4.877240
H	1.103868	-0.734591	-5.777484
H	2.245476	-1.488286	-4.639644
H	0.745282	-2.342057	-5.054379
Pd	-0.963176	-0.995789	-1.079542
C	-3.862186	-1.596343	-2.078731
O	-4.296815	-2.120460	-1.038202
O	-2.684913	-1.142431	-2.321261
C	-4.817176	-1.419686	-3.280626
H	-5.744126	-1.980990	-3.120909
H	-5.056995	-0.354371	-3.395751
H	-4.331295	-1.746111	-4.207933
C	0.977855	4.754457	-0.690796
C	-0.000791	3.785535	-0.407432
C	-1.147704	4.193050	0.295890
C	-1.303487	5.521527	0.706626
C	-0.318705	6.473880	0.422075
C	0.825807	6.082916	-0.282749
H	1.868134	4.458561	-1.243763
H	-1.918451	3.455041	0.506591
H	-2.201880	5.813083	1.248784
H	-0.441830	7.507734	0.741681
H	1.598897	6.813496	-0.517724
C	0.177710	2.344095	-0.835671
H	-0.793313	1.842716	-0.866397
H	0.583044	2.294219	-1.852549
C	1.123998	1.576741	0.127497
H	0.671918	1.499225	1.122743
H	2.047985	2.152511	0.237006
C	1.485225	0.196495	-0.385270
H	1.888468	0.178933	-1.392903
C	0.821318	-0.988204	0.062775
H	0.548029	-1.000562	1.117296
H	1.271103	-1.923702	-0.275431
C	5.097032	-0.723816	1.792066
C	5.541371	-0.939830	0.490578
C	6.783212	-1.505088	0.231542
C	7.581613	-1.857658	1.332915
C	7.133285	-1.641167	2.644839
C	5.874929	-1.065960	2.890591
C	3.722023	-0.090647	1.683170
C	4.443874	-0.441864	-0.431087
H	7.116741	-1.668957	-0.790330

H	8.559945	-2.306666	1.169524
H	7.769800	-1.925742	3.481071
H	5.513945	-0.894591	3.901831
N	3.417730	0.049737	0.345971
O	4.501942	-0.474398	-1.659705
O	3.034773	0.242007	2.647252
C	-3.780834	-0.172092	2.104101
C	-3.405770	-1.469205	2.436361
C	-4.011425	-2.154761	3.480168
C	-5.026657	-1.493637	4.191973
C	-5.404752	-0.184828	3.856823
C	-4.777901	0.497255	2.800308
C	-2.919732	0.249632	0.938503
C	-2.302215	-1.863529	1.485274
H	-3.709098	-3.169505	3.726950
H	-5.529884	-2.001913	5.013216
H	-6.195727	0.305155	4.422725
H	-5.061122	1.511038	2.527892
N	-2.073818	-0.792467	0.634316
O	-1.708397	-2.936292	1.513088
O	-2.979219	1.355623	0.398929

8M-int

B3LYP SCF energy: -1998.33135091 a.u.
B3LYP enthalpy: -1997.786646 a.u.
B3LYP free energy: -1997.907423 a.u.
B3LYP free energy after quasi-harmonic correction: -1997.891578 a.u.
M06 SCF energy in solution: -1997.80160078 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.688619	0.688727	3.656732
O	-0.830241	1.840657	3.205182
O	-0.158907	-0.332370	3.088122
C	-1.253467	0.384949	5.059715
H	-2.340808	0.250059	4.979655
H	-0.816154	-0.526523	5.480428
H	-1.069400	1.235810	5.726178
Pd	0.973118	-0.491215	1.333975
C	3.952063	-0.319826	2.488661
O	4.551292	-0.978591	1.614827
O	2.704935	-0.053202	2.583711
C	4.782040	0.286428	3.648688
H	4.688676	1.380315	3.635563
H	4.385796	-0.059631	4.612374
H	5.838173	0.007475	3.560466
C	-1.287470	4.683825	-0.801775
C	-0.334132	3.653485	-0.889359
C	0.737747	3.822941	-1.783926
C	0.842214	4.976842	-2.568527
C	-0.118694	5.990333	-2.476074
C	-1.186179	5.839041	-1.583143
H	-2.113551	4.577018	-0.100024
H	1.494357	3.043427	-1.841056
H	1.684387	5.086408	-3.250448

H	-0.033411	6.889408	-3.085148
H	-1.936254	6.623956	-1.490433
C	-0.462336	2.396553	-0.055373
H	0.512911	1.908164	0.026766
H	-0.771714	2.640524	0.967361
C	-1.477703	1.409785	-0.673091
H	-1.113962	1.063623	-1.647893
H	-2.419245	1.949860	-0.858461
C	-1.793444	0.194587	0.227006
H	-2.021882	0.552197	1.233196
C	-0.738245	-0.913512	0.289924
H	-0.480612	-1.245325	-0.721400
H	-1.154067	-1.767183	0.844936
C	-4.755223	-1.521823	-1.441873
C	-5.265391	-1.288295	-0.168737
C	-6.543442	-1.696517	0.189474
C	-7.307613	-2.360592	-0.783280
C	-6.792558	-2.597328	-2.066814
C	-5.499134	-2.176292	-2.414635
C	-3.367937	-0.944785	-1.495415
C	-4.213332	-0.559460	0.617226
H	-6.927862	-1.506879	1.188021
H	-8.312897	-2.698526	-0.540311
H	-7.405548	-3.116169	-2.800908
H	-5.086070	-2.353597	-3.403932
N	-3.115693	-0.395720	-0.234365
O	-4.313984	-0.177964	1.771117
O	-2.632196	-0.949228	-2.467748
C	3.531600	-2.213152	-1.690890
C	3.724342	-0.872534	-2.005360
C	4.626872	-0.478432	-2.983396
C	5.349240	-1.484371	-3.648337
C	5.154433	-2.837081	-3.331570
C	4.232253	-3.218873	-2.341740
C	2.478968	-2.260569	-0.608290
C	2.796143	-0.077978	-1.117345
H	4.767566	0.574276	-3.216728
H	6.071454	-1.213236	-4.417375
H	5.728347	-3.598218	-3.858772
H	4.071504	-4.262911	-2.083616
N	2.103726	-0.959564	-0.321605
O	2.687791	1.149567	-1.160230
O	2.034141	-3.297356	-0.122524

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B3LYP SCF energy: -813.52649975 a.u.
B3LYP enthalpy: -813.355494 a.u.
B3LYP free energy: -813.424026 a.u.
B3LYP free energy after quasi-harmonic correction: -813.417185 a.u.
M06 SCF energy in solution: -813.38224355 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.776218	0.026970	0.011961
O	-2.122332	1.030933	-0.423350

O	-2.139212	-0.984076	0.455909
C	-4.285696	0.021115	-0.026272
H	-4.618944	-0.470631	-0.948909
H	-4.683696	-0.543709	0.822037
H	-4.670645	1.044652	-0.019707
Pd	-0.296739	0.004810	0.006472
C	1.556255	2.223739	0.103353
O	1.143461	2.516041	1.228539
O	1.151121	1.246915	-0.657292
C	2.689464	3.026535	-0.549308
H	3.636868	2.494382	-0.394088
H	2.535608	3.122804	-1.629094
H	2.762679	4.014306	-0.084878
C	1.509404	-2.250680	-0.111676
O	1.073552	-2.537278	-1.229692
O	1.134825	-1.264863	0.652862
C	2.637146	-3.073694	0.524990
H	3.591839	-2.559518	0.354575
H	2.497969	-3.165560	1.607132
H	2.684856	-4.063289	0.061137

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B3LYP SCF energy: -1201.82539661 a.u.
B3LYP enthalpy: -1201.451026 a.u.
B3LYP free energy: -1201.544956 a.u.
B3LYP free energy after quasi-harmonic correction: -1201.533554 a.u.
M06 SCF energy in solution: -1201.46740389 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.029691	-2.723207	0.576413
O	0.903675	-2.886985	1.059412
O	2.420844	-1.743359	-0.185757
C	3.152685	-3.726189	0.858278
H	3.808273	-3.842705	-0.010484
H	3.763569	-3.342955	1.685424
H	2.730148	-4.690855	1.153974
Pd	1.336238	-0.040436	-0.480170
C	-0.256193	2.451147	-0.200272
O	-0.863806	2.035258	0.791214
O	0.535036	1.769984	-0.976870
C	-0.385188	3.912424	-0.641212
H	0.509351	4.457853	-0.315403
H	-0.438221	3.991918	-1.732150
H	-1.266120	4.370253	-0.182394
C	3.559530	1.354372	0.757298
O	4.086402	1.410286	-0.359137
O	2.400157	0.843122	1.047059
C	4.281622	1.904454	1.993752
H	3.590638	2.470694	2.627422
H	4.663334	1.066313	2.590621
H	5.121497	2.535382	1.689078
C	-4.671806	-1.472147	0.156371
C	-3.631982	-0.555731	0.382735
C	-3.971439	0.757473	0.751847

C	-5.310479	1.138216	0.883835
C	-6.337254	0.216262	0.651463
C	-6.012178	-1.094367	0.287294
H	-4.426285	-2.497417	-0.117676
H	-3.170524	1.470199	0.937071
H	-5.551967	2.158729	1.174984
H	-7.378532	0.513850	0.758215
H	-6.800477	-1.824091	0.111327
C	-2.182007	-0.957133	0.214233
H	-1.550187	-0.365536	0.882649
H	-2.048310	-2.011732	0.486657
C	-1.680516	-0.746663	-1.232489
H	-1.745778	0.311483	-1.507032
H	-2.346580	-1.295222	-1.921033
C	-0.285071	-1.271039	-1.462548
H	-0.083890	-2.242997	-1.016621
C	0.612079	-0.775690	-2.393699
H	0.375019	0.107413	-2.983207
H	1.450686	-1.380061	-2.730742

12A-TS

B3LYP SCF energy: -1714.29999420 a.u.
B3LYP enthalpy: -1713.814033 a.u.
B3LYP free energy: -1713.931950 a.u.
B3LYP free energy after quasi-harmonic correction: -1713.914532 a.u.
M06 SCF energy in solution: -1713.89012570 a.u.
Imaginary frequency: -314.0519 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.202727	-1.537509	2.782815
O	2.043701	-0.401237	3.251767
O	2.199692	-1.897162	1.542095
C	2.399910	-2.734203	3.732417
H	1.461992	-3.302119	3.792889
H	3.171858	-3.410828	3.348729
H	2.666073	-2.382643	4.734649
Pd	2.034515	-0.621437	-0.059197
C	2.129268	1.592596	-2.117390
O	2.335652	2.514168	-1.310296
O	1.852455	0.359657	-1.864715
C	2.185453	1.877631	-3.628917
H	3.057430	1.368044	-4.058499
H	1.294930	1.476110	-4.126421
H	2.266194	2.953656	-3.814035
C	4.813941	-1.573080	-0.912169
O	4.380698	-2.558096	-1.535035
O	4.155081	-0.662460	-0.290716
C	6.344774	-1.373936	-0.811098
H	6.605960	-0.311069	-0.872714
H	6.687463	-1.742738	0.165682
H	6.858534	-1.938518	-1.597362
C	-1.611881	3.783208	1.956836
C	-0.538011	3.391501	1.139686
C	-0.039431	4.325547	0.212012

C	-0.601069	5.601766	0.109032
C	-1.672474	5.977787	0.929080
C	-2.176629	5.059684	1.856375
H	-2.006765	3.074765	2.683816
H	0.795750	4.030387	-0.421221
H	-0.197093	6.308218	-0.614926
H	-2.107459	6.973065	0.847298
H	-3.008381	5.336600	2.503305
C	0.061420	2.006079	1.230209
H	1.134014	2.052222	1.019313
H	-0.047341	1.613903	2.249352
C	-0.578339	1.009445	0.236871
H	-0.426921	1.363902	-0.788976
H	-1.671231	0.994786	0.404446
C	-0.037812	-0.403253	0.396006
H	-0.108382	-0.763359	1.423620
C	-0.365028	-1.390269	-0.588953
H	-0.332363	-1.112571	-1.637041
H	-0.127315	-2.424183	-0.369006
C	-4.573207	-1.316000	-1.129346
C	-4.513174	-1.967185	0.099667
C	-5.662749	-2.266609	0.819213
C	-6.896480	-1.886216	0.264822
C	-6.956801	-1.229471	-0.973807
C	-5.785017	-0.935589	-1.691137
C	-3.144232	-1.170408	-1.616373
C	-3.046208	-2.231092	0.383447
H	-5.600975	-2.774824	1.778444
H	-7.819106	-2.100489	0.801659
H	-7.925264	-0.942848	-1.380289
H	-5.816700	-0.425059	-2.650560
N	-2.312312	-1.732570	-0.671860
O	-2.624702	-2.809260	1.382366
O	-2.822596	-0.653467	-2.684448

12A-TS-cis

B3LYP SCF energy: -1714.26472221 a.u.
B3LYP enthalpy: -1713.779871 a.u.
B3LYP free energy: -1713.895639 a.u.
B3LYP free energy after quasi-harmonic correction: -1713.880098 a.u.
M06 SCF energy in solution: -1713.85879045 a.u.
Imaginary frequency: -251.0094 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.734692	3.624835	-1.519348
O	1.808230	3.173838	-1.960215
O	-0.183809	2.996020	-0.873906
C	0.394009	5.108838	-1.724796
H	-0.655316	5.226991	-2.018044
H	0.531266	5.627729	-0.767792
H	1.052941	5.554885	-2.477104
Pd	-0.100947	1.178947	0.089628
C	0.334616	-1.138670	1.962397
O	1.462670	-0.780558	2.340177

O	-0.403439	-0.600862	1.052390
C	-0.321297	-2.385203	2.576615
H	-1.312287	-2.131566	2.971891
H	-0.463537	-3.141068	1.794910
H	0.306271	-2.790474	3.376938
C	-0.610130	3.113115	2.372958
O	0.479688	3.692420	2.260277
O	-1.057569	2.094854	1.721468
C	-1.636461	3.638606	3.402942
H	-1.141956	4.281833	4.139034
H	-2.400868	4.226341	2.876365
H	-2.146099	2.808409	3.905502
C	5.366581	-1.266391	-1.097911
C	4.300199	-1.077928	-0.202462
C	4.308781	-1.811675	0.998813
C	5.346822	-2.703693	1.284177
C	6.402027	-2.883758	0.380792
C	6.407479	-2.158110	-0.815110
H	5.379665	-0.700173	-2.028429
H	3.488832	-1.664467	1.699998
H	5.332686	-3.259789	2.220531
H	7.210102	-3.578247	0.607131
H	7.222883	-2.283171	-1.526958
C	3.163389	-0.132083	-0.518447
H	2.804054	0.335530	0.404388
H	3.519572	0.672768	-1.174811
C	1.965781	-0.837097	-1.193860
H	1.566352	-1.605124	-0.522476
H	2.328872	-1.372510	-2.089807
C	0.868284	0.145516	-1.595293
H	1.222585	1.169031	-1.809548
C	-0.078546	-0.267010	-2.543359
H	-0.701618	0.471711	-3.037013
H	0.035654	-1.213529	-3.063719
C	-4.016000	-1.321063	-0.831659
C	-3.303287	-2.445765	-0.423465
C	-3.855493	-3.375658	0.447265
C	-5.159313	-3.139753	0.915357
C	-5.875718	-2.004868	0.506366
C	-5.307229	-1.077395	-0.383183
C	-3.116237	-0.566698	-1.793045
C	-1.959817	-2.386584	-1.127909
H	-3.288438	-4.248958	0.760566
H	-5.619187	-3.840931	1.610418
H	-6.881635	-1.839996	0.889944
H	-5.848709	-0.191261	-0.705706
N	-1.922436	-1.241109	-1.885240
O	-1.099815	-3.267347	-1.057630
O	-3.450991	0.445780	-2.411238

12b-TS

B3LYP SCF energy: -1201.77625819 a.u.
B3LYP enthalpy: -1201.408501 a.u.
B3LYP free energy: -1201.502732 a.u.
B3LYP free energy after quasi-harmonic correction: -1201.490365 a.u.

M06 SCF energy in solution: -1201.41978952 a.u.
Imaginary frequency: -1323.2695 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.511902	2.665987	0.608155
O	-1.455474	2.868571	1.222364
O	-2.781420	1.691444	-0.204575
C	-3.698250	3.620754	0.788807
H	-4.330898	3.646936	-0.103517
H	-4.310275	3.260070	1.625493
H	-3.337544	4.624162	1.035173
Pd	-1.589786	0.073487	-0.488883
C	0.353967	-2.254356	-0.236731
O	1.333501	-1.605121	0.306743
O	-0.597344	-1.753585	-0.872875
C	0.389606	-3.758474	-0.056998
H	-0.061557	-3.996185	0.914597
H	-0.205929	-4.241507	-0.835389
H	1.417524	-4.132166	-0.059830
C	-3.864592	-1.636986	0.358517
O	-4.230847	-1.704437	-0.822772
O	-2.820044	-1.028118	0.820855
C	-4.710056	-2.301936	1.458186
H	-4.078310	-2.702448	2.258537
H	-5.369239	-1.545110	1.903672
H	-5.332220	-3.094622	1.031010
C	5.328967	1.306740	-0.246188
C	4.242549	0.694982	0.398153
C	4.446508	-0.568273	0.978604
C	5.694788	-1.193637	0.919221
C	6.769341	-0.570037	0.275052
C	6.580734	0.685052	-0.310209
H	5.190637	2.285720	-0.701938
H	3.613799	-1.068494	1.465896
H	5.828035	-2.171932	1.376550
H	7.740964	-1.057367	0.230062
H	7.406584	1.182559	-0.814903
C	2.889434	1.377717	0.448641
H	2.470414	1.279973	1.460060
H	3.045166	2.455591	0.290106
C	1.884313	0.824072	-0.575079
H	1.443142	-0.475765	-0.045664
H	2.331855	0.401085	-1.481599
C	0.649910	1.468549	-0.737777
H	0.340420	2.182903	0.028465
C	-0.324588	1.205718	-1.748703
H	-0.004342	0.604447	-2.603907
H	-0.979440	2.036445	-2.012077

12M-TS

B3LYP SCF energy: -1714.29661338 a.u.
B3LYP enthalpy: -1713.810722 a.u.
B3LYP free energy: -1713.928553 a.u.
B3LYP free energy after quasi-harmonic correction: -1713.911302 a.u.

M06 SCF energy in solution: -1713.88513086 a.u.
Imaginary frequency: -230.0208 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.157379	-1.736113	2.649881
O	1.323164	-0.560381	3.006643
O	1.164675	-2.214976	1.450873
C	0.847871	-2.809352	3.709422
H	1.273676	-2.516036	4.674966
H	-0.241732	-2.887411	3.822270
H	1.230345	-3.789147	3.404290
Pd	1.671672	-1.218570	-0.274430
C	2.562687	0.570795	-2.556176
O	2.634264	1.618344	-1.891404
O	2.143475	-0.585392	-2.181215
C	3.042728	0.582427	-4.019679
H	2.476171	-0.130253	-4.628360
H	2.962530	1.591667	-4.437755
H	4.098211	0.279468	-4.043515
C	4.380429	-2.622489	-0.188694
O	3.972008	-3.642909	-0.769762
O	3.732122	-1.556016	0.115203
C	5.854482	-2.566504	0.276824
H	6.310143	-1.610444	-0.008147
H	5.890520	-2.630378	1.372684
H	6.425731	-3.398295	-0.149898
C	0.209392	4.235560	1.913545
C	0.814102	3.472000	0.900342
C	1.527307	4.151369	-0.104461
C	1.623773	5.546718	-0.092755
C	1.013752	6.295580	0.920999
C	0.304880	5.631211	1.928200
H	-0.336685	3.722728	2.704034
H	2.008559	3.564183	-0.883825
H	2.183970	6.051598	-0.878779
H	1.093113	7.382028	0.928906
H	-0.169913	6.198581	2.728069
C	0.694036	1.963258	0.876135
H	1.578349	1.529780	0.401735
H	0.651984	1.564915	1.895509
C	-0.567068	1.509424	0.090921
H	-0.462810	1.773688	-0.966983
H	-1.433749	2.051855	0.482713
C	-0.837583	0.023248	0.227902
H	-0.933434	-0.323976	1.252748
C	-0.372039	-0.936049	-0.728789
H	-0.403713	-0.608573	-1.768750
H	-0.760586	-1.946713	-0.580653
C	-4.936673	-0.353021	-1.001172
C	-5.016645	-0.917067	0.268915
C	-6.172959	-1.545742	0.712392
C	-7.266542	-1.596768	-0.168782
C	-7.185571	-1.028738	-1.449316
C	-6.008915	-0.394498	-1.882860
C	-3.547316	0.244473	-1.126628
C	-3.677005	-0.671894	0.937827

H	-6.221207	-1.982908	1.706817
H	-8.189179	-2.083832	0.142609
H	-8.046458	-1.083137	-2.113697
H	-5.931370	0.048610	-2.872823
N	-2.876619	0.023313	0.057697
O	-3.394756	-1.035135	2.078911
O	-3.134957	0.830974	-2.125276

12M-TS-cis

B3LYP SCF energy: -1714.26882779 a.u.
B3LYP enthalpy: -1713.783203 a.u.
B3LYP free energy: -1713.898327 a.u.
B3LYP free energy after quasi-harmonic correction: -1713.883171 a.u.
M06 SCF energy in solution: -1713.86407455 a.u.
Imaginary frequency: -229.4923 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.665637	2.693526	-0.768014
O	-2.541279	2.338451	0.051154
O	-0.422318	2.395659	-0.794573
C	-2.073355	3.598859	-1.946103
H	-1.384851	4.448217	-2.020854
H	-1.996329	3.030248	-2.881753
H	-3.101235	3.955619	-1.821941
Pd	0.895164	1.325919	0.392679
C	2.686984	0.272681	2.560772
O	2.171192	0.946133	3.465215
O	2.364931	0.237760	1.308677
C	3.834001	-0.698169	2.887251
H	4.609977	-0.657064	2.114345
H	4.261137	-0.461472	3.867473
H	3.431819	-1.718993	2.904394
C	2.775113	3.425638	-0.757004
O	2.413604	4.322485	0.020908
O	2.411142	2.192682	-0.794624
C	3.784550	3.772211	-1.876947
H	4.335954	4.685069	-1.625149
H	4.479872	2.942752	-2.050134
H	3.231619	3.942767	-2.811002
C	-5.747076	-1.860741	0.721082
C	-4.867448	-0.772094	0.620617
C	-5.215806	0.291957	-0.232221
C	-6.409249	0.258686	-0.957680
C	-7.280424	-0.833091	-0.848546
C	-6.943745	-1.895654	-0.004772
H	-5.489615	-2.692304	1.375993
H	-4.533788	1.137984	-0.315565
H	-6.660001	1.090576	-1.613571
H	-8.208972	-0.855549	-1.416851
H	-7.609530	-2.752514	0.089182
C	-3.565545	-0.724364	1.390268
H	-3.422529	0.284886	1.788714
H	-3.615860	-1.414583	2.244918
C	-2.336264	-1.077512	0.507590

H	-2.310054	-0.404552	-0.352809
H	-2.432130	-2.100094	0.130220
C	-1.061841	-0.926737	1.305686
H	-0.828026	-1.745412	1.980841
C	-0.576296	0.361417	1.641314
H	-0.038878	0.424747	2.587036
H	-1.298974	1.156380	1.435761
C	1.817179	-2.525364	-1.632365
C	2.282807	-3.067343	-0.437483
C	3.507985	-3.716861	-0.365411
C	4.272052	-3.801571	-1.541449
C	3.804120	-3.251426	-2.744379
C	2.558629	-2.604065	-2.803291
C	0.451454	-1.934182	-1.338503
C	1.211088	-2.804859	0.600825
H	3.863230	-4.132211	0.574617
H	5.244676	-4.291279	-1.520021
H	4.420532	-3.320317	-3.639553
H	2.186491	-2.165285	-3.725800
N	0.182264	-2.121370	0.001742
O	1.259685	-3.198704	1.770973
O	-0.287903	-1.436460	-2.185396

13

B3LYP SCF energy: -1714.31494928 a.u.
B3LYP enthalpy: -1713.826808 a.u.
B3LYP free energy: -1713.945701 a.u.
B3LYP free energy after quasi-harmonic correction: -1713.927212 a.u.
M06 SCF energy in solution: -1713.92246336 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.064141	-1.278844	2.926253
O	1.677910	-0.176323	3.351922
O	2.226630	-1.660740	1.709993
C	2.386733	-2.401619	3.936970
H	1.594417	-3.161449	3.898312
H	3.328433	-2.896646	3.671958
H	2.444379	-1.997790	4.953630
Pd	2.007748	-0.561687	-0.037022
C	1.939335	1.461991	-2.321421
O	2.036991	2.483631	-1.617010
O	1.779526	0.244356	-1.945148
C	2.004563	1.599449	-3.856055
H	2.926757	1.128554	-4.220430
H	1.162908	1.072591	-4.321809
H	1.994229	2.654276	-4.150580
C	4.907426	-1.463378	-0.821139
O	4.565474	-2.520079	-1.390203
O	4.176024	-0.568953	-0.275518
C	6.424221	-1.155618	-0.708797
H	6.616859	-0.087963	-0.870202
H	6.763436	-1.401087	0.307616
H	6.997755	-1.756939	-1.424142
C	-1.642791	3.686721	2.042159

C	-0.643721	3.276149	1.143524
C	-0.234654	4.187918	0.150281
C	-0.810747	5.458433	0.064798
C	-1.808125	5.853333	0.966698
C	-2.222303	4.958690	1.959002
H	-1.963678	2.997125	2.821951
H	0.543297	3.878293	-0.546484
H	-0.476069	6.147142	-0.710070
H	-2.253437	6.845320	0.898186
H	-2.993472	5.250931	2.671524
C	-0.027374	1.897686	1.213894
H	1.048854	1.961350	1.024621
H	-0.139482	1.475941	2.219367
C	-0.629188	0.923956	0.176384
H	-0.479793	1.336650	-0.828443
H	-1.726363	0.891568	0.337715
C	-0.034350	-0.485882	0.260649
H	-0.193454	-0.893810	1.266219
C	-0.625864	-1.445772	-0.771844
H	-0.414713	-1.113034	-1.790318
H	-0.227902	-2.453477	-0.631589
C	-4.398500	-1.257031	-1.052565
C	-4.263142	-2.109822	0.039997
C	-5.369474	-2.604922	0.717122
C	-6.638046	-2.209730	0.263137
C	-6.774404	-1.350486	-0.837432
C	-5.646338	-0.861849	-1.515721
C	-3.019170	-0.933469	-1.554764
C	-2.794110	-2.342330	0.259300
H	-5.248324	-3.269521	1.568288
H	-7.528965	-2.572242	0.771710
H	-7.769223	-1.057725	-1.166669
H	-5.736308	-0.194787	-2.368728
N	-2.124552	-1.589168	-0.706481
O	-2.293986	-3.072829	1.097914
O	-2.745990	-0.259432	-2.533927

13b

B3LYP SCF energy: -972.71592352 a.u.
B3LYP enthalpy: -972.411662 a.u.
B3LYP free energy: -972.491744 a.u.
B3LYP free energy after quasi-harmonic correction: -972.482920 a.u.
M06 SCF energy in solution: -972.42239057 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-4.231274	-0.751424	0.030447
O	-4.071443	-1.908780	-0.395636
O	-3.322061	0.119843	0.309009
C	-5.657565	-0.218746	0.253398
H	-5.730409	0.295018	1.218814
H	-5.892632	0.518538	-0.525104
H	-6.385616	-1.034118	0.203562
Pd	-1.251167	-0.207937	0.053834
C	-0.193276	2.645299	-0.080678

O	0.771365	2.372750	0.662176
O	-1.092387	1.838451	-0.522122
C	-0.396916	4.097210	-0.544096
H	-0.655718	4.130811	-1.608381
H	-1.238761	4.533526	0.009000
H	0.500052	4.694263	-0.353026
C	4.120967	-1.412307	-0.832062
C	3.260706	-0.375773	-0.442576
C	3.746774	0.604072	0.441167
C	5.058214	0.541285	0.919382
C	5.909463	-0.497408	0.522755
C	5.435680	-1.475541	-0.356503
H	3.757605	-2.178345	-1.515449
H	3.079130	1.408921	0.743945
H	5.418356	1.308739	1.601737
H	6.931307	-0.542448	0.894099
H	6.087648	-2.287452	-0.673468
C	1.825946	-0.298452	-0.933280
H	1.588121	0.747314	-1.148390
H	1.715935	-0.861759	-1.869597
C	0.828758	-0.813811	0.093292
H	1.054117	-0.545356	1.125278
C	-0.003669	-1.932140	-0.158360
H	-0.012371	-2.372771	-1.156368
C	-1.065094	-2.218643	0.737136
H	-0.923425	-2.089854	1.810921
H	-1.855728	-2.899770	0.438506

13M

B3LYP SCF energy: -1714.31209009 a.u.
B3LYP enthalpy: -1713.824059 a.u.
B3LYP free energy: -1713.941905 a.u.
B3LYP free energy after quasi-harmonic correction: -1713.924605 a.u.
M06 SCF energy in solution: -1713.91918335 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.063278	-1.720990	2.635177
O	1.105325	-0.543909	3.035502
O	1.159557	-2.162865	1.432584
C	0.811263	-2.841062	3.665910
H	-0.273274	-2.972410	3.783306
H	1.239090	-3.792089	3.331122
H	1.227332	-2.556852	4.639141
Pd	1.690287	-1.155116	-0.307702
C	2.386823	0.689668	-2.644406
O	2.209703	1.768647	-2.046000
O	2.192408	-0.502833	-2.220085
C	2.932432	0.743233	-4.086947
H	4.011322	0.945892	-4.046007
H	2.777364	-0.205341	-4.611180
H	2.458508	1.565154	-4.637006
C	4.556231	-2.415658	-0.096178
O	4.274083	-3.495989	-0.652843
O	3.801531	-1.413960	0.149874

C	6.017343	-2.193588	0.376622
H	6.469006	-1.376369	-0.202228
H	6.030065	-1.888262	1.430807
H	6.614254	-3.103537	0.244709
C	0.040863	4.144381	2.050397
C	0.550814	3.431355	0.951372
C	1.149281	4.163401	-0.091519
C	1.222344	5.558981	-0.034007
C	0.704390	6.257205	1.064246
C	0.113679	5.540540	2.111041
H	-0.408954	3.590062	2.873046
H	1.564822	3.614456	-0.934345
H	1.694720	6.104373	-0.850258
H	0.767126	7.344087	1.107509
H	-0.284291	6.067249	2.978155
C	0.445299	1.923815	0.875779
H	1.289235	1.521778	0.307633
H	0.497196	1.480772	1.876231
C	-0.865905	1.490731	0.183845
H	-0.861626	1.836279	-0.856293
H	-1.709686	1.988216	0.687967
C	-1.114467	-0.032919	0.222112
H	-0.982027	-0.389326	1.246062
C	-0.290900	-0.889496	-0.742140
H	-0.364536	-0.494186	-1.761556
H	-0.689695	-1.915829	-0.726311
C	-4.685944	-0.496627	-1.025282
C	-4.762696	-1.090146	0.230629
C	-5.937010	-1.672000	0.689883
C	-7.051445	-1.643390	-0.163862
C	-6.973659	-1.045768	-1.430959
C	-5.779473	-0.459500	-1.880159
C	-3.291704	0.040583	-1.196818
C	-3.418908	-0.943558	0.885881
H	-5.981524	-2.131753	1.673517
H	-7.989136	-2.090940	0.159204
H	-7.852091	-1.038494	-2.073064
H	-5.703434	0.006694	-2.858838
N	-2.597613	-0.269923	-0.023310
O	-3.119711	-1.331470	2.003177
O	-2.878055	0.642384	-2.173156

11-di

B3LYP SCF energy: -1786.77033834 a.u.
B3LYP enthalpy: -1786.279218 a.u.
B3LYP free energy: -1786.404681 a.u.
B3LYP free energy after quasi-harmonic correction: -1786.386344 a.u.
M06 SCF energy in solution: -1786.26437302 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.793201	-0.206012	-2.582683
O	0.518739	-0.126372	-2.412549
O	2.713355	-0.091896	-1.732776
C	2.216540	-0.495622	-4.014274

H	3.242723	-0.158971	-4.178654
H	2.174473	-1.579948	-4.174237
H	1.532936	-0.021404	-4.724244
Pd	-0.243623	0.019670	-0.521422
C	-1.210185	-2.707882	-0.193523
O	-2.354999	-2.230646	-0.146635
O	-0.105775	-2.055115	-0.370464
C	-0.984994	-4.214003	-0.034794
H	-0.427337	-4.604088	-0.893781
H	-0.376908	-4.402230	0.857498
H	-1.943336	-4.732925	0.053642
C	3.165386	2.995647	0.587661
O	4.000963	2.619586	1.409404
O	2.306921	2.237098	-0.044279
C	3.034867	4.472357	0.202098
H	3.141390	4.592509	-0.882493
H	2.041551	4.848162	0.477166
H	3.800507	5.060207	0.715049
Pd	2.427483	0.237628	0.341898
C	0.181437	0.331725	2.352165
O	1.426621	0.446933	2.195950
O	-0.737371	0.201243	1.461689
C	-0.326031	0.331257	3.785717
H	-1.341489	0.732432	3.840570
H	-0.348468	-0.706001	4.141841
H	0.353483	0.900671	4.424767
C	3.763200	-2.263573	0.620219
O	2.583652	-1.722243	0.766125
O	4.789374	-1.692738	0.245930
C	3.754991	-3.754223	0.967651
H	4.771715	-4.153265	0.917220
H	3.342369	-3.909361	1.971166
H	3.111259	-4.294068	0.263056
C	-6.328735	1.196888	-0.650855
C	-5.245868	0.330631	-0.433057
C	-5.382550	-0.682980	0.530457
C	-6.569196	-0.817541	1.257574
C	-7.640401	0.054744	1.034898
C	-7.517035	1.063985	0.074632
H	-6.242499	1.981222	-1.402024
H	-4.551782	-1.366886	0.691168
H	-6.658491	-1.610798	1.996875
H	-8.563722	-0.053706	1.600044
H	-8.345403	1.744495	-0.112609
C	-3.945654	0.483681	-1.192461
H	-3.431255	-0.481571	-1.227729
H	-4.154034	0.796351	-2.226389
C	-2.994292	1.513073	-0.544236
H	-2.835929	1.270347	0.512687
H	-3.462895	2.511552	-0.568540
C	-1.664400	1.605227	-1.253045
H	-1.677430	1.375818	-2.320035
C	-0.521481	2.199667	-0.740050
H	-0.514015	2.618588	0.262485
H	0.300386	2.498100	-1.380122

12A-TS-di

B3LYP SCF energy: -2299.25844778 a.u.
B3LYP enthalpy: -2298.655328 a.u.
B3LYP free energy: -2298.804405 a.u.
B3LYP free energy after quasi-harmonic correction: -2298.780104 a.u.
M06 SCF energy in solution: -2298.68654946 a.u.
Imaginary frequency: -245.1599 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.291726	-0.371811	-2.593180
O	-1.389232	0.458382	-2.237185
O	-2.978662	-1.173291	-1.897345
C	-2.550911	-0.417390	-4.097329
H	-3.534352	-0.849648	-4.299661
H	-2.472958	0.585453	-4.528442
H	-1.785137	-1.048982	-4.565340
Pd	-0.929377	0.783821	-0.235381
C	-2.483190	3.275890	0.003008
O	-1.395364	3.887621	0.013301
O	-2.670033	2.009067	-0.083878
C	-3.793295	4.080316	0.067300
H	-4.178130	4.215829	-0.952583
H	-4.553613	3.540556	0.640936
H	-3.612112	5.068363	0.503569
C	-1.288403	-3.998771	0.023812
O	-2.237959	-4.529426	0.607361
O	-1.173656	-2.742154	-0.302225
C	-0.059686	-4.817447	-0.390537
H	0.194381	-4.628801	-1.439773
H	0.805729	-4.513300	0.211047
H	-0.251081	-5.883468	-0.235574
Pd	-2.698749	-1.476128	0.177079
C	-1.268136	-0.229680	2.536023
O	-1.984651	-1.204123	2.163112
O	-0.721208	0.693942	1.844301
C	-0.966354	-0.157487	4.030271
H	0.057448	-0.513368	4.199924
H	-1.022582	0.880180	4.374340
H	-1.660831	-0.787341	4.591996
C	-5.464777	-0.602669	0.382472
O	-4.248766	-0.295179	0.714060
O	-5.853717	-1.596022	-0.241722
C	-6.465366	0.465392	0.851959
H	-7.488432	0.085436	0.766534
H	-6.256512	0.765612	1.885031
H	-6.356524	1.358223	0.223638
C	3.856087	4.241840	-0.684668
C	2.478462	4.055144	-0.481417
C	1.777148	5.024490	0.257648
C	2.439428	6.141810	0.776685
C	3.812649	6.315779	0.568515
C	4.520412	5.358430	-0.166699
H	4.413109	3.500963	-1.256651
H	0.707955	4.889099	0.410326
H	1.877382	6.881214	1.344908

H	4.325671	7.186672	0.973643
H	5.589172	5.480188	-0.337162
C	1.755942	2.840816	-1.022717
H	0.688093	3.067971	-1.102476
H	2.125985	2.609699	-2.032474
C	1.928514	1.585437	-0.138570
H	1.624662	1.813008	0.891351
H	2.998197	1.317187	-0.095273
C	1.148850	0.387665	-0.661376
H	1.149106	0.291602	-1.748897
C	1.186192	-0.835654	0.042098
H	1.246602	-0.825602	1.123782
H	0.761617	-1.724771	-0.401135
C	5.315501	-2.149968	0.739537
C	5.332718	-2.157368	-0.652713
C	6.490708	-2.447674	-1.362247
C	7.652162	-2.735910	-0.625546
C	7.634640	-2.728080	0.777420
C	6.455112	-2.431916	1.481420
C	3.897891	-1.796914	1.151877
C	3.924774	-1.810578	-1.106610
H	6.490525	-2.449207	-2.449612
H	8.579237	-2.967885	-1.147124
H	8.548280	-2.954011	1.324676
H	6.427664	-2.420908	2.568333
N	3.146355	-1.627179	0.012581
O	3.580512	-1.721826	-2.284970
O	3.520076	-1.691461	2.319353

12M-TS-di

B3LYP SCF energy: -2299.26662565 a.u.
B3LYP enthalpy: -2298.663556 a.u.
B3LYP free energy: -2298.811312 a.u.
B3LYP free energy after quasi-harmonic correction: -2298.787930 a.u.
M06 SCF energy in solution: -2298.69549568 a.u.
Imaginary frequency: -224.7267 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.804382	-1.234277	-2.382674
O	-1.011103	-0.259057	-2.165009
O	-2.610104	-1.812996	-1.596312
C	-1.770388	-1.763847	-3.813452
H	-2.342160	-2.691674	-3.892539
H	-2.207204	-1.010678	-4.480439
H	-0.733150	-1.924246	-4.125735
Pd	-0.922626	0.693600	-0.322864
C	-1.690020	3.401507	-1.206832
O	-0.502850	3.728663	-0.998436
O	-2.225145	2.249380	-1.032506
C	-2.665542	4.453843	-1.765299
H	-2.791648	4.287531	-2.843657
H	-3.651801	4.354109	-1.298853
H	-2.271119	5.463707	-1.610931
C	-1.854558	-3.600983	1.771367

O	-2.978339	-3.824038	2.233451
O	-1.504957	-2.626862	0.984647
C	-0.669485	-4.514860	2.115507
H	-0.158833	-4.840424	1.201814
H	0.062993	-3.960122	2.714775
H	-1.017601	-5.385093	2.680144
Pd	-2.893036	-1.241149	0.421720
C	-1.972494	0.755414	2.461370
O	-2.729032	-0.245005	2.276011
O	-1.145350	1.310895	1.668222
C	-2.081950	1.411069	3.835807
H	-1.122289	1.844673	4.131716
H	-2.819193	2.221770	3.774531
H	-2.425315	0.685575	4.578485
C	-5.416877	-0.151139	-0.563436
O	-4.243032	0.163347	-0.107944
O	-5.893699	-1.280761	-0.718627
C	-6.243362	1.101286	-0.894741
H	-7.079954	0.835448	-1.549024
H	-6.644018	1.524237	0.036274
H	-5.612852	1.864665	-1.361641
C	4.707419	3.854774	0.524213
C	3.409882	3.663369	0.025332
C	2.490449	4.724245	0.126432
C	2.870019	5.938006	0.706345
C	4.169279	6.119344	1.197069
C	5.088568	5.069908	1.105252
H	5.425943	3.039355	0.457623
H	1.477055	4.584218	-0.248267
H	2.144188	6.746372	0.775506
H	4.460168	7.066876	1.648066
H	6.101348	5.193881	1.486024
C	2.990746	2.350059	-0.600272
H	2.401833	2.558326	-1.502351
H	3.874599	1.778627	-0.907685
C	2.132230	1.481684	0.338688
H	1.266045	2.068739	0.667769
H	2.691278	1.203232	1.238684
C	1.610946	0.227965	-0.331643
H	1.658516	0.202084	-1.416972
C	0.629313	-0.611779	0.279234
H	0.629725	-0.665474	1.366621
H	0.433327	-1.567910	-0.197851
C	4.937954	-2.536414	0.319922
C	4.803010	-2.636509	-1.062290
C	5.502176	-3.588453	-1.792783
C	6.354574	-4.454464	-1.087157
C	6.490555	-4.353385	0.305656
C	5.777518	-3.383845	1.030828
C	4.043271	-1.393424	0.761762
C	3.824338	-1.555710	-1.480664
H	5.385824	-3.657549	-2.871598
H	6.915792	-5.216654	-1.624922
H	7.155275	-5.038588	0.828834
H	5.871112	-3.296470	2.110517
N	3.432623	-0.866343	-0.355076
O	3.473237	-1.345138	-2.641907

O	3.924755	-1.015579	1.927407

13-di

B3LYP SCF energy: -2299.28532196 a.u.
B3LYP enthalpy: -2298.680621 a.u.
B3LYP free energy: -2298.825048 a.u.
B3LYP free energy after quasi-harmonic correction: -2298.803534 a.u.
M06 SCF energy in solution: -2298.73353128 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.845398	0.113042	-2.651479
O	-1.171181	0.964791	-1.999835
O	-2.472275	-0.916105	-2.246536
C	-1.885466	0.326312	-4.166502
H	-2.800347	-0.097975	-4.590471
H	-1.808403	1.391944	-4.402613
H	-1.026801	-0.189226	-4.616200
Pd	-0.874913	0.928444	0.135459
C	-2.100182	3.593458	0.677170
O	-0.932245	4.037866	0.554348
O	-2.488273	2.385560	0.561835
C	-3.219306	4.611754	0.980136
H	-3.430851	5.190400	0.070370
H	-4.139581	4.112900	1.300585
H	-2.885227	5.318830	1.749560
C	-1.330562	-3.940258	-0.876870
O	-2.387712	-4.376919	-1.342966
O	-1.122362	-2.774391	-0.341387
C	-0.061529	-4.807918	-0.878299
H	0.757817	-4.277378	-1.376300
H	0.254470	-5.005322	0.154604
H	-0.256845	-5.758440	-1.384544
Pd	-2.628705	-1.390203	-0.211750
C	-1.769992	-0.682075	2.561478
O	-2.495034	-1.474304	1.882461
O	-0.982133	0.232023	2.172808
C	-1.881183	-0.850754	4.077595
H	-0.918489	-0.645682	4.556418
H	-2.609700	-0.120709	4.453022
H	-2.233994	-1.854511	4.331031
C	-5.301197	-0.306680	0.320840
O	-4.117468	-0.030355	-0.127081
O	-5.732895	-1.391636	0.729758
C	-6.219066	0.926361	0.268324
H	-6.659387	1.000953	-0.735556
H	-7.031326	0.818540	0.995329
H	-5.646218	1.839734	0.454948
C	4.038851	3.637023	-1.321818
C	2.717712	3.593127	-0.846853
C	2.241343	4.686776	-0.099661
C	3.069981	5.782144	0.162583
C	4.386619	5.812884	-0.314030
C	4.869190	4.732994	-1.060858
H	4.419342	2.800327	-1.907002

H	1.213564	4.663623	0.261000
H	2.681399	6.619220	0.740438
H	5.027631	6.669083	-0.108431
H	5.889877	4.743225	-1.441547
C	1.821809	2.400940	-1.101582
H	0.782467	2.737619	-1.152920
H	2.067229	1.948181	-2.072769
C	1.942654	1.317100	-0.004003
H	1.768731	1.779202	0.978465
H	2.993863	0.969500	0.011960
C	0.989169	0.126638	-0.199542
H	0.992095	-0.204450	-1.243946
C	1.313313	-1.054654	0.711470
H	1.214746	-0.785927	1.764166
H	0.648372	-1.890368	0.484179
C	4.952879	-2.012669	1.040398
C	4.701247	-2.428220	-0.264417
C	5.692308	-3.003599	-1.048185
C	6.966146	-3.150344	-0.476767
C	7.220182	-2.730495	0.837582
C	6.207296	-2.152429	1.619065
C	3.676135	-1.450615	1.595221
C	3.259425	-2.136224	-0.570393
H	5.480833	-3.323863	-2.064712
H	7.769543	-3.594883	-1.060180
H	8.217219	-2.854589	1.254662
H	6.389996	-1.821333	2.637694
N	2.721967	-1.549802	0.579503
O	2.679662	-2.373980	-1.614959
O	3.506464	-1.008900	2.720058

13M-di

B3LYP SCF energy: -2299.28645840 a.u.
B3LYP enthalpy: -2298.680862 a.u.
B3LYP free energy: -2298.830780 a.u.
B3LYP free energy after quasi-harmonic correction: -2298.805512 a.u.
M06 SCF energy in solution: -2298.73262839 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.198242	0.472512	-2.503481
O	0.660668	-0.501363	-1.890003
O	1.920745	1.416594	-2.058314
C	0.904497	0.532925	-4.002453
H	1.604658	1.204964	-4.505867
H	0.958044	-0.471216	-4.435873
H	-0.117377	0.907012	-4.144208
Pd	0.914208	-0.870392	0.195329
C	2.366006	-3.528526	0.089258
O	1.311159	-4.075865	0.493581
O	2.556847	-2.295751	-0.166622
C	3.593868	-4.438721	-0.125656
H	3.326504	-5.267675	-0.793834
H	4.439290	-3.883595	-0.544032
H	3.889926	-4.878006	0.836361

C	0.959559	4.153966	0.477786
O	2.019506	4.763337	0.657555
O	0.800167	2.901078	0.182867
C	-0.386877	4.888246	0.610193
H	-1.009885	4.707823	-0.273893
H	-0.932865	4.500979	1.479982
H	-0.220888	5.962691	0.736609
Pd	2.406377	1.634699	-0.026633
C	2.167448	0.392771	2.667279
O	2.604091	1.417249	2.050165
O	1.484783	-0.585641	2.244428
C	2.553598	0.334190	4.146880
H	1.813464	-0.237895	4.714362
H	3.521981	-0.175840	4.231084
H	2.661330	1.342992	4.556940
C	5.051090	0.675445	-0.859913
O	3.980653	0.383365	-0.190175
O	5.314341	1.721106	-1.466117
C	6.069915	-0.475075	-0.808683
H	6.771835	-0.391266	-1.645310
H	6.636371	-0.409875	0.130426
H	5.556330	-1.441180	-0.824235
C	-1.711436	-5.186273	0.361206
C	-2.459258	-4.207899	-0.316483
C	-3.771329	-4.526842	-0.708993
C	-4.330485	-5.777073	-0.427873
C	-3.580193	-6.740535	0.256452
C	-2.270591	-6.437860	0.644638
H	-0.683469	-4.958393	0.638611
H	-4.361584	-3.785908	-1.247044
H	-5.348829	-5.999508	-0.744492
H	-4.010535	-7.716042	0.478689
H	-1.672513	-7.181797	1.168346
C	-1.855329	-2.849099	-0.616966
H	-0.789527	-2.865291	-0.361936
H	-1.920417	-2.650181	-1.696819
C	-2.558972	-1.701083	0.137265
H	-2.476346	-1.861770	1.218459
H	-3.631170	-1.724779	-0.105109
C	-1.997482	-0.306188	-0.226617
H	-1.744761	-0.291901	-1.290432
C	-0.789830	0.173363	0.586525
H	-0.970724	0.044178	1.660250
H	-0.593222	1.226933	0.375024
C	-4.685308	2.217691	0.656598
C	-4.533164	2.453519	-0.707264
C	-5.254300	3.444282	-1.359769
C	-6.146255	4.207939	-0.590772
C	-6.300119	3.970416	0.783303
C	-5.566825	2.962400	1.428588
C	-3.773577	1.085073	1.033914
C	-3.523923	1.475074	-1.230342
H	-5.121221	3.620023	-2.423621
H	-6.723696	4.999038	-1.064021
H	-6.995143	4.580601	1.355972
H	-5.673502	2.769775	2.492551
N	-3.103737	0.711712	-0.135763

O	-3.161939	1.351908	-2.388765
O	-3.668096	0.578634	2.137602

14-TS

B3LYP SCF energy: -1485.80566700 a.u.
B3LYP enthalpy: -1485.377368 a.u.
B3LYP free energy: -1485.480220 a.u.
B3LYP free energy after quasi-harmonic correction: -1485.465356 a.u.
M06 SCF energy in solution: -1485.32896492 a.u.
Imaginary frequency: -529.2830 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.855647	-2.570605	1.455261
O	2.328571	-1.933475	2.384513
O	3.014342	-2.176740	0.236520
C	3.420383	-3.974261	1.723030
H	3.177638	-4.655498	0.899788
H	4.514752	-3.912104	1.784904
H	3.035266	-4.370187	2.667485
Pd	2.472383	-0.191169	-0.290495
C	4.813102	1.473927	-1.055457
O	4.489215	0.272804	-0.716673
O	4.053325	2.452322	-1.188934
C	6.319964	1.652685	-1.289138
H	6.699853	0.858433	-1.941664
H	6.530581	2.632633	-1.726866
H	6.847622	1.565231	-0.330952
C	-1.606466	1.842786	2.208363
C	-0.791927	2.495278	1.269007
C	-1.319387	3.606683	0.592993
C	-2.620954	4.052114	0.842072
C	-3.421934	3.391280	1.778788
C	-2.908397	2.284131	2.462237
H	-1.212848	0.982528	2.745400
H	-0.700625	4.127184	-0.135505
H	-3.007866	4.915984	0.305584
H	-4.434552	3.736396	1.976038
H	-3.520639	1.763816	3.195809
C	0.613898	2.001474	0.976362
H	1.260572	2.848785	0.723079
H	1.039461	1.525763	1.866133
C	0.627060	0.991021	-0.173895
H	0.241066	1.385984	-1.114582
C	0.422965	-0.401100	0.074830
H	0.336290	-0.737198	1.107607
C	-0.248327	-1.295719	-0.947912
H	0.029937	-1.013294	-1.965972
H	0.031235	-2.337852	-0.779630
C	-3.923815	-0.599361	-1.271167
C	-3.938965	-1.612582	-0.312541
C	-5.126697	-2.071879	0.240635
C	-6.317984	-1.474736	-0.199342
C	-6.302504	-0.455579	-1.163094

C	-5.095371	-0.002083	-1.716419
C	-2.498835	-0.352981	-1.659950
C	-2.523483	-2.038705	-0.066373
H	-5.125836	-2.862246	0.985838
H	-7.268359	-1.804951	0.212763
H	-7.240994	-0.009856	-1.483403
H	-5.070514	0.787819	-2.461556
N	-1.727803	-1.236328	-0.895158
O	-2.126012	-2.913542	0.680850
O	-2.075595	0.435301	-2.487651
H	2.164359	1.276615	-0.780154

14M-TS

B3LYP SCF energy: -1485.79236517 a.u.
B3LYP enthalpy: -1485.365218 a.u.
B3LYP free energy: -1485.465320 a.u.
B3LYP free energy after quasi-harmonic correction: -1485.453209 a.u.
M06 SCF energy in solution: -1485.31758344 a.u.
Imaginary frequency: -590.0231 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.283057	4.188622	-1.384721
O	1.433122	3.791280	-1.639650
O	-0.652557	3.543652	-0.773233
C	-0.138946	5.608064	-1.798558
H	-1.119627	5.590748	-2.287934
H	-0.235868	6.231409	-0.900429
H	0.606586	6.052784	-2.464422
Pd	-0.357383	1.623925	0.054537
C	-2.144748	1.645459	2.410526
O	-1.194544	2.325917	1.872184
O	-2.634530	0.576722	1.993838
C	-2.720629	2.286364	3.681602
H	-3.464220	3.040797	3.392470
H	-3.216913	1.531493	4.299322
H	-1.937835	2.794005	4.254636
C	-3.763489	-2.245078	0.349518
C	-3.121854	-2.145588	-0.897319
C	-3.415057	-3.101297	-1.882217
C	-4.320467	-4.138178	-1.633309
C	-4.949927	-4.232220	-0.387964
C	-4.668650	-3.280983	0.599319
H	-3.550432	-1.496247	1.110750
H	-2.933104	-3.029320	-2.856477
H	-4.536337	-4.867836	-2.411552
H	-5.656860	-5.035737	-0.191111
H	-5.160084	-3.340607	1.568251
C	-2.120634	-1.035857	-1.141302
H	-2.174962	-0.706952	-2.186690
H	-2.370390	-0.177684	-0.506433
C	-0.681916	-1.477741	-0.806908
H	-0.324336	-2.202123	-1.554661
H	-0.687101	-1.989083	0.161873
C	0.341975	-0.337459	-0.744797

C	0.366504	0.736994	-1.680544
H	-0.415619	0.786667	-2.434659
H	1.304131	1.209023	-1.952723
C	3.845024	-1.568352	-0.329609
C	3.420109	-1.576146	0.996693
C	4.262944	-1.966111	2.029554
C	5.568098	-2.347990	1.686575
C	5.996700	-2.340132	0.350256
C	5.132956	-1.949651	-0.683505
C	2.705143	-1.118039	-1.186038
C	1.993021	-1.134739	1.032409
H	3.917938	-1.968758	3.059396
H	6.260223	-2.654895	2.466762
H	7.014743	-2.640417	0.114974
H	5.452216	-1.938658	-1.721596
N	1.650047	-0.807114	-0.298540
O	1.258081	-1.083559	1.997016
O	2.675352	-1.062687	-2.399918
H	-0.177547	0.210378	0.741478

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B3LYP SCF energy: -1485.81742497 a.u.
B3LYP enthalpy: -1485.386693 a.u.
B3LYP free energy: -1485.489006 a.u.
B3LYP free energy after quasi-harmonic correction: -1485.475453 a.u.
M06 SCF energy in solution: -1485.32987776 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.251418	1.304522	2.566494
O	1.032964	1.596084	2.528328
O	2.938826	0.731780	1.651105
C	3.055243	1.647088	3.831190
H	3.339111	0.717748	4.341480
H	3.984130	2.162675	3.561332
H	2.464705	2.265958	4.513496
Pd	2.488096	-0.282216	-0.246246
C	5.092489	-1.457383	-1.200980
O	4.509892	-0.693000	-0.326681
O	4.572387	-2.076560	-2.136590
C	6.608379	-1.545199	-0.967714
H	6.807376	-1.930695	0.039332
H	7.074082	-2.196676	-1.712363
H	7.051816	-0.543725	-1.022107
C	-1.481198	2.908865	0.423351
C	-0.715201	2.760395	-0.745491
C	-1.260303	3.190853	-1.964081
C	-2.539460	3.753773	-2.021439
C	-3.294676	3.896386	-0.853185
C	-2.759300	3.472480	0.368668
H	-1.055089	2.586942	1.371420
H	-0.676735	3.084416	-2.877094
H	-2.944159	4.081286	-2.977112
H	-4.289255	4.336038	-0.893796
H	-3.336661	3.585489	1.284213

C	0.669084	2.134517	-0.665878
H	1.326422	2.591374	-1.416018
H	1.086809	2.322998	0.325133
C	0.615194	0.632849	-0.905354
H	0.441706	0.335577	-1.939197
C	0.354268	-0.305694	0.094589
H	0.243800	0.047275	1.119811
C	-0.217893	-1.675633	-0.215283
H	0.011264	-1.978960	-1.238968
H	0.169099	-2.428867	0.474549
C	-3.947718	-1.461692	-0.518359
C	-3.819478	-1.863184	0.811710
C	-4.929756	-2.053528	1.623419
C	-6.192139	-1.822710	1.056005
C	-6.320865	-1.418463	-0.281087
C	-5.191086	-1.232821	-1.092135
C	-2.574646	-1.363764	-1.107558
C	-2.360865	-2.030564	1.107622
H	-4.817451	-2.366210	2.657556
H	-7.085349	-1.957096	1.661076
H	-7.311901	-1.244551	-0.692841
H	-5.277335	-0.917492	-2.127904
N	-1.686849	-1.696004	-0.075067
O	-1.843596	-2.402508	2.144856
O	-2.267536	-1.084566	-2.252210
H	2.356710	-1.095928	-1.536683

15M

B3LYP SCF energy: -1485.80623274 a.u.
B3LYP enthalpy: -1485.376685 a.u.
B3LYP free energy: -1485.476912 a.u.
B3LYP free energy after quasi-harmonic correction: -1485.465219 a.u.
M06 SCF energy in solution: -1485.32465505 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.988949	-1.718096	-0.323538
O	-3.058119	-0.892233	0.610467
O	-1.964108	-1.973054	-1.052189
C	-4.234535	-2.544588	-0.679718
H	-4.385146	-2.562830	-1.765412
H	-4.076809	-3.581244	-0.355361
H	-5.123968	-2.146081	-0.182115
Pd	0.142206	-1.607857	-0.579260
C	1.300587	-3.949385	0.898889
O	0.219220	-3.411735	0.419029
O	2.457258	-3.514506	0.837708
C	1.014654	-5.277384	1.614162
H	0.491055	-5.962575	0.937255
H	1.945499	-5.734601	1.960796
H	0.351614	-5.098407	2.469115
C	4.645220	0.771661	0.594571
C	4.024617	1.502887	-0.432253
C	4.554136	2.757631	-0.768842

C	5.669193	3.273923	-0.100268
C	6.276012	2.537396	0.921189
C	5.758923	1.283338	1.265235
H	4.250588	-0.206021	0.864274
H	4.088751	3.335397	-1.566003
H	6.063675	4.248907	-0.379304
H	7.144055	2.934770	1.442655
H	6.224697	0.699221	2.055742
C	2.803382	0.947808	-1.135550
H	2.729293	1.382834	-2.140702
H	2.919672	-0.135246	-1.254465
C	1.509464	1.232941	-0.349827
H	1.337072	2.320289	-0.342620
H	1.635973	0.938867	0.695577
C	0.236556	0.585163	-0.898244
C	0.157685	-0.114287	-2.104149
H	1.051358	-0.243640	-2.706027
H	-0.791584	-0.231888	-2.611905
C	-2.980433	2.297208	-0.157665
C	-2.572415	1.941943	1.124608
C	-3.331992	2.257168	2.241918
C	-4.533386	2.948312	2.031828
C	-4.945030	3.308728	0.739419
C	-4.166169	2.985202	-0.380546
C	-1.957283	1.818677	-1.130969
C	-1.262283	1.239889	1.022829
H	-3.008271	1.960962	3.235132
H	-5.161343	3.204356	2.881990
H	-5.883799	3.841368	0.606499
H	-4.475023	3.252050	-1.387272
N	-0.959160	1.183015	-0.366596
O	-0.534110	0.874023	1.920748
O	-1.955032	1.980565	-2.339853
H	1.656699	-1.557444	-0.371482

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B3LYP SCF energy: -1485.80624105 a.u.
B3LYP enthalpy: -1485.377982 a.u.
B3LYP free energy: -1485.479411 a.u.
B3LYP free energy after quasi-harmonic correction: -1485.466034 a.u.
M06 SCF energy in solution: -1485.32647363 a.u.
Imaginary frequency: -501.8904 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-3.270266	2.563878	0.983672
O	-2.101856	2.963975	1.152830
O	-3.652933	1.439123	0.490815
C	-4.442613	3.470314	1.395445
H	-5.131793	3.601154	0.552675
H	-5.009832	2.990562	2.202796
H	-4.079086	4.444827	1.734879
Pd	-2.510867	-0.229136	-0.155088
C	-4.251348	-2.628204	-0.350589
O	-4.312750	-1.359765	-0.138642

O	-3.230235	-3.304748	-0.587885
C	-5.617487	-3.325369	-0.287026
H	-6.304758	-2.862646	-1.005296
H	-5.519844	-4.392972	-0.502929
H	-6.054211	-3.189824	0.709883
C	2.006124	2.060372	-2.015388
C	0.935334	2.390378	-1.171428
C	1.141012	3.363173	-0.176973
C	2.384138	3.985064	-0.035880
C	3.445949	3.648533	-0.884497
C	3.252206	2.682789	-1.876532
H	1.862438	1.310503	-2.791773
H	0.312972	3.618097	0.481724
H	2.524633	4.735690	0.739434
H	4.413162	4.134691	-0.773735
H	4.068450	2.413883	-2.544485
C	-0.417718	1.708845	-1.288746
H	-1.202579	2.458226	-1.155399
H	-0.531581	1.269719	-2.288027
C	-0.420057	-0.752001	-0.526028
H	-0.184282	-1.011463	-1.558047
C	-0.596677	0.630543	-0.225404
H	-0.395603	0.970670	0.789737
C	0.185590	-1.720336	0.485156
H	-0.150264	-1.490456	1.497461
H	-0.089104	-2.751696	0.247320
C	3.828420	-1.163109	1.163813
C	3.886182	-1.750013	-0.100433
C	5.095500	-1.963370	-0.748303
C	6.264060	-1.563346	-0.082830
C	6.205810	-0.972858	1.188272
C	4.977427	-0.764955	1.833599
C	2.391278	-1.087129	1.575264
C	2.486721	-2.058811	-0.532314
H	5.127940	-2.420476	-1.733151
H	7.230357	-1.710636	-0.558815
H	7.127646	-0.669949	1.678486
H	4.919342	-0.306460	2.816456
N	1.655242	-1.627341	0.507489
O	2.119791	-2.586964	-1.567583
O	1.931881	-0.671803	2.622181
H	-1.869523	-1.574647	-0.668387

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B3LYP SCF energy: -1485.83733389 a.u.
B3LYP enthalpy: -1485.403602 a.u.
B3LYP free energy: -1485.504039 a.u.
B3LYP free energy after quasi-harmonic correction: -1485.491648 a.u.
M06 SCF energy in solution: -1485.34984006 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.417751	1.213725	2.803176
O	1.034696	0.073569	3.111962

O	2.020474	1.572749	1.717482
C	1.164497	2.391269	3.754386
H	2.073613	2.991548	3.873458
H	0.396551	3.044085	3.320589
H	0.822450	2.029114	4.728353
Pd	2.631249	0.432525	0.127511
C	4.706173	0.052088	-1.468929
O	5.014087	0.883408	-0.584591
O	3.539723	-0.492900	-1.527933
C	5.705465	-0.333516	-2.551039
H	6.717751	-0.360486	-2.135656
H	5.451311	-1.299666	-2.997055
H	5.688153	0.427910	-3.341679
C	-0.735654	-3.698694	-0.114311
C	-0.241428	-2.711128	0.751569
C	-0.996767	-2.392195	1.896010
C	-2.204860	-3.042732	2.158767
C	-2.688037	-4.024722	1.284433
C	-1.947230	-4.350605	0.145000
H	-0.163310	-3.962222	-1.002210
H	-0.615492	-1.631130	2.574190
H	-2.770653	-2.784882	3.052357
H	-3.629615	-4.530184	1.490699
H	-2.310355	-5.110821	-0.544373
C	1.064362	-1.980218	0.485219
H	1.616703	-1.909815	1.426497
H	1.675321	-2.553626	-0.224169
C	0.387746	-0.517189	-1.508702
H	-0.353590	-1.310957	-1.689197
C	0.858247	-0.546922	-0.052196
H	0.165935	-0.012298	0.606075
C	-0.227782	0.816713	-1.962584
H	0.349524	1.662530	-1.579564
H	-0.255653	0.870565	-3.056426
C	-3.483587	1.740614	-0.342658
C	-3.901002	0.764327	-1.246698
C	-5.230881	0.374735	-1.333137
C	-6.144205	0.998286	-0.469622
C	-5.723983	1.980063	0.440043
C	-4.377717	2.368543	0.513813
C	-2.007731	1.932756	-0.514214
C	-2.701347	0.305461	-2.015816
H	-5.543651	-0.388692	-2.039704
H	-7.193463	0.715163	-0.502148
H	-6.453440	2.443779	1.099549
H	-4.039162	3.125598	1.215258
N	-1.608956	1.003727	-1.490932
O	-2.664805	-0.491296	-2.938869
O	-1.293144	2.743878	0.040739
H	1.235874	-0.736982	-2.169208

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B3LYP SCF energy: -1485.80667064 a.u.
B3LYP enthalpy: -1485.378447 a.u.
B3LYP free energy: -1485.479961 a.u.

B3LYP free energy after quasi-harmonic correction: -1485.466685 a.u.
M06 SCF energy in solution: -1485.32838369 a.u.
Imaginary frequency: -664.4659 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.918320	-2.426367	2.142303
O	2.267691	-1.391023	2.743098
O	1.648444	-2.540719	0.888234
C	1.805880	-3.745034	2.921936
H	1.719906	-3.551577	3.995516
H	0.952164	-4.335436	2.571835
H	2.712053	-4.339095	2.744601
Pd	1.936106	-0.844359	-0.366669
C	3.887957	-1.337972	-2.554066
O	3.403422	-1.880288	-1.489267
O	3.594551	-0.227977	-3.036150
C	4.951796	-2.202944	-3.246548
H	5.852442	-2.239082	-2.620436
H	4.592271	-3.232346	-3.356955
H	5.211943	-1.787830	-4.224555
C	1.267322	1.261655	-0.300009
H	0.756637	1.669269	-1.175177
C	0.497287	0.364730	0.522164
H	0.698402	0.366957	1.592872
C	-0.923196	-0.006021	0.141643
H	-1.030296	-0.041605	-0.949543
H	-1.160943	-1.003464	0.530339
C	-5.461739	-0.209396	0.372460
C	-5.310120	0.494114	-0.823431
C	-6.332939	0.565684	-1.759594
C	-7.530881	-0.100820	-1.459532
C	-7.683335	-0.807735	-0.257713
C	-6.642771	-0.870501	0.681813
C	-4.186619	-0.086943	1.147782
C	-3.934552	1.083824	-0.842353
H	-6.202798	1.115196	-2.687407
H	-8.353741	-0.071355	-2.169248
H	-8.622223	-1.316086	-0.053374
H	-6.748890	-1.416374	1.614804
N	-3.325255	0.685014	0.354703
O	-3.427412	1.784256	-1.700394
O	-3.929750	-0.538820	2.248547
H	2.149685	0.405224	-1.333595
C	2.253153	2.219068	0.297643
C	2.421677	3.484180	-0.285080
C	2.998742	1.900221	1.448107
C	3.299006	4.421731	0.269422
H	1.865360	3.734304	-1.186524
C	3.871193	2.838185	2.000977
H	2.905819	0.912504	1.896749
C	4.026171	4.102882	1.418643
H	3.416220	5.395617	-0.201547
H	4.441859	2.573404	2.888385
H	4.713913	4.826305	1.851674
C	-1.939658	1.007082	0.711784
H	-1.736062	2.011173	0.328931

H	-1.889522	1.028541	1.803856

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B3LYP SCF energy: -1485.81920939 a.u.
B3LYP enthalpy: -1485.388354 a.u.
B3LYP free energy: -1485.490618 a.u.
B3LYP free energy after quasi-harmonic correction: -1485.477364 a.u.
M06 SCF energy in solution: -1485.33254508 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.875611	0.067545	2.711856
O	2.036688	0.975448	2.925975
O	3.043502	-0.594535	1.631486
C	3.842901	-0.324170	3.841423
H	3.697849	-1.380545	4.099055
H	4.878813	-0.217786	3.496925
H	3.681318	0.295981	4.728335
Pd	1.906822	-0.917090	-0.226515
C	2.707117	-3.646132	-1.209597
O	2.939650	-2.701774	-0.349278
O	1.847226	-3.672122	-2.098698
C	3.663396	-4.835165	-1.030049
H	3.586431	-5.224474	-0.008008
H	3.430310	-5.626644	-1.747742
H	4.698778	-4.502057	-1.170554
C	1.197225	1.063169	-0.898927
H	0.743783	0.902045	-1.876710
C	0.466438	0.641148	0.216518
H	0.768317	0.969785	1.212695
C	-0.953063	0.130346	0.092421
H	-1.137874	-0.254395	-0.917111
H	-1.123005	-0.690676	0.799178
C	-5.451174	-0.045498	0.700896
C	-5.415007	0.300335	-0.650727
C	-6.509758	0.101996	-1.481377
C	-7.659868	-0.463674	-0.910079
C	-7.696190	-0.811291	0.448289
C	-6.583709	-0.603907	1.278118
C	-4.124601	0.298085	1.303877
C	-4.064324	0.873283	-0.946444
H	-6.469352	0.373618	-2.532231
H	-8.536370	-0.637986	-1.528965
H	-8.600351	-1.250057	0.862611
H	-6.599769	-0.870497	2.330923
N	-3.352294	0.828949	0.259866
O	-3.647473	1.311650	-2.003718
O	-3.768234	0.169882	2.460402
H	1.175904	-1.376686	-1.490792
C	2.316805	2.034088	-0.930800
C	2.830511	2.417119	-2.184371
C	2.864372	2.624467	0.225040
C	3.857561	3.357268	-2.289414
H	2.422132	1.961330	-3.084355
C	3.890259	3.563802	0.116699

H	2.501352	2.330709	1.206679
C	4.393084	3.937613	-1.135714
H	4.239921	3.632406	-3.270295
H	4.303150	4.004036	1.021886
H	5.194780	4.669493	-1.210229
C	-1.958756	1.261262	0.400734
H	-1.813338	2.099056	-0.286881
H	-1.834418	1.618298	1.426629

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B3LYP SCF energy: -585.61408736 a.u.
B3LYP enthalpy: -585.491965 a.u.
B3LYP free energy: -585.548395 a.u.
B3LYP free energy after quasi-harmonic correction: -585.543202 a.u.
M06 SCF energy in solution: -585.53029489 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.681825	0.266386	-0.009681
O	-2.130179	-0.893630	-0.010977
O	-2.015480	1.331162	-0.013429
C	-4.204321	0.315801	0.023288
H	-4.533093	0.580377	1.036559
H	-4.568309	1.093951	-0.656027
H	-4.636914	-0.652626	-0.244421
Pd	-0.118404	-0.277540	-0.004349
C	2.881896	0.043514	0.006678
O	1.710072	0.600626	0.000924
O	3.157118	-1.161263	0.011952
C	4.009425	1.090818	0.004381
H	3.909565	1.752397	0.873530
H	4.986216	0.599265	0.025532
H	3.933282	1.719876	-0.891112
H	0.552536	-1.640696	0.000232

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B3LYP SCF energy: -585.59255950 a.u.
B3LYP enthalpy: -585.473874 a.u.
B3LYP free energy: -585.526192 a.u.
B3LYP free energy after quasi-harmonic correction: -585.523026 a.u.
M06 SCF energy in solution: -585.52831027 a.u.
Imaginary frequency: -518.8043 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.923414	-0.035464	0.000645
O	1.868297	0.703350	0.000384
O	2.980784	-1.277997	0.000925
C	4.230094	0.782362	-0.000674
H	4.259697	1.443020	0.875221
H	5.101638	0.120431	0.010018
H	4.268391	1.424163	-0.890262
Pd	-0.021501	-0.172530	-0.000135

C	-2.843339	0.116337	0.000000
O	-2.075577	-0.866276	-0.000616
O	-2.404473	1.344139	0.000759
C	-4.343835	-0.058846	-0.000092
H	-4.601536	-1.120640	-0.000811
H	-4.775244	0.426042	0.883182
H	-4.775289	0.427259	-0.882671
H	-1.238874	1.164022	0.000628

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B3LYP SCF energy: -585.59290438 a.u.
B3LYP enthalpy: -585.469159 a.u.
B3LYP free energy: -585.524854 a.u.
B3LYP free energy after quasi-harmonic correction: -585.520616 a.u.
M06 SCF energy in solution: -585.53522916 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.740423	0.539944	-0.004640
O	-2.346793	1.719041	-0.009710
O	-2.036430	-0.537953	-0.002284
C	-4.258127	0.256254	0.010280
H	-4.525305	-0.420974	-0.810760
H	-4.530472	-0.248426	0.946739
H	-4.828123	1.186698	-0.077150
Pd	0.035741	-0.653524	-0.001406
C	2.698970	0.394703	0.001743
O	2.191543	-0.735072	-0.000333
O	1.972680	1.496752	0.003049
C	4.189957	0.613251	0.003520
H	4.483995	1.198927	-0.875246
H	4.483286	1.186377	0.890831
H	4.707974	-0.348364	-0.002789
H	0.974279	1.140820	0.001828

23A-TS

B3LYP SCF energy: -1265.64328452 a.u.
B3LYP enthalpy: -1265.105308 a.u.
B3LYP free energy: -1265.205528 a.u.
B3LYP free energy after quasi-harmonic correction: -1265.195066 a.u.
M06 SCF energy in solution: -1265.14857972 a.u.
Imaginary frequency: -258.9241 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	3.000098	-2.859740	-1.061436
O	2.443261	-3.435303	-0.088852
O	2.568459	-1.699891	-1.443515
C	4.174548	-3.468517	-1.783689
H	4.214096	-4.544598	-1.599051
H	4.111602	-3.266512	-2.857123
H	5.101187	-3.015121	-1.410344
Pd	1.081886	-1.600003	-0.007229
C	-0.386715	-1.254724	2.569856

O	0.151610	-0.167775	2.830082
O	-0.283687	-1.918719	1.455570
C	-1.258079	-1.951413	3.610616
H	-1.967500	-2.642093	3.147546
H	-0.605751	-2.530338	4.276321
H	-1.782904	-1.208018	4.217349
C	-4.272497	0.334768	-2.078663
C	-3.560682	-0.358703	-1.088273
C	-4.254725	-0.774080	0.059666
C	-5.615701	-0.499413	0.216199
C	-6.311570	0.196925	-0.777583
C	-5.635052	0.612151	-1.928012
H	-3.756393	0.652804	-2.983226
H	-3.721695	-1.324617	0.832180
H	-6.134493	-0.834767	1.111162
H	-7.371611	0.407264	-0.659276
H	-6.168072	1.145709	-2.711614
C	-2.077794	-0.630398	-1.230707
H	-1.837686	-1.622526	-0.832406
H	-1.803843	-0.637100	-2.294608
C	-1.210978	0.411699	-0.492062
H	-1.452093	0.404055	0.575079
H	-1.493710	1.411943	-0.867168
C	0.282042	0.212141	-0.698961
H	0.555981	0.176953	-1.758168
C	1.223041	0.898259	0.150478
H	1.004930	0.911942	1.210746
H	2.274411	0.860166	-0.115757
N	1.134588	2.911840	-0.066500
H	0.268905	3.011457	-0.599725
C	2.267268	3.396674	-0.918026
H	3.183825	3.030419	-0.440140
C	0.940870	3.606954	1.250881
H	0.893282	4.684378	1.044218
C	2.164054	2.774806	-2.316617
H	3.005197	3.112432	-2.931131
H	2.186971	1.683282	-2.293365
H	1.240322	3.091030	-2.820083
C	2.349481	4.929100	-1.024384
H	3.149727	5.198550	-1.722573
H	1.413406	5.351379	-1.412672
H	2.574885	5.411544	-0.069071
C	-0.401267	3.207280	1.875131
H	-0.595813	3.852578	2.739189
H	-1.229471	3.349470	1.168900
H	-0.410685	2.171072	2.225408
C	2.114767	3.351095	2.202325
H	1.957990	3.923323	3.123209
H	2.189173	2.295119	2.479468
H	3.073195	3.670401	1.778061

23A-TS-cis

B3LYP SCF energy: -1265.62572649 a.u.
B3LYP enthalpy: -1265.089519 a.u.
B3LYP free energy: -1265.190609 a.u.

B3LYP free energy after quasi-harmonic correction: -1265.179616 a.u.
M06 SCF energy in solution: -1265.12566745 a.u.
Imaginary frequency: -198.0903 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.177606	-3.232871	-0.000860
O	1.826225	-2.857903	1.155256
O	1.758475	-2.561318	-1.021641
C	3.039558	-4.446712	-0.212622
H	3.679461	-4.611482	0.658038
H	2.394254	-5.325335	-0.336041
H	3.642334	-4.337103	-1.118281
Pd	0.654353	-1.255645	0.155239
C	0.238828	0.456750	2.426940
O	1.392805	0.881945	2.252774
O	-0.412546	-0.295894	1.589427
C	-0.541840	0.790010	3.689710
H	-0.579637	-0.098723	4.331056
H	-0.051979	1.600038	4.234758
H	-1.573883	1.064185	3.448875
C	-5.070757	-0.214073	-1.659839
C	-4.119741	-0.345238	-0.636951
C	-4.492797	0.013198	0.668352
C	-5.776542	0.492204	0.942374
C	-6.713972	0.621114	-0.087790
C	-6.356857	0.265008	-1.391380
H	-4.804042	-0.496933	-2.676874
H	-3.769038	-0.092868	1.473991
H	-6.047249	0.759045	1.961291
H	-7.714434	0.989631	0.124784
H	-7.079913	0.354094	-2.198783
C	-2.716928	-0.834918	-0.927817
H	-2.358590	-1.453850	-0.096654
H	-2.727462	-1.474194	-1.821513
C	-1.716535	0.319170	-1.142788
H	-1.711976	0.949878	-0.248158
H	-2.072999	0.947679	-1.974498
C	-0.306134	-0.170431	-1.445879
H	-0.257704	-1.115899	-2.003009
C	0.686415	0.738320	-1.865826
H	1.559299	0.359413	-2.382427
H	0.446953	1.779625	-2.045428
N	2.140632	1.884663	-0.403169
H	1.911865	1.433500	0.494745
C	1.714347	3.308143	-0.365897
H	1.670900	3.655081	-1.409157
C	3.570055	1.641987	-0.726653
H	4.181767	2.206670	-0.006237
C	0.310466	3.428297	0.240950
H	-0.040044	4.463206	0.158885
H	-0.418461	2.787900	-0.261948
H	0.326544	3.155537	1.300966
C	2.679004	4.233665	0.403929
H	2.255793	5.244096	0.446405
H	2.814506	3.878855	1.432653
H	3.662969	4.312144	-0.068380

C	3.927640	0.164663	-0.538597
H	5.011162	0.038186	-0.650108
H	3.647692	-0.186097	0.460313
H	3.436385	-0.478709	-1.275158
C	3.938343	2.132966	-2.134171
H	5.006641	1.964180	-2.311236
H	3.385229	1.589946	-2.909286
H	3.748363	3.203165	-2.270060

23M-TS

B3LYP SCF energy: -1265.63118392 a.u.
B3LYP enthalpy: -1265.092849 a.u.
B3LYP free energy: -1265.192242 a.u.
B3LYP free energy after quasi-harmonic correction: -1265.182086 a.u.
M06 SCF energy in solution: -1265.14235107 a.u.
Imaginary frequency: -206.3725 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.446807	-2.374602	-1.872776
O	2.043454	-3.258823	-1.072524
O	2.290880	-1.125100	-1.571312
C	3.136587	-2.731831	-3.165563
H	2.752293	-3.681828	-3.546367
H	3.005969	-1.940404	-3.908696
H	4.210596	-2.851836	-2.976058
Pd	1.403050	-1.529435	0.272282
C	-0.440642	-2.083918	2.545446
O	-1.288573	-1.271418	2.150338
O	0.722855	-2.305652	2.005831
C	-0.706104	-2.968191	3.761194
H	-0.995367	-3.968833	3.416989
H	0.195529	-3.078751	4.371201
H	-1.522622	-2.552644	4.356984
C	-3.677312	0.144196	-2.290061
C	-3.042818	-0.278295	-1.112807
C	-3.837899	-0.696734	-0.032077
C	-5.231517	-0.686551	-0.131756
C	-5.854681	-0.260465	-1.310161
C	-5.072701	0.154097	-2.391680
H	-3.074356	0.457725	-3.141238
H	-3.351536	-1.033669	0.880831
H	-5.832620	-1.018983	0.711497
H	-6.939358	-0.258147	-1.386442
H	-5.546062	0.478070	-3.315754
C	-1.532827	-0.268656	-0.987242
H	-1.190038	-1.173719	-0.478654
H	-1.073227	-0.251673	-1.983939
C	-1.047084	0.961280	-0.172693
H	-1.486454	0.910156	0.826600
H	-1.438527	1.848535	-0.682870
C	0.463358	1.047737	-0.086006
H	0.941841	1.017312	-1.060508
C	1.206695	0.402423	0.979014
H	0.707838	0.370707	1.942659

H	2.255591	0.702962	1.059451
N	0.796313	3.035597	-0.013194
H	0.301848	3.287554	-0.871821
C	2.251526	3.376571	-0.227997
H	2.730568	3.238768	0.748211
C	0.173111	3.821485	1.122849
H	0.765596	4.736934	1.218919
C	2.931459	2.458057	-1.253365
H	3.952527	2.818282	-1.419916
H	2.999958	1.414978	-0.943087
H	2.415257	2.493675	-2.221925
C	2.431828	4.837243	-0.688264
H	3.500639	5.061373	-0.772726
H	1.986265	4.984223	-1.681204
H	2.000231	5.575908	-0.007759
C	-1.259967	4.255210	0.791865
H	-1.604485	4.960799	1.555894
H	-1.315774	4.769961	-0.176298
H	-1.958334	3.414777	0.780619
C	0.252168	3.100408	2.471614
H	-0.044922	3.804543	3.257445
H	-0.419267	2.239850	2.520945
H	1.267035	2.759402	2.698542

23M-TS-cis

B3LYP SCF energy: -1265.63084119 a.u.
B3LYP enthalpy: -1265.093963 a.u.
B3LYP free energy: -1265.195707 a.u.
B3LYP free energy after quasi-harmonic correction: -1265.184277 a.u.
M06 SCF energy in solution: -1265.12739639 a.u.
Imaginary frequency: -157.3620 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.776983	-3.049322	1.196514
O	2.018449	-2.907502	1.009123
O	-0.039865	-2.289353	0.543207
C	0.229409	-4.093407	2.131476
H	-0.710880	-3.757309	2.577387
H	0.028149	-5.010150	1.563368
H	0.962117	-4.325795	2.908340
Pd	1.492928	-1.344552	-0.499884
C	3.750415	0.364641	-1.282546
O	3.263477	1.328350	-0.667548
O	3.203981	-0.804771	-1.418044
C	5.119050	0.475888	-1.941077
H	5.342310	1.521620	-2.166902
H	5.876792	0.103966	-1.240344
H	5.174200	-0.134133	-2.846770
C	-5.107700	1.229325	-0.916482
C	-4.191914	0.174103	-1.036232
C	-4.559519	-1.089132	-0.546466
C	-5.808103	-1.291443	0.046475
C	-6.712616	-0.230551	0.160445
C	-6.358729	1.031650	-0.323802

H	-4.842993	2.214146	-1.297430
H	-3.863335	-1.921180	-0.633474
H	-6.076381	-2.278281	0.415593
H	-7.685679	-0.388105	0.618512
H	-7.056412	1.861822	-0.245478
C	-2.827654	0.393831	-1.656213
H	-2.564848	-0.455523	-2.297238
H	-2.852526	1.282464	-2.299462
C	-1.720757	0.571055	-0.568839
H	-1.662814	-0.347095	0.025920
H	-2.015224	1.389842	0.092069
C	-0.397428	0.865297	-1.204116
H	-0.223543	1.888268	-1.504629
C	0.371515	-0.145761	-1.834993
H	1.077720	0.195454	-2.589593
H	-0.213098	-1.025104	-2.132964
N	0.741299	1.849243	0.695194
H	1.625858	1.538364	0.271682
C	0.753076	3.331623	0.791725
H	-0.218417	3.639085	1.196644
C	0.460874	1.044809	1.915353
H	0.085866	0.087173	1.534512
C	-0.638935	1.644386	2.801068
H	-0.909276	0.916483	3.574313
H	-0.311460	2.556606	3.312927
H	-1.547971	1.876843	2.236338
C	1.718556	0.699525	2.741047
H	1.464706	-0.069437	3.481951
H	2.508676	0.295923	2.100053
H	2.121510	1.562304	3.280119
C	1.861904	3.881609	1.715360
H	1.852887	4.978525	1.690056
H	1.726130	3.576922	2.756057
H	2.846632	3.538073	1.378295
C	0.909817	3.956744	-0.605448
H	1.043477	5.040332	-0.511945
H	1.788755	3.549950	-1.118168
H	0.027476	3.799653	-1.234818

24-TS

B3LYP SCF energy: -741.67582681 a.u.
B3LYP enthalpy: -741.500726 a.u.
B3LYP free energy: -741.559406 a.u.
B3LYP free energy after quasi-harmonic correction: -741.554907 a.u.
M06 SCF energy in solution: -741.4906404 a.u.
Imaginary frequency: -745.9980 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.755511	0.696195	-0.066988
C	1.755444	-0.696255	-0.066935
C	2.921117	-1.422320	0.141498
C	4.107097	-0.701830	0.356175
C	4.107164	0.701573	0.356127
C	2.921254	1.422162	0.141396

C	0.332997	1.138644	-0.328133
C	0.332885	-1.138586	-0.328031
H	2.907145	-2.509285	0.138948
H	5.039988	-1.235878	0.525810
H	5.040106	1.235543	0.525728
H	2.907387	2.509128	0.138771
N	-0.437365	0.000059	-0.468212
H	-1.679558	0.000106	-0.541120
O	-0.037428	-2.305407	-0.410780
O	-0.037196	2.305493	-0.411004
C	-3.691147	0.000273	0.327027
O	-3.322995	0.000667	1.509528
O	-2.929199	0.000094	-0.723083
C	-5.189005	-0.000510	-0.013875
H	-5.432881	0.879712	-0.621871
H	-5.433279	-0.885965	-0.614129
H	-5.792713	0.003380	0.898486

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B3LYP SCF energy: -1265.65129492 a.u.
B3LYP enthalpy: -1265.110109 a.u.
B3LYP free energy: -1265.209971 a.u.
B3LYP free energy after quasi-harmonic correction: -1265.199253 a.u.
M06 SCF energy in solution: -1265.17251742 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	3.323917	-2.427487	-1.148456
O	2.918860	-3.115532	-0.178724
O	2.711033	-1.333470	-1.472187
C	4.540376	-2.825602	-1.952958
H	4.761696	-3.885148	-1.804075
H	4.385220	-2.614614	-3.015541
H	5.404047	-2.237764	-1.617500
Pd	1.266355	-1.464082	0.021612
C	-0.178512	-1.262684	2.654060
O	0.175662	-0.088602	2.875329
O	-0.001662	-1.927940	1.558409
C	-0.884455	-2.061243	3.747554
H	-1.553081	-2.815481	3.323312
H	-0.124558	-2.584998	4.341339
H	-1.433376	-1.390534	4.414565
C	-4.152954	-0.087155	-2.112910
C	-3.406662	-0.710128	-1.100990
C	-4.094826	-1.214458	0.014651
C	-5.482924	-1.093701	0.118882
C	-6.213142	-0.465562	-0.895732
C	-5.542793	0.036311	-2.014819
H	-3.640521	0.295262	-2.994503
H	-3.534020	-1.713201	0.802498
H	-5.995675	-1.496533	0.989211
H	-7.293892	-0.376110	-0.818240
H	-6.101112	0.516576	-2.815238
C	-1.898503	-0.813014	-1.187205
H	-1.560249	-1.780234	-0.799744

H	-1.583474	-0.763573	-2.238423
C	-1.181765	0.298219	-0.391071
H	-1.462389	0.230018	0.664535
H	-1.591533	1.263995	-0.754343
C	0.339737	0.264706	-0.542833
H	0.604487	0.314346	-1.606766
C	1.094211	1.296605	0.273774
H	0.890603	1.137712	1.330848
H	2.170777	1.247395	0.105125
N	0.707242	2.798743	-0.035926
H	-0.175082	2.743852	-0.555910
C	1.716777	3.476537	-0.966374
H	2.665328	3.439865	-0.422978
C	0.382855	3.596882	1.237615
H	0.133024	4.598033	0.879097
C	1.861818	2.689345	-2.273473
H	2.584107	3.210716	-2.910319
H	2.227482	1.672272	-2.122913
H	0.912087	2.641256	-2.820961
C	1.341083	4.935627	-1.253227
H	2.018494	5.325012	-2.019773
H	0.320283	5.018721	-1.648524
H	1.432712	5.588104	-0.381052
C	-0.857675	3.025598	1.930642
H	-1.146469	3.718007	2.729371
H	-1.707229	2.950297	1.241365
H	-0.679515	2.044450	2.381280
C	1.590515	3.680824	2.171826
H	1.318959	4.307940	3.027527
H	1.872165	2.698282	2.561402
H	2.464061	4.139264	1.696298

25M

B3LYP SCF energy: -1265.63748708 a.u.
B3LYP enthalpy: -1265.096383 a.u.
B3LYP free energy: -1265.195211 a.u.
B3LYP free energy after quasi-harmonic correction: -1265.185399 a.u.
M06 SCF energy in solution: -1265.16209559 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.624548	-2.683850	-2.060187
O	1.037742	-3.532932	-1.348027
O	1.796489	-1.474407	-1.624320
C	2.171452	-3.033701	-3.425917
H	3.258611	-3.164764	-3.357725
H	1.728076	-3.965821	-3.783615
H	1.977707	-2.225232	-4.138250
Pd	0.878565	-1.801990	0.233218
C	-1.018289	-1.900252	2.525710
O	-1.596619	-0.858979	2.174489
O	0.024928	-2.430483	1.963977
C	-1.535272	-2.710971	3.713092
H	-2.151714	-3.536707	3.336079
H	-0.709482	-3.149493	4.281349

H	-2.154512	-2.082936	4.359023
C	-3.593430	1.353447	-2.179176
C	-3.034411	0.712038	-1.064162
C	-3.872646	0.390602	0.017477
C	-5.232353	0.709964	-0.021213
C	-5.779390	1.352474	-1.137825
C	-4.955196	1.672581	-2.219848
H	-2.959631	1.595386	-3.031453
H	-3.448646	-0.114623	0.882785
H	-5.868534	0.449548	0.821646
H	-6.839038	1.594966	-1.166351
H	-5.370455	2.163462	-3.097185
C	-1.555589	0.385677	-1.010101
H	-1.405732	-0.636617	-0.646240
H	-1.128297	0.436837	-2.020763
C	-0.792907	1.345803	-0.071249
H	-1.217444	1.247676	0.928931
H	-0.987806	2.372162	-0.420594
C	0.726087	1.069875	-0.044581
H	1.021132	0.751914	-1.040947
C	1.219307	0.053936	0.960331
H	0.752776	0.165512	1.939812
H	2.313080	0.064662	1.048363
N	1.517457	2.472453	0.058985
H	0.929397	3.109469	-0.489294
C	2.861024	2.424923	-0.693614
H	3.436374	1.639654	-0.197987
C	1.614487	3.154854	1.440181
H	1.957865	4.160771	1.185020
C	2.650996	2.042189	-2.168444
H	3.584334	2.229568	-2.709007
H	2.403805	0.988414	-2.310985
H	1.874691	2.661393	-2.638314
C	3.610995	3.762659	-0.608942
H	4.523547	3.680670	-1.207318
H	3.017354	4.583422	-1.033100
H	3.915833	4.038731	0.402702
C	0.249133	3.308306	2.114868
H	0.383551	3.962861	2.983351
H	-0.492720	3.778240	1.461407
H	-0.150833	2.357124	2.471070
C	2.638187	2.527825	2.392646
H	2.809926	3.243147	3.205349
H	2.273989	1.599244	2.833657
H	3.605891	2.329848	1.924406

26

B3LYP SCF energy: -1265.69154294 a.u.
B3LYP enthalpy: -1265.152607 a.u.
B3LYP free energy: -1265.253549 a.u.
B3LYP free energy after quasi-harmonic correction: -1265.242993 a.u.
M06 SCF energy in solution: -1265.19125180 a.u.

Cartesian coordinates

ATOM	X	Y	Z

C	-2.634358	2.659361	0.353682
O	-3.032637	2.114992	1.395718
O	-1.883452	2.110869	-0.557799
C	-3.007963	4.101597	0.037694
H	-3.776379	4.450092	0.730954
H	-2.120438	4.738214	0.135909
H	-3.361049	4.189746	-0.994725
Pd	-0.952083	0.279117	-0.513332
C	0.199889	-2.271957	-1.433025
O	-0.397846	-2.151273	-2.503727
O	0.149874	-1.425531	-0.432282
C	1.065065	-3.494331	-1.144235
H	1.842016	-3.281864	-0.405244
H	0.423999	-4.291454	-0.746856
H	1.511266	-3.855934	-2.074333
C	5.106080	1.546235	0.327743
C	4.062690	0.616875	0.457154
C	4.390789	-0.714036	0.756912
C	5.722224	-1.107778	0.918519
C	6.752091	-0.171956	0.783798
C	6.439348	1.158349	0.488140
H	4.872355	2.586334	0.106277
H	3.593337	-1.445905	0.869561
H	5.954290	-2.143578	1.154348
H	7.788001	-0.475128	0.912667
H	7.232280	1.895622	0.388138
C	2.619950	1.030354	0.252723
H	1.964862	0.394145	0.856425
H	2.477654	2.062495	0.601146
C	2.174874	0.932187	-1.222332
H	2.262204	-0.099706	-1.576559
H	2.866498	1.532098	-1.835931
C	0.793609	1.470562	-1.491030
H	0.567852	2.444743	-1.056996
C	-0.068083	0.981473	-2.448061
H	0.163360	0.088729	-3.021926
H	-0.904912	1.585512	-2.787415
N	-2.325325	-0.561192	0.926307
H	-2.712811	0.335728	1.269515
C	-1.633756	-1.218336	2.087877
H	-1.044080	-2.042244	1.677711
C	-3.471602	-1.330555	0.326582
H	-4.188624	-1.493660	1.142526
C	-0.680964	-0.209831	2.739700
H	-0.125286	-0.695515	3.549605
H	0.046356	0.177004	2.019622
H	-1.231098	0.640151	3.159707
C	-2.617719	-1.759489	3.139430
H	-2.050331	-2.139910	3.996516
H	-3.282341	-0.966438	3.504855
H	-3.233022	-2.583430	2.765930
C	-4.181098	-0.485294	-0.736031
H	-5.073850	-1.018510	-1.082744
H	-4.498420	0.481996	-0.334240
H	-3.534547	-0.309673	-1.603020
C	-3.054967	-2.690377	-0.236745
H	-3.953380	-3.233508	-0.552884

H	-2.406178	-2.576271	-1.109842
H	-2.540579	-3.311660	0.504180

26b

B3LYP SCF energy: -1169.86328080 a.u.
B3LYP enthalpy: -1169.309519 a.u.
B3LYP free energy: -1169.401704 a.u.
B3LYP free energy after quasi-harmonic correction: -1169.396295 a.u.
M06 SCF energy in solution: -1169.42902701 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.341751	-3.001281	-0.350233
O	-1.531152	-2.925247	-0.703078
O	0.407942	-2.016744	0.045178
C	0.380461	-4.343642	-0.367776
H	-0.341338	-5.158160	-0.460408
H	1.061598	-4.375727	-1.227189
H	0.984517	-4.471633	0.535914
Pd	-0.001460	-0.000289	0.032960
C	0.340950	2.990837	-0.413398
O	1.525873	2.902365	-0.779290
O	-0.411553	2.015893	-0.000822
C	-0.351027	4.348925	-0.386035
H	-1.387941	4.270928	-0.726389
H	-0.369096	4.720642	0.646115
H	0.199743	5.061756	-1.004050
N	-2.121626	-0.289160	0.036875
H	-2.131328	-1.281623	-0.259322
C	-2.836425	0.493127	-1.030957
H	-2.687657	1.549415	-0.794935
C	-2.755254	-0.232730	1.399934
H	-3.786798	-0.589427	1.279169
C	-2.195933	0.200090	-2.392807
H	-2.713136	0.769522	-3.173617
H	-1.141371	0.490045	-2.407722
H	-2.265915	-0.865381	-2.641766
C	-4.343095	0.183318	-1.083612
H	-4.787968	0.709576	-1.935923
H	-4.521590	-0.890436	-1.224063
H	-4.879723	0.509088	-0.187134
C	-2.057900	-1.207141	2.354999
H	-2.610060	-1.241616	3.301553
H	-2.028117	-2.220368	1.942462
H	-1.031143	-0.891745	2.569890
C	-2.797209	1.183359	1.979214
H	-3.285313	1.154382	2.960665
H	-1.789440	1.590046	2.098691
H	-3.362323	1.876619	1.348025
N	2.119363	0.288629	0.032238
H	2.129721	1.272564	-0.291142
C	2.834657	-0.523499	-1.012675
H	2.679751	-1.572767	-0.750492
C	2.749970	0.267928	1.397398
H	3.784123	0.614057	1.268765

C	2.200257	-0.261672	-2.383776
H	2.713982	-0.856934	-3.147461
H	1.142911	-0.541694	-2.393618
H	2.280407	0.795875	-2.661588
C	4.342934	-0.222511	-1.067717
H	4.787682	-0.771122	-1.905866
H	4.527506	0.846699	-1.233024
H	4.875003	-0.529859	-0.162014
C	2.057506	1.273948	2.323016
H	2.606330	1.329286	3.270572
H	2.038759	2.275884	1.882970
H	1.027151	0.973791	2.542165
C	2.781101	-1.131292	2.016901
H	3.268036	-1.078484	2.997919
H	1.770019	-1.526727	2.146111
H	3.341663	-1.846193	1.406013

27A-TS

B3LYP SCF energy: -1558.10152718 a.u.
B3LYP enthalpy: -1557.343075 a.u.
B3LYP free energy: -1557.464762 a.u.
B3LYP free energy after quasi-harmonic correction: -1557.452307 a.u.
M06 SCF energy in solution: -1557.46677989 a.u.
Imaginary frequency: -263.3743 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.721044	1.125240	-2.456789
O	3.599959	0.247499	-2.448651
O	1.718018	1.219023	-1.638177
C	2.768135	2.246823	-3.492069
H	3.594492	2.083827	-4.187378
H	1.823056	2.294136	-4.044644
H	2.902192	3.211817	-2.988585
Pd	1.148443	-0.140593	-0.176657
C	-0.026059	-1.202601	2.369282
O	-0.205078	-0.061433	2.825489
O	0.458730	-1.498289	1.202366
C	-0.397876	-2.418622	3.216342
H	-0.149062	-3.358972	2.718538
H	0.125670	-2.359975	4.177049
H	-1.472419	-2.392828	3.432208
C	-4.289987	-2.251404	-1.965461
C	-3.181758	-2.404736	-1.118257
C	-3.256826	-3.365396	-0.096948
C	-4.404424	-4.143757	0.076664
C	-5.502930	-3.976468	-0.772888
C	-5.441250	-3.027102	-1.797136
H	-4.246348	-1.522241	-2.773055
H	-2.402675	-3.505360	0.562475
H	-4.438782	-4.885241	0.871512
H	-6.394500	-4.584778	-0.642322
H	-6.285480	-2.895304	-2.470054
C	-1.949325	-1.539619	-1.276532
H	-1.050861	-2.118364	-1.036935

H	-1.854408	-1.220946	-2.323686
C	-1.975357	-0.288758	-0.372716
H	-2.029790	-0.595258	0.676643
H	-2.918289	0.250817	-0.580540
C	-0.794438	0.644380	-0.604694
H	-0.683664	0.912017	-1.658157
C	-0.563675	1.733606	0.312462
H	-0.613190	1.492258	1.366990
H	0.212788	2.442846	0.043257
N	-1.997799	3.055373	0.319828
H	-2.722960	2.556606	-0.199421
C	-1.605570	4.264764	-0.479033
H	-0.669937	4.626028	-0.036288
C	-2.529347	3.314184	1.703249
H	-3.340996	4.045758	1.601072
C	-1.332723	3.859654	-1.933035
H	-1.043270	4.745976	-2.507830
H	-0.528429	3.126724	-2.019821
H	-2.235506	3.443849	-2.401094
C	-2.645537	5.396288	-0.427291
H	-2.323912	6.208002	-1.089104
H	-3.626664	5.051137	-0.779185
H	-2.767891	5.821562	0.573066
C	-3.140879	2.037089	2.291080
H	-3.669198	2.292442	3.216589
H	-3.874884	1.591907	1.607543
H	-2.386375	1.283405	2.534706
C	-1.454214	3.909304	2.618491
H	-1.900901	4.130826	3.593924
H	-0.630787	3.208103	2.783843
H	-1.042690	4.845865	2.226371
N	3.187442	-0.979469	0.087369
H	3.563405	-0.654868	-0.817067
C	3.196449	-2.477898	0.062729
H	2.596877	-2.810662	0.914953
C	4.007835	-0.343778	1.165947
H	5.033399	-0.728827	1.071882
C	2.513080	-2.959649	-1.223098
H	2.464218	-4.054805	-1.231722
H	1.491181	-2.574180	-1.297405
H	3.066418	-2.631090	-2.110953
C	4.607417	-3.084034	0.164626
H	4.543028	-4.172432	0.048897
H	5.260711	-2.701419	-0.630351
H	5.087695	-2.888658	1.128947
C	4.078129	1.171861	0.949991
H	4.749587	1.616472	1.694467
H	4.463111	1.415618	-0.045704
H	3.089585	1.631553	1.059188
C	3.496649	-0.675563	2.570344
H	4.177412	-0.243798	3.314193
H	2.499532	-0.256180	2.736284
H	3.451230	-1.754693	2.752783

27M-TS

B3LYP SCF energy: -1558.08592221 a.u.
B3LYP enthalpy: -1557.327371 a.u.
B3LYP free energy: -1557.447891 a.u.
B3LYP free energy after quasi-harmonic correction: -1557.436240 a.u.
M06 SCF energy in solution: -1557.45722863 a.u.
Imaginary frequency: -214.2421 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.055065	1.773706	-2.337991
O	3.048233	1.087793	-2.631600
O	1.337411	1.677209	-1.261340
C	1.583566	2.863770	-3.300802
H	2.217504	2.878563	-4.189917
H	0.543370	2.686011	-3.597714
H	1.622764	3.843222	-2.809814
Pd	1.511880	0.331358	0.333973
C	0.893674	-1.952017	2.105998
O	0.147917	-2.431570	1.237588
O	1.554116	-0.837906	2.018226
C	1.129506	-2.703369	3.415253
H	0.242325	-3.286809	3.677006
H	1.963306	-3.403564	3.276843
H	1.393043	-2.021484	4.228627
C	-4.738314	-2.070212	-1.661588
C	-3.452496	-1.958742	-1.110296
C	-2.862522	-3.106833	-0.553461
C	-3.545417	-4.326745	-0.556983
C	-4.825096	-4.425551	-1.112083
C	-5.421620	-3.290071	-1.666449
H	-5.211077	-1.191685	-2.098485
H	-1.871463	-3.056118	-0.109720
H	-3.071282	-5.202890	-0.121388
H	-5.351850	-5.376636	-1.111202
H	-6.416957	-3.350624	-2.100436
C	-2.718363	-0.628227	-1.147762
H	-1.997490	-0.632540	-1.979072
H	-3.448212	0.158207	-1.389950
C	-1.950694	-0.297912	0.143916
H	-1.142495	-1.025398	0.280721
H	-2.583149	-0.432740	1.025122
C	-1.266042	1.055610	0.152253
H	-1.021011	1.399340	-0.849037
C	-0.194311	1.293021	1.112339
H	-0.366536	0.885826	2.109091
H	0.162981	2.324819	1.154734
N	-2.664725	2.361861	0.347661
H	-3.163614	2.228057	-0.535058
C	-2.063257	3.753103	0.294849
H	-1.402712	3.819887	1.164921
C	-3.680427	2.175180	1.460096
H	-4.148736	3.151296	1.598294
C	-1.232445	3.931328	-0.982632
H	-0.871824	4.964379	-1.028419
H	-0.359889	3.277913	-1.033087
H	-1.850706	3.765051	-1.876704
C	-3.112463	4.879681	0.375497

H	-2.615141	5.831757	0.163864
H	-3.901908	4.749067	-0.376649
H	-3.581850	4.982966	1.357389
C	-4.820677	1.235153	1.047790
H	-5.596922	1.271448	1.820326
H	-5.285109	1.563122	0.108731
H	-4.516405	0.193838	0.934296
C	-3.039870	1.798812	2.799598
H	-3.805639	1.866261	3.580924
H	-2.643026	0.781450	2.807250
H	-2.227668	2.481094	3.069205
N	3.426345	-0.555304	-0.366246
H	3.454774	-0.063478	-1.273665
C	3.355727	-2.021702	-0.662975
H	3.177014	-2.532922	0.288686
C	4.639254	-0.110441	0.394178
H	5.520827	-0.376786	-0.207616
C	2.164656	-2.295702	-1.588337
H	2.096051	-3.369988	-1.796025
H	1.227145	-1.986567	-1.118244
H	2.281130	-1.767549	-2.542611
C	4.648473	-2.572800	-1.292509
H	4.506892	-3.629013	-1.550389
H	4.894251	-2.032102	-2.215724
H	5.510774	-2.514044	-0.620504
C	4.638337	1.416773	0.530157
H	5.582844	1.744898	0.981597
H	4.539519	1.902237	-0.446340
H	3.814993	1.756208	1.169689
C	4.765839	-0.788712	1.761497
H	5.653698	-0.401159	2.275963
H	3.882647	-0.593288	2.375787
H	4.885069	-1.874715	1.675734

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B3LYP SCF energy: -1558.10646794 a.u.
B3LYP enthalpy: -1557.345491 a.u.
B3LYP free energy: -1557.467362 a.u.
B3LYP free energy after quasi-harmonic correction: -1557.454359 a.u.
M06 SCF energy in solution: -1557.48330839 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.654607	1.249566	-2.447747
O	3.540476	0.378973	-2.488623
O	1.666742	1.307625	-1.610608
C	2.678543	2.406089	-3.447961
H	3.511486	2.287732	-4.144651
H	1.735786	2.443895	-4.006219
H	2.783512	3.359103	-2.915200
Pd	1.141560	-0.120251	-0.174838
C	0.018963	-1.221558	2.391210
O	-0.235708	-0.087236	2.839034
O	0.495294	-1.499358	1.221683
C	-0.211615	-2.445210	3.277770

H	-0.232589	-3.371305	2.697274
H	0.608430	-2.509608	4.004229
H	-1.141460	-2.329515	3.843493
C	-4.246134	-2.181072	-2.008442
C	-3.160355	-2.335584	-1.132805
C	-3.259577	-3.304752	-0.121127
C	-4.408098	-4.088832	0.015235
C	-5.484170	-3.919906	-0.862645
C	-5.398509	-2.962798	-1.877717
H	-4.182985	-1.446999	-2.810398
H	-2.422700	-3.447338	0.559507
H	-4.460487	-4.836943	0.802901
H	-6.375995	-4.533441	-0.761228
H	-6.224223	-2.829957	-2.573154
C	-1.927140	-1.465697	-1.251643
H	-1.027467	-2.053408	-1.040494
H	-1.832494	-1.098171	-2.282583
C	-1.946635	-0.260068	-0.287903
H	-1.995337	-0.622504	0.743853
H	-2.905784	0.271015	-0.464782
C	-0.754544	0.678673	-0.484379
H	-0.705244	0.988134	-1.533634
C	-0.705960	1.868450	0.444773
H	-0.648147	1.532785	1.477751
H	0.142347	2.517777	0.224854
N	-1.971421	2.834964	0.373199
H	-2.683301	2.294635	-0.129961
C	-1.696721	4.081216	-0.469440
H	-0.860934	4.578475	0.031478
C	-2.575327	3.122756	1.754562
H	-3.428929	3.774854	1.554491
C	-1.264252	3.686956	-1.885957
H	-1.081664	4.603466	-2.457419
H	-0.348927	3.092498	-1.902807
H	-2.054607	3.126881	-2.402096
C	-2.905407	5.024512	-0.516729
H	-2.692863	5.826605	-1.230799
H	-3.807165	4.506234	-0.868318
H	-3.126826	5.498465	0.443228
C	-3.112676	1.836199	2.388633
H	-3.677027	2.111967	3.286576
H	-3.802754	1.312376	1.716613
H	-2.319236	1.144443	2.687287
C	-1.584578	3.853415	2.661730
H	-2.089748	4.087164	3.604918
H	-0.716568	3.231459	2.898556
H	-1.236282	4.799828	2.234601
N	3.231292	-0.932497	0.041003
H	3.575516	-0.583205	-0.865566
C	3.267027	-2.427523	-0.011286
H	2.691762	-2.787619	0.847356
C	4.062958	-0.303367	1.110234
H	5.094997	-0.667892	0.999650
C	2.562133	-2.898302	-1.289731
H	2.529653	-3.993983	-1.317715
H	1.534353	-2.524310	-1.333243
H	3.090539	-2.544771	-2.183393

C	4.688340	-3.016539	0.048009
H	4.637518	-4.104202	-0.082830
H	5.316941	-2.612078	-0.756316
H	5.190220	-2.828522	1.003037
C	4.103927	1.216771	0.916690
H	4.776103	1.664015	1.659355
H	4.471246	1.481111	-0.080540
H	3.107339	1.654747	1.042158
C	3.577365	-0.662246	2.517823
H	4.257152	-0.225734	3.260087
H	2.572976	-0.266346	2.697909
H	3.555599	-1.744446	2.686489

28M

B3LYP SCF energy: -1558.08866425 a.u.
B3LYP enthalpy: -1557.327885 a.u.
B3LYP free energy: -1557.448184 a.u.
B3LYP free energy after quasi-harmonic correction: -1557.436624 a.u.
M06 SCF energy in solution: -1557.46902211 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.941868	1.701380	-2.412299
O	2.934816	1.019931	-2.717426
O	1.267648	1.641993	-1.306856
C	1.411515	2.737084	-3.406570
H	2.036252	2.753565	-4.302278
H	0.380045	2.494653	-3.689642
H	1.402496	3.733711	-2.949857
Pd	1.510163	0.352297	0.333507
C	0.893510	-1.872824	2.185876
O	0.070614	-2.329108	1.375296
O	1.600640	-0.795701	2.040210
C	1.174771	-2.618372	3.491187
H	0.296771	-3.197250	3.791165
H	2.002614	-3.320304	3.327745
H	1.471655	-1.931437	4.289127
C	-4.752347	-2.016216	-1.743874
C	-3.501260	-1.875591	-1.122821
C	-2.918174	-3.008277	-0.529327
C	-3.573285	-4.243383	-0.567803
C	-4.816683	-4.371863	-1.193497
C	-5.406841	-3.250570	-1.783513
H	-5.219520	-1.148909	-2.208815
H	-1.954925	-2.936310	-0.030887
H	-3.104852	-5.107515	-0.103130
H	-5.321335	-5.334489	-1.219504
H	-6.374882	-3.334066	-2.271992
C	-2.797100	-0.527418	-1.129899
H	-2.119934	-0.473847	-1.995632
H	-3.562462	0.246692	-1.307354
C	-1.975761	-0.236882	0.137910
H	-1.129583	-0.927227	0.195553
H	-2.562848	-0.457282	1.033995
C	-1.351280	1.160900	0.200374

H	-1.048506	1.450234	-0.807750
C	-0.165799	1.285887	1.123829
H	-0.329301	0.821505	2.095720
H	0.148027	2.327607	1.265496
N	-2.534812	2.255576	0.457155
H	-3.166001	2.065175	-0.327212
C	-2.092695	3.716847	0.263513
H	-1.630637	3.994862	1.215831
C	-3.418124	2.120408	1.721674
H	-3.708650	3.146023	1.949917
C	-1.082119	3.894662	-0.871114
H	-0.837511	4.961120	-0.933658
H	-0.153654	3.338131	-0.739219
H	-1.517580	3.604753	-1.836241
C	-3.315094	4.607462	-0.020447
H	-2.977837	5.644482	-0.115372
H	-3.780893	4.330006	-0.975224
H	-4.085410	4.590971	0.754859
C	-4.705811	1.353280	1.399035
H	-5.369205	1.396936	2.269574
H	-5.245183	1.806777	0.557425
H	-4.527769	0.300404	1.168876
C	-2.706337	1.598549	2.970972
H	-3.405934	1.712345	3.807759
H	-2.432071	0.544834	2.905531
H	-1.809512	2.176629	3.205116
N	3.417965	-0.571240	-0.417829
H	3.414345	-0.106114	-1.338546
C	3.335772	-2.043786	-0.666965
H	3.191035	-2.525073	0.306173
C	4.654372	-0.108371	0.288546
H	5.521537	-0.399272	-0.323587
C	2.109633	-2.343084	-1.537544
H	2.030648	-3.422926	-1.711033
H	1.191152	-2.014653	-1.043145
H	2.190685	-1.843515	-2.510907
C	4.602192	-2.621597	-1.325861
H	4.448906	-3.684982	-1.545607
H	4.816396	-2.110333	-2.273560
H	5.488696	-2.545044	-0.687760
C	4.660763	1.423049	0.368941
H	5.611172	1.765600	0.797012
H	4.550344	1.872116	-0.623809
H	3.843686	1.786788	1.003185
C	4.813174	-0.737490	1.676222
H	5.710150	-0.329760	2.158743
H	3.941528	-0.525670	2.301724
H	4.935395	-1.825570	1.625507

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B3LYP SCF energy: -1265.67121500 a.u.
B3LYP enthalpy: -1265.132508 a.u.
B3LYP free energy: -1265.232773 a.u.
B3LYP free energy after quasi-harmonic correction: -1265.222830 a.u.
M06 SCF energy in solution: -1265.18499444 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.738879	0.368947	2.517599
O	-0.234352	-0.375778	2.363268
O	1.570684	0.727006	1.572692
C	1.070948	0.969626	3.878561
H	0.635447	0.359516	4.673842
H	2.151323	1.069822	4.018855
H	0.635022	1.974895	3.933667
Pd	0.945146	0.296427	-0.347091
C	0.162034	2.980674	-0.467035
O	1.277431	3.119778	-0.976440
O	-0.375408	1.823222	-0.156340
C	-0.726864	4.167756	-0.125801
H	-1.780947	3.943111	-0.314089
H	-0.621574	4.393040	0.942499
H	-0.413487	5.042760	-0.700186
C	-4.863765	-1.647603	-0.768204
C	-3.875483	-0.896969	-0.113111
C	-4.282001	0.126750	0.756393
C	-5.638409	0.395752	0.961124
C	-6.613381	-0.356816	0.298963
C	-6.221477	-1.382414	-0.566880
H	-4.568106	-2.454565	-1.437311
H	-3.526155	0.707146	1.280742
H	-5.933326	1.189740	1.643133
H	-7.668530	-0.150544	0.460708
H	-6.971540	-1.979438	-1.080444
C	-2.403321	-1.160196	-0.352761
H	-1.823430	-0.858436	0.525692
H	-2.241233	-2.238279	-0.496154
C	-1.873188	-0.401424	-1.589567
H	-2.042150	0.672271	-1.471322
H	-2.442700	-0.722273	-2.477764
C	-0.421343	-0.659039	-1.903238
H	-0.125166	-1.709548	-1.883393
C	0.435721	0.246885	-2.502018
H	0.113885	1.258352	-2.731125
H	1.331588	-0.090015	-3.014162
N	2.491202	-1.206500	-0.502900
H	2.281975	-1.697354	-1.376785
C	2.433949	-2.262599	0.580071
H	2.547396	-1.721632	1.521682
C	3.870392	-0.600057	-0.714634
H	4.532408	-1.439788	-0.962730
C	1.061523	-2.938615	0.568580
H	1.026382	-3.704088	1.351282
H	0.263355	-2.222558	0.775324
H	0.873868	-3.442596	-0.390716
C	3.549279	-3.312412	0.447280
H	3.397157	-4.090198	1.203369
H	3.523491	-3.801445	-0.536505
H	4.551012	-2.901494	0.601595
C	3.867362	0.348226	-1.917212
H	4.891577	0.695269	-2.094342
H	3.537591	-0.157610	-2.833811

H	3.235441	1.226305	-1.746778
C	4.413619	0.094797	0.535226
H	5.420334	0.466563	0.312206
H	3.784614	0.935645	0.834268
H	4.495653	-0.584142	1.389790

30A-TS

B3LYP SCF energy: -1558.07399449 a.u.
B3LYP enthalpy: -1557.315895 a.u.
B3LYP free energy: -1557.437767 a.u.
B3LYP free energy after quasi-harmonic correction: -1557.425012 a.u.
M06 SCF energy in solution: -1557.45586295 a.u.
Imaginary frequency: -268.8281 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	3.044123	-2.385176	1.001968
O	2.570660	-2.998251	0.033789
O	2.826230	-1.135130	1.284438
C	3.959972	-3.096977	1.996626
H	4.692257	-2.410269	2.432349
H	3.344902	-3.491644	2.815387
H	4.464025	-3.938210	1.512725
Pd	1.219973	-0.211087	0.295927
C	-0.261861	-0.486550	2.867822
O	-0.280687	0.741053	3.070123
O	0.085201	-1.080912	1.769726
C	-0.673967	-1.450320	3.978002
H	-1.073115	-2.383819	3.571869
H	0.217868	-1.695602	4.568327
H	-1.401677	-0.976362	4.642797
C	-3.740544	-2.583232	-2.167319
C	-2.799988	-2.577344	-1.126007
C	-3.063201	-3.358251	0.010874
C	-4.233008	-4.116680	0.106134
C	-5.164365	-4.109139	-0.937605
C	-4.913158	-3.340043	-2.077568
H	-3.547120	-1.996443	-3.064311
H	-2.336854	-3.374102	0.820716
H	-4.413635	-4.720253	0.992574
H	-6.072013	-4.703483	-0.866575
H	-5.624842	-3.335466	-2.900127
C	-1.548568	-1.728380	-1.202592
H	-0.717906	-2.239131	-0.704193
H	-1.260747	-1.592202	-2.253767
C	-1.742443	-0.347912	-0.542056
H	-2.004356	-0.496167	0.509346
H	-2.620112	0.126445	-1.020093
C	-0.540814	0.591911	-0.646101
H	-0.283681	0.780777	-1.696482
C	-0.558723	1.778424	0.180618
H	-0.726159	1.623880	1.240221
H	0.181348	2.545061	-0.023292
N	-2.083175	2.943430	-0.105720
H	-2.707137	2.336793	-0.641612

C	-1.715003	4.113240	-0.971323
H	-0.846402	4.579692	-0.491496
C	-2.783173	3.275293	1.188447
H	-3.619382	3.936969	0.931474
C	-1.301761	3.616203	-2.362112
H	-0.992530	4.466093	-2.979532
H	-0.471186	2.908725	-2.321971
H	-2.141763	3.124970	-2.871064
C	-2.827551	5.167130	-1.100395
H	-2.511861	5.932297	-1.818204
H	-3.757316	4.722033	-1.477699
H	-3.045146	5.676441	-0.157659
C	-3.384224	2.012420	1.815539
H	-4.040107	2.309094	2.641655
H	-3.995289	1.453822	1.095438
H	-2.617879	1.348902	2.223579
C	-1.857471	4.012356	2.162042
H	-2.438164	4.310750	3.041877
H	-1.041878	3.371445	2.510365
H	-1.433453	4.924802	1.727195
N	2.521932	0.548835	-1.268737
H	1.873696	1.081368	-1.854377
C	3.057835	-0.551441	-2.162357
H	3.648414	-1.202606	-1.515595
C	3.570205	1.551136	-0.832568
H	3.986637	1.984369	-1.752345
C	1.894611	-1.374639	-2.714427
H	2.283830	-2.157975	-3.373953
H	1.353089	-1.865229	-1.904631
H	1.205402	-0.752177	-3.303550
C	3.929758	-0.018396	-3.311690
H	4.209148	-0.854154	-3.962546
H	3.381393	0.708686	-3.927770
H	4.857664	0.450586	-2.971598
C	2.924420	2.696167	-0.050333
H	3.687760	3.445305	0.189616
H	2.149786	3.201387	-0.642330
H	2.480651	2.342066	0.885998
C	4.712134	0.916935	-0.036682
H	5.431069	1.701191	0.229227
H	4.340249	0.440026	0.872869
H	5.251783	0.161001	-0.616508

30M-TS

B3LYP SCF energy: -1558.05542798 a.u.
B3LYP enthalpy: -1557.297233 a.u.
B3LYP free energy: -1557.417156 a.u.
B3LYP free energy after quasi-harmonic correction: -1557.405744 a.u.
M06 SCF energy in solution: -1557.44890064 a.u.
Imaginary frequency: -214.2322 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	3.158273	-2.551804	-0.534607
O	2.828245	-2.299463	-1.703035

O	2.973609	-1.789409	0.499957
C	3.845911	-3.877035	-0.203056
H	4.367482	-4.264756	-1.082783
H	4.537852	-3.771072	0.638238
H	3.074587	-4.602215	0.085973
Pd	1.593425	-0.209742	0.606048
C	0.115973	-2.476445	1.774937
O	-0.277601	-2.828991	0.653626
O	0.689955	-1.345323	2.057575
C	-0.050581	-3.393114	2.984076
H	0.880379	-3.957365	3.121179
H	-0.226004	-2.818076	3.898563
H	-0.864930	-4.102845	2.815086
C	-4.989552	-1.139586	-1.570254
C	-3.652360	-1.353303	-1.203206
C	-3.256186	-2.648728	-0.827826
C	-4.183606	-3.694433	-0.823268
C	-5.514436	-3.470792	-1.191893
C	-5.916712	-2.186865	-1.567448
H	-5.311435	-0.143219	-1.871000
H	-2.228903	-2.845036	-0.528823
H	-3.859070	-4.689822	-0.530341
H	-6.229930	-4.289451	-1.187259
H	-6.947394	-1.997943	-1.858653
C	-2.656980	-0.205797	-1.235134
H	-1.954085	-0.352297	-2.068006
H	-3.215863	0.712422	-1.475042
C	-1.832118	-0.052705	0.060599
H	-1.161157	-0.915887	0.142510
H	-2.473930	-0.110629	0.944284
C	-0.941624	1.179008	0.108323
H	-0.652839	1.487921	-0.894331
C	0.148213	1.269358	1.081368
H	-0.124119	0.973762	2.092447
H	0.635529	2.250827	1.090889
N	-2.175107	2.616978	0.281864
H	-2.764683	2.398899	-0.523883
C	-1.570517	3.978305	0.010682
H	-1.116407	4.288418	0.958461
C	-3.096061	2.650213	1.500077
H	-3.294586	3.710123	1.682920
C	-0.488914	3.954730	-1.075615
H	-0.165113	4.982840	-1.269670
H	0.392859	3.383771	-0.784711
H	-0.873331	3.549365	-2.019580
C	-2.651427	4.993278	-0.409324
H	-2.198732	5.985383	-0.511540
H	-3.072572	4.722042	-1.386382
H	-3.476007	5.085706	0.302158
C	-4.444524	1.994297	1.180947
H	-5.117817	2.120115	2.035816
H	-4.924596	2.467209	0.314441
H	-4.358274	0.922952	0.982144
C	-2.465665	2.113388	2.788101
H	-3.154631	2.331494	3.612437
H	-2.299366	1.034723	2.768241
H	-1.514226	2.603791	3.011562

N	2.712837	1.148861	-0.660081
H	2.109021	1.973989	-0.665598
C	2.839590	0.728386	-2.106657
H	3.381380	-0.218027	-2.101007
C	4.002860	1.625163	-0.030751
H	4.360440	2.466938	-0.640261
C	1.451435	0.434721	-2.674456
H	1.550092	0.049535	-3.694864
H	0.949160	-0.333172	-2.080876
H	0.831539	1.343634	-2.718798
C	3.566413	1.770872	-2.971028
H	3.535740	1.450611	-4.018482
H	3.080378	2.756331	-2.913555
H	4.620052	1.894293	-2.702167
C	3.732558	2.166287	1.376486
H	4.654415	2.599677	1.782018
H	2.970928	2.957161	1.369539
H	3.393917	1.371599	2.049456
C	5.082305	0.542366	-0.015073
H	5.986028	0.949894	0.453881
H	4.746904	-0.332679	0.547480
H	5.352379	0.213211	-1.023740

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B3LYP SCF energy: -1558.07851293 a.u.
B3LYP enthalpy: -1557.317663 a.u.
B3LYP free energy: -1557.438799 a.u.
B3LYP free energy after quasi-harmonic correction: -1557.426094 a.u.
M06 SCF energy in solution: -1557.47176746 a.u.
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Cartesian coordinates

ATOM	X	Y	Z
C	3.193616	-2.204655	1.021326
O	2.740418	-2.871805	0.076481
O	2.921043	-0.961604	1.268856
C	4.152028	-2.850422	2.023542
H	4.852040	-2.118746	2.439256
H	3.563659	-3.258725	2.855400
H	4.694957	-3.675918	1.554163
Pd	1.235545	-0.120903	0.293791
C	-0.171092	-0.353150	2.933100
O	-0.287150	0.881600	3.079824
O	0.175502	-0.969007	1.853666
C	-0.453340	-1.283342	4.111250
H	-0.809217	-2.260379	3.772252
H	0.485685	-1.441156	4.656609
H	-1.172785	-0.827539	4.797783
C	-3.546848	-2.714564	-2.129533
C	-2.623439	-2.639649	-1.075628
C	-2.854034	-3.424832	0.065772
C	-3.975849	-4.253330	0.152624
C	-4.891076	-4.313999	-0.903844
C	-4.671548	-3.542137	-2.048388
H	-3.375840	-2.127432	-3.030962

H	-2.138431	-3.389435	0.884552
H	-4.130682	-4.859521	1.042182
H	-5.760506	-4.963672	-0.839248
H	-5.369360	-3.590844	-2.881409
C	-1.423994	-1.718484	-1.143908
H	-0.563341	-2.184676	-0.653418
H	-1.146374	-1.551389	-2.192989
C	-1.689991	-0.360267	-0.462704
H	-1.935206	-0.544731	0.587907
H	-2.613244	0.044422	-0.931971
C	-0.530632	0.645289	-0.555989
H	-0.334959	0.847304	-1.620676
C	-0.797703	1.930257	0.206149
H	-0.795517	1.729927	1.276931
H	-0.058394	2.705339	0.004746
N	-2.194783	2.645229	-0.084985
H	-2.770963	1.917777	-0.522331
C	-2.085700	3.784696	-1.095712
H	-1.391444	4.498431	-0.642475
C	-2.936737	3.029997	1.206853
H	-3.846036	3.527548	0.863517
C	-1.493209	3.281991	-2.416269
H	-1.438154	4.121427	-3.117118
H	-0.487118	2.879556	-2.297115
H	-2.122143	2.507105	-2.871138
C	-3.435530	4.470646	-1.348598
H	-3.321090	5.169749	-2.183216
H	-4.208601	3.745377	-1.633784
H	-3.795935	5.047557	-0.493454
C	-3.359040	1.779725	1.982537
H	-4.051671	2.091753	2.772380
H	-3.891234	1.064271	1.344201
H	-2.510414	1.281312	2.458917
C	-2.117924	3.998144	2.061732
H	-2.732120	4.302694	2.915960
H	-1.216981	3.522617	2.459196
H	-1.837852	4.909326	1.521343
N	2.463496	0.645662	-1.330039
H	1.773475	1.106300	-1.928737
C	3.066864	-0.449468	-2.182433
H	3.693738	-1.041124	-1.513156
C	3.441258	1.731670	-0.940518
H	3.826181	2.161439	-1.876151
C	1.955485	-1.360497	-2.702402
H	2.388599	-2.134335	-3.345725
H	1.454883	-1.862463	-1.873718
H	1.222998	-0.797662	-3.299988
C	3.905291	0.092095	-3.352897
H	4.240560	-0.749151	-3.969578
H	3.311319	0.755885	-3.997860
H	4.799514	0.635059	-3.032941
C	2.716749	2.854517	-0.195752
H	3.420060	3.671031	0.005922
H	1.898304	3.270890	-0.798570
H	2.309139	2.500196	0.757051
C	4.624468	1.205061	-0.125801
H	5.279372	2.047251	0.129122

H	4.283845	0.715375	0.789687
H	5.224278	0.482064	-0.688227

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B3LYP SCF energy: -1558.05683349 a.u.
B3LYP enthalpy: -1557.296807 a.u.
B3LYP free energy: -1557.416950 a.u.
B3LYP free energy after quasi-harmonic correction: -1557.405696 a.u.
M06 SCF energy in solution: -1557.45917226 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	3.055385	-2.656159	-0.513803
O	2.815906	-2.373093	-1.699496
O	2.862716	-1.891474	0.513921
C	3.626150	-4.031312	-0.161882
H	4.159972	-4.453870	-1.018055
H	4.282819	-3.979672	0.712411
H	2.790102	-4.697860	0.085576
Pd	1.568465	-0.220282	0.590067
C	-0.028492	-2.422369	1.744291
O	-0.388995	-2.794086	0.617590
O	0.555110	-1.296978	2.024914
C	-0.256546	-3.313069	2.964236
H	0.651452	-3.905695	3.132460
H	-0.434882	-2.718258	3.865535
H	-1.089200	-3.999363	2.786500
C	-5.072195	-0.992652	-1.573402
C	-3.736420	-1.217001	-1.206618
C	-3.352398	-2.512541	-0.819494
C	-4.290953	-3.548500	-0.805280
C	-5.619813	-3.314933	-1.174276
C	-6.009928	-2.030214	-1.560332
H	-5.384573	0.004311	-1.882748
H	-2.327153	-2.717891	-0.518869
H	-3.975661	-4.544274	-0.503808
H	-6.343451	-4.126320	-1.161698
H	-7.039158	-1.833371	-1.851446
C	-2.729546	-0.079735	-1.255509
H	-2.070736	-0.209484	-2.126687
H	-3.294553	0.847700	-1.450118
C	-1.837726	0.036957	0.000590
H	-1.133625	-0.800638	0.005620
H	-2.429909	-0.090821	0.911126
C	-0.985693	1.310344	0.057605
H	-0.659368	1.528150	-0.961857
C	0.201138	1.310649	0.990470
H	-0.071940	1.073906	2.016893
H	0.706361	2.287451	0.983702
N	-2.014528	2.584284	0.268392
H	-2.670304	2.435806	-0.504466
C	-1.390698	3.958902	-0.000785
H	-0.890796	4.231109	0.933923
C	-2.908793	2.630513	1.536385
H	-3.029435	3.696826	1.731287

C	-0.367463	3.946135	-1.140659
H	-0.024086	4.973566	-1.301560
H	0.508620	3.337234	-0.922488
H	-0.811915	3.598034	-2.080787
C	-2.483916	4.985536	-0.345850
H	-2.019980	5.969726	-0.466002
H	-2.963981	4.732986	-1.300360
H	-3.264310	5.088817	0.411837
C	-4.299839	2.067956	1.221848
H	-4.953493	2.243005	2.083010
H	-4.756816	2.572379	0.360676
H	-4.288944	0.993326	1.025677
C	-2.302432	2.037536	2.809018
H	-3.008249	2.247291	3.621613
H	-2.157051	0.957553	2.762347
H	-1.350503	2.506262	3.068175
N	2.787626	1.079357	-0.645354
H	2.230669	1.936511	-0.657774
C	2.917919	0.652862	-2.088163
H	3.402422	-0.324432	-2.072722
C	4.087577	1.481225	0.012068
H	4.510497	2.297944	-0.590214
C	1.525146	0.436553	-2.679652
H	1.618191	0.054638	-3.701933
H	0.975225	-0.307718	-2.097697
H	0.953190	1.376766	-2.724465
C	3.718243	1.651169	-2.939331
H	3.692561	1.330378	-3.986821
H	3.286791	2.662650	-2.893662
H	4.771088	1.716746	-2.647679
C	3.814224	2.043395	1.410705
H	4.747776	2.430430	1.836250
H	3.094039	2.872093	1.382440
H	3.418170	1.270281	2.077370
C	5.099993	0.336310	0.058935
H	6.015114	0.692087	0.547844
H	4.698959	-0.514193	0.616559
H	5.373514	-0.014889	-0.941365

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B3LYP SCF energy: -1433.55847338 a.u.
B3LYP enthalpy: -1433.237617 a.u.
B3LYP free energy: -1433.319438 a.u.
B3LYP free energy after quasi-harmonic correction: -1433.312773 a.u.
M06 SCF energy in solution: -1433.26194539 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-3.533660	-1.866305	-0.105686
O	-3.969457	-1.636436	1.028684
O	-2.490164	-1.331001	-0.669627
C	-4.241881	-2.865311	-1.024959
H	-4.893381	-2.305604	-1.707703
H	-3.523667	-3.421582	-1.635730
H	-4.856409	-3.550960	-0.434445

Pd	-1.523636	0.290782	0.103948
C	0.399842	2.526546	0.288561
O	1.126975	2.043168	-0.586264
O	-0.614275	1.951221	0.865006
C	0.639378	3.946389	0.806509
H	-0.042660	4.623773	0.277534
H	0.419104	4.022525	1.876246
H	1.669006	4.255694	0.604460
C	4.246195	-2.069838	-0.155301
C	3.389000	-0.972978	-0.336868
C	3.961293	0.297575	-0.522730
C	5.349917	0.459456	-0.523024
C	6.193984	-0.641641	-0.338712
C	5.635971	-1.910492	-0.154886
H	3.819042	-3.062736	-0.019785
H	3.301442	1.150210	-0.668880
H	5.774234	1.450245	-0.673236
H	7.274495	-0.513113	-0.343228
H	6.280644	-2.776520	-0.016840
C	1.884322	-1.139813	-0.313142
H	1.418900	-0.418642	-0.991863
H	1.620717	-2.148612	-0.661294
C	1.282117	-0.924868	1.093110
H	1.489017	0.093938	1.436073
H	1.782239	-1.608143	1.800976
C	-0.197188	-1.217493	1.156461
H	-0.510791	-2.125078	0.640504
C	-1.094627	-0.647305	2.042339
H	-0.780326	0.164392	2.695115
H	-2.056562	-1.112402	2.243607
Cl	-2.588848	1.638087	-1.516209

33A-TS

B3LYP SCF energy: -1946.03049192 a.u.
B3LYP enthalpy: -1945.597731 a.u.
B3LYP free energy: -1945.705222 a.u.
B3LYP free energy after quasi-harmonic correction: -1945.690976 a.u.
M06 SCF energy in solution: -1945.68940641 a.u.
Imaginary frequency: -317.7677 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.276182	-2.282666	-2.413497
O	-2.292459	-1.188884	-2.995879
O	-2.159273	-2.514353	-1.147867
C	-2.414181	-3.584753	-3.224941
H	-1.633165	-4.299329	-2.939143
H	-3.383472	-4.047500	-2.998744
H	-2.353992	-3.373155	-4.297437
Pd	-2.167026	-1.091263	0.330567
C	-2.512829	1.249549	2.220059
O	-2.870480	2.070950	1.360094
O	-2.049355	0.060482	2.041698
C	-2.605625	1.623450	3.709895
H	-3.488680	1.130466	4.137130

H	-1.727126	1.264433	4.257766
H	-2.710271	2.707125	3.828469
C	0.572090	3.690849	-2.244213
C	-0.358992	3.190921	-1.318133
C	-0.941301	4.097968	-0.412346
C	-0.596833	5.452680	-0.435441
C	0.334522	5.936679	-1.363118
C	0.918828	5.046605	-2.270363
H	1.027927	3.004214	-2.956370
H	-1.668613	3.717838	0.303222
H	-1.062104	6.135798	0.274044
H	0.599723	6.993104	-1.379538
H	1.643169	5.406723	-3.000308
C	-0.720225	1.723122	-1.271967
H	-1.774961	1.607825	-1.004223
H	-0.589725	1.271405	-2.263473
C	0.118150	0.930955	-0.243190
H	-0.053209	1.336541	0.760122
H	1.190627	1.085643	-0.465678
C	-0.180483	-0.559233	-0.272638
H	-0.109073	-0.979445	-1.276659
C	0.372091	-1.400772	0.750256
H	0.340181	-1.055056	1.778157
H	0.293463	-2.472781	0.613081
C	4.517318	-0.637420	1.026517
C	4.499642	-1.383310	-0.148814
C	5.647929	-1.569087	-0.907711
C	6.835274	-0.973712	-0.449714
C	6.852828	-0.221495	0.734742
C	5.683350	-0.044414	1.492957
C	3.107398	-0.665973	1.583886
C	3.078375	-1.881324	-0.330265
H	5.619544	-2.153699	-1.824011
H	7.754809	-1.094156	-1.020027
H	7.785575	0.231529	1.066404
H	5.681525	0.537754	2.411189
N	2.326725	-1.412848	0.727214
O	2.703996	-2.594802	-1.257227
O	2.762029	-0.126503	2.632920
Cl	-4.489916	-1.703182	0.903398

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B3LYP SCF energy: -1946.04390505 a.u.
B3LYP enthalpy: -1945.608872 a.u.
B3LYP free energy: -1945.714783 a.u.
B3LYP free energy after quasi-harmonic correction: -1945.702000 a.u.
M06 SCF energy in solution: -1945.72194268 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.266504	-1.978156	2.594728
O	2.007677	-0.896930	3.151814
O	2.331541	-2.244023	1.339520
C	2.572330	-3.217116	3.465098
H	1.971138	-4.073440	3.135214

H	3.628018	-3.491526	3.341214
H	2.373353	-3.004678	4.521188
Pd	2.200937	-0.968513	-0.290831
C	2.210357	1.182799	-2.467937
O	2.399086	2.167417	-1.731038
O	1.949082	-0.029536	-2.132010
C	2.288321	1.367075	-3.996420
H	3.234273	0.937248	-4.351173
H	1.472923	0.829203	-4.494487
H	2.255716	2.429797	-4.260235
C	-0.660957	3.538847	2.375908
C	0.164676	3.081286	1.335153
C	0.560848	4.008566	0.350848
C	0.137891	5.339220	0.410572
C	-0.688845	5.780628	1.452806
C	-1.086500	4.871490	2.438540
H	-0.966778	2.837045	3.150775
H	1.207917	3.662007	-0.453871
H	0.459286	6.038485	-0.360492
H	-1.014902	6.819322	1.497073
H	-1.724600	5.199023	3.259184
C	0.611410	1.639697	1.247927
H	1.664018	1.596193	0.950276
H	0.543692	1.152736	2.227497
C	-0.199848	0.831111	0.210924
H	-0.080821	1.297479	-0.774037
H	-1.274007	0.927262	0.472574
C	0.199566	-0.646177	0.148491
H	0.050207	-1.113945	1.128135
C	-0.572165	-1.429013	-0.913161
H	-0.362539	-1.049339	-1.915360
H	-0.320171	-2.491022	-0.866513
C	-4.281517	-0.662005	-0.939967
C	-4.224560	-1.623817	0.065627
C	-5.358437	-2.007407	0.769154
C	-6.571633	-1.385095	0.433401
C	-6.628871	-0.416632	-0.579961
C	-5.474796	-0.042617	-1.286779
C	-2.897066	-0.506002	-1.503482
C	-2.800424	-2.095049	0.167156
H	-5.299026	-2.758741	1.551990
H	-7.480876	-1.654731	0.966695
H	-7.581487	0.052069	-0.817949
H	-5.503293	0.706824	-2.073028
N	-2.072093	-1.363497	-0.771767
O	-2.378369	-2.970920	0.903658
O	-2.574122	0.202615	-2.442102
Cl	4.631333	-1.433527	-0.849681

33M-TS

B3LYP SCF energy: -1946.02688513 a.u.
B3LYP enthalpy: -1945.594236 a.u.
B3LYP free energy: -1945.701072 a.u.
B3LYP free energy after quasi-harmonic correction: -1945.687357 a.u.
M06 SCF energy in solution: -1945.68772454 a.u.

Imaginary frequency: -264.7279 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.117315	-2.191309	2.468255
O	1.315545	-1.017635	2.814103
O	1.209306	-2.695640	1.281848
C	0.644884	-3.214342	3.515962
H	1.074161	-2.968695	4.493342
H	-0.448532	-3.151620	3.597209
H	0.915332	-4.235610	3.227785
Pd	1.969456	-1.664947	-0.326955
C	3.192427	0.316994	-2.221153
O	3.184054	1.257773	-1.408437
O	2.669106	-0.851746	-2.092792
C	3.915599	0.498836	-3.567932
H	3.396630	-0.038336	-4.369750
H	4.001782	1.562339	-3.815256
H	4.924552	0.074534	-3.479295
C	-0.308654	4.488166	1.544204
C	0.475115	3.423953	1.069187
C	1.727455	3.729171	0.500664
C	2.171589	5.052053	0.424609
C	1.382104	6.102680	0.909503
C	0.134523	5.814002	1.470194
H	-1.282910	4.270630	1.979837
H	2.349643	2.929438	0.103688
H	3.142505	5.260516	-0.021210
H	1.733364	7.131775	0.846175
H	-0.496805	6.617974	1.847312
C	-0.004195	1.991032	1.182019
H	0.619679	1.451555	1.908621
H	-1.027648	1.980987	1.580287
C	0.044483	1.211644	-0.144756
H	1.073116	1.190267	-0.518912
H	-0.560934	1.704497	-0.913309
C	-0.405780	-0.228180	0.012174
H	-0.515629	-0.571710	1.034906
C	-0.012009	-1.225830	-0.943941
H	0.049220	-0.891033	-1.980850
H	-0.511197	-2.190674	-0.828083
C	-4.510475	-0.151931	-1.124334
C	-4.623347	-0.686973	0.155225
C	-5.832463	-1.173322	0.635252
C	-6.946074	-1.109750	-0.219466
C	-6.832270	-0.570701	-1.510054
C	-5.601854	-0.081369	-1.980522
C	-3.065527	0.279183	-1.291321
C	-3.249686	-0.589582	0.790508
H	-5.905330	-1.589095	1.637323
H	-7.910502	-1.483395	0.120743
H	-7.710043	-0.533803	-2.153234
H	-5.498647	0.337572	-2.978630
N	-2.394890	-0.000558	-0.118680
O	-2.985159	-0.970636	1.928600
O	-2.614413	0.798197	-2.310815
Cl	4.238292	-2.502100	0.165075

34M

B3LYP SCF energy: -1946.04101279 a.u.
B3LYP enthalpy: -1945.606152 a.u.
B3LYP free energy: -1945.711925 a.u.
B3LYP free energy after quasi-harmonic correction: -1945.699523 a.u.
M06 SCF energy in solution: -1945.71887803 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.785967	-2.220674	-2.553484
O	-1.004318	-1.077529	-2.992838
O	-0.849474	-2.640211	-1.341239
C	-0.316330	-3.311775	-3.538178
H	0.781814	-3.302758	-3.576328
H	-0.641652	-4.305006	-3.210201
H	-0.696242	-3.099587	-4.543783
Pd	-1.626840	-1.733870	0.360859
C	-2.638589	-0.031566	2.695151
O	-2.636977	1.066794	2.106961
O	-2.239536	-1.171018	2.267599
C	-3.210781	-0.097462	4.126885
H	-4.270244	-0.380595	4.065007
H	-2.696058	-0.858923	4.723678
H	-3.139872	0.881908	4.613552
C	-1.326911	3.729878	-2.172514
C	-1.603233	2.963283	-1.027069
C	-2.305058	3.579026	0.026852
C	-2.704157	4.916089	-0.065696
C	-2.416727	5.670248	-1.210780
C	-1.726138	5.067864	-2.268212
H	-0.800508	3.261631	-3.003127
H	-2.539644	2.983446	0.907004
H	-3.251125	5.370006	0.759958
H	-2.733465	6.710413	-1.281107
H	-1.504028	5.636722	-3.170922
C	-1.145716	1.525828	-0.914230
H	-1.870104	0.953083	-0.327337
H	-1.091054	1.055064	-1.901668
C	0.231698	1.434136	-0.220740
H	0.145988	1.798041	0.809281
H	0.932888	2.102225	-0.745820
C	0.831747	0.011811	-0.223552
H	0.777880	-0.393420	-1.236029
C	0.241285	-0.987123	0.772614
H	0.217601	-0.558775	1.780490
H	0.868403	-1.891907	0.778268
C	4.417357	0.422697	1.005595
C	4.624803	-0.205879	-0.217920
C	5.898894	-0.541055	-0.657101
C	6.978396	-0.222862	0.182744
C	6.769242	0.411415	1.416704
C	5.474597	0.745151	1.846142
C	2.938133	0.645036	1.164314
C	3.282781	-0.393216	-0.866639

H	6.044782	-1.033079	-1.614989
H	7.991996	-0.471366	-0.125350
H	7.623675	0.645929	2.048385
H	5.296199	1.235667	2.799313
N	2.331648	0.133357	0.013130
O	3.079522	-0.899954	-1.957331
O	2.400301	1.183148	2.117127
Cl	-3.881542	-2.815832	-0.038072

35M-TS

B3LYP SCF energy: -1088.96165936 a.u.
B3LYP enthalpy: -1088.586293 a.u.
B3LYP free energy: -1088.673528 a.u.
M06 SCF energy in solution: -1088.53959712 a.u.
M06 enthalpy in solution: -1088.164231 a.u.
M06 free energy in solution: -1088.251466 a.u.
Imaginary frequency: -27.2776 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.951283	-1.392060	1.877066
O	3.032674	-0.143495	2.076536
O	2.304638	-1.822685	0.847382
C	3.619187	-2.381425	2.792153
H	3.727015	-1.964159	3.797278
H	3.057701	-3.319476	2.833257
H	4.622197	-2.603163	2.403808
Pd	1.829075	0.089966	0.143645
C	2.256685	2.792392	-0.871020
O	3.302063	2.388384	-1.403651
O	1.416768	2.059421	-0.197981
C	1.867182	4.265114	-0.929458
H	2.367264	4.761769	-1.765865
H	0.783490	4.392630	-1.015874
H	2.185739	4.755069	0.000395
C	-1.563506	-0.332222	-0.675282
H	-1.878149	0.375119	-1.454010
C	-0.369044	-1.123934	-1.161621
H	-0.183873	-2.039007	-0.598260
C	0.847291	-0.406281	-1.584653
H	0.633664	0.501896	-2.156044
H	1.558257	-1.052098	-2.112196
H	-1.198787	0.276651	0.160885
O	-1.009891	-1.893110	-2.562876
C	-2.752282	-1.190247	-0.199007
H	-3.131028	-1.788671	-1.035033
H	-2.395067	-1.889749	0.567641
C	-3.876244	-0.346450	0.367494
C	-4.931288	0.091250	-0.449582
C	-3.874284	0.040174	1.718178
C	-5.954549	0.895109	0.065448
H	-4.953638	-0.203520	-1.497225
C	-4.894838	0.843332	2.238094
H	-3.068418	-0.294267	2.369161
C	-5.939491	1.274671	1.412225

H	-6.764432	1.220230	-0.583793
H	-4.876196	1.128168	3.287662
H	-6.735335	1.896537	1.815194
H	-0.812040	-1.285533	-3.309431
C	-0.455114	-3.219135	-2.865340
H	-0.820005	-3.885108	-2.084553
H	-0.847853	-3.517034	-3.838991
H	0.636080	-3.174563	-2.875137

35A-TS

B3LYP SCF energy: -1088.95747964 a.u.
B3LYP enthalpy: -1088.581694 a.u.
B3LYP free energy: -1088.666980 a.u.
M06 SCF energy in solution: -1088.53679999 a.u.
M06 enthalpy in solution: -1088.161014 a.u.
M06 free energy in solution: -1088.246300 a.u.
Imaginary frequency: -74.0186 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	3.016715	-2.300578	-0.693816
O	3.038834	-2.046254	0.545862
O	2.263299	-1.598536	-1.470573
C	3.822970	-3.428627	-1.280274
H	4.028115	-3.258738	-2.341022
H	4.761771	-3.554177	-0.732675
H	3.249674	-4.360597	-1.186718
Pd	1.475763	-0.406687	0.053305
C	1.572145	1.327683	2.399995
O	2.715531	1.664130	2.053688
O	0.782897	0.533978	1.734617
C	0.982519	1.821502	3.715749
H	-0.111227	1.829013	3.696870
H	1.302647	1.147795	4.521994
H	1.357689	2.823029	3.947714
C	-1.311620	0.596544	-0.620181
H	-1.371174	1.037718	0.381787
H	-1.941933	1.218152	-1.276152
C	0.129714	0.644915	-1.119484
H	0.245895	0.148043	-2.091168
C	0.781942	1.961185	-1.098582
H	0.686927	2.530587	-0.176862
H	1.776673	2.015483	-1.537635
O	-0.051803	3.009338	-2.100723
C	-1.903552	-0.828397	-0.597003
H	-1.316311	-1.445501	0.094603
H	-1.794770	-1.274333	-1.594788
C	-3.362735	-0.848748	-0.191534
C	-4.380803	-0.751820	-1.155174
C	-3.735235	-0.932278	1.160923
C	-5.729283	-0.734899	-0.781789
H	-4.113929	-0.693763	-2.209069
C	-5.081923	-0.915115	1.540341
H	-2.962760	-1.015061	1.923476
C	-6.085140	-0.815432	0.569377

H	-6.500556	-0.663716	-1.545645
H	-5.347113	-0.983661	2.593110
H	-7.132433	-0.805492	0.862079
H	-0.086260	2.591798	-2.989936
C	0.527436	4.357965	-2.214779
H	1.556716	4.289348	-2.573725
H	-0.102476	4.917031	-2.907927
H	0.480755	4.790002	-1.215930

36M-TS

B3LYP SCF energy: -1206.91790489 a.u.
B3LYP enthalpy: -1206.454861 a.u.
B3LYP free energy: -1206.547873 a.u.
M06 SCF energy in solution: -1206.43363587 a.u.
M06 enthalpy in solution: -1205.970592 a.u.
M06 free energy in solution: -1206.063604 a.u.
Imaginary frequency: -198.0303 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	3.744463	-0.139805	-1.805184
O	3.541496	-1.356444	-1.514178
O	3.055315	0.771804	-1.208582
C	4.793572	0.272720	-2.800849
H	5.019856	-0.546469	-3.488669
H	4.472717	1.155979	-3.361677
H	5.713046	0.533654	-2.260068
Pd	1.992439	-0.579109	-0.017034
C	1.540516	-2.661868	1.977227
O	2.567785	-2.279064	2.558717
O	1.040716	-2.135188	0.896163
C	0.733131	-3.831010	2.528860
H	-0.012321	-4.193682	1.815919
H	1.405380	-4.650318	2.805955
H	0.215748	-3.505491	3.440780
C	-1.438888	0.108306	0.208248
H	-1.831241	-0.035875	1.223184
C	-0.280373	1.079627	0.256803
H	-0.050733	1.567754	-0.687475
C	0.881522	0.743025	1.093695
H	0.605603	0.271260	2.041530
H	1.564111	1.582822	1.246256
H	-1.006427	-0.856296	-0.084640
O	-1.055923	2.480008	1.023723
C	-2.572178	0.480201	-0.766173
H	-3.019026	1.431417	-0.460028
H	-2.144864	0.626179	-1.766363
C	-3.648864	-0.584805	-0.824537
C	-4.745732	-0.547351	0.052278
C	-3.563318	-1.647487	-1.739038
C	-5.728008	-1.543385	0.019703
H	-4.833226	0.271893	0.763840
C	-4.543533	-2.645275	-1.776961
H	-2.724309	-1.690643	-2.431350
C	-5.630026	-2.597182	-0.896004

H	-6.570474	-1.493504	0.706007
H	-4.460396	-3.456850	-2.496421
H	-6.394295	-3.370262	-0.925320
H	-0.775937	2.413990	1.961739
C	-0.856371	3.922131	0.576542
C	0.635064	4.221235	0.468750
H	1.146456	4.071479	1.426232
H	1.118261	3.604959	-0.295342
H	0.760830	5.271502	0.181814
C	-1.530772	4.752393	1.665439
H	-1.038133	4.617217	2.636555
H	-1.458955	5.813448	1.401439
H	-2.590418	4.493576	1.763312
C	-1.574241	4.046667	-0.759841
H	-1.130083	3.402547	-1.525333
H	-2.638070	3.808040	-0.664369
H	-1.486187	5.082957	-1.104442

36A-TS

B3LYP SCF energy: -1206.91574018 a.u.
B3LYP enthalpy: -1206.452446 a.u.
B3LYP free energy: -1206.545804 a.u.
M06 SCF energy in solution: -1206.42988557 a.u.
M06 enthalpy in solution: -1205.966591 a.u.
M06 free energy in solution: -1206.059949 a.u.
Imaginary frequency: -254.0493 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.804708	-2.726188	-1.389696
O	2.742627	-2.954216	-0.145670
O	2.135082	-1.741087	-1.884525
C	3.621835	-3.594276	-2.307831
H	3.913600	-3.049765	-3.210382
H	4.511667	-3.964559	-1.790047
H	3.020481	-4.462091	-2.609539
Pd	1.333965	-1.130404	-0.053223
C	1.449211	-0.391713	2.758296
O	2.621937	-0.034569	2.563619
O	0.628798	-0.822064	1.842621
C	0.861241	-0.379673	4.164258
H	-0.232361	-0.388039	4.155959
H	1.207403	-1.275094	4.697535
H	1.221475	0.494879	4.715625
C	-1.329161	0.313966	-0.353920
H	-1.393337	0.374153	0.738899
H	-1.868954	1.187453	-0.752186
C	0.128847	0.394948	-0.789458
H	0.247639	0.265074	-1.872124
C	0.915823	1.514592	-0.274783
H	0.825037	1.729019	0.784734
H	1.923550	1.625654	-0.663770
O	0.208570	2.981390	-0.870340
C	-2.043852	-0.961548	-0.847651
H	-1.536304	-1.837542	-0.424379

H	-1.940049	-1.027425	-1.938918
C	-3.512249	-0.991971	-0.478069
C	-4.493079	-0.523549	-1.368274
C	-3.928550	-1.465397	0.778118
C	-5.847471	-0.523159	-1.015448
H	-4.193015	-0.159668	-2.349471
C	-5.280838	-1.467270	1.136483
H	-3.185758	-1.840669	1.479885
C	-6.246760	-0.994828	0.240067
H	-6.589468	-0.158596	-1.722501
H	-5.580356	-1.841373	2.113045
H	-7.298839	-0.998835	0.515213
H	0.286020	2.918946	-1.846642
C	0.688386	4.363924	-0.440802
C	2.204076	4.434550	-0.590879
H	2.534573	5.451142	-0.348921
H	2.713888	3.745523	0.089714
H	2.514607	4.216926	-1.619815
C	-0.030927	5.323469	-1.384418
H	0.235925	6.352445	-1.119084
H	0.269242	5.160478	-2.427205
H	-1.118290	5.219040	-1.304868
C	0.224742	4.521909	1.000475
H	-0.858262	4.382683	1.083620
H	0.728129	3.820393	1.673395
H	0.467351	5.536087	1.336044

37M-TS

B3LYP SCF energy: -1201.88309467 a.u.
B3LYP enthalpy: -1201.510593 a.u.
B3LYP free energy: -1201.601867 a.u.
M06 SCF energy in solution: -1201.43288395 a.u.
M06 enthalpy in solution: -1201.060382 a.u.
M06 free energy in solution: -1201.151656 a.u.
Imaginary frequency: -156.0119 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-3.413120	0.287420	1.893348
O	-3.248947	-0.949239	1.662123
O	-2.757570	1.140607	1.181343
C	-4.372525	0.780387	2.937148
H	-5.355244	0.930337	2.470447
H	-4.484071	0.044391	3.738320
H	-4.042955	1.738549	3.349071
Pd	-1.856302	-0.311833	-0.004353
C	-1.824348	-2.568470	-1.785346
O	-2.955115	-2.200716	-2.132979
O	-1.073835	-1.950770	-0.911805
C	-1.168429	-3.805370	-2.380550
H	-1.915928	-4.435570	-2.869750
H	-0.427553	-3.496445	-3.129552
H	-0.640994	-4.382764	-1.614272
C	1.382956	0.182035	-0.456349
H	2.026049	0.472309	-1.296386

C	0.170419	1.070756	-0.486166
H	0.028705	1.775514	0.325763
C	-0.881370	0.906235	-1.414657
H	-0.686613	0.323318	-2.314610
H	-1.572211	1.738861	-1.547947
H	1.074134	-0.852646	-0.648013
C	1.096545	3.975156	-0.755279
O	1.301237	2.861064	-1.350286
O	0.494372	4.127990	0.337013
C	1.614326	5.224218	-1.483313
H	0.840839	5.574873	-2.180865
H	1.820412	6.034250	-0.775660
H	2.514196	5.007623	-2.069072
C	2.175629	0.272742	0.862526
H	2.460270	1.318632	1.029826
H	1.521117	-0.022093	1.692849
C	3.415110	-0.597437	0.860889
C	4.638740	-0.105277	0.375976
C	3.367796	-1.924640	1.318972
C	5.780608	-0.913291	0.347843
H	4.698189	0.922842	0.023237
C	4.506746	-2.737313	1.293262
H	2.431200	-2.323540	1.704739
C	5.718687	-2.234188	0.806708
H	6.718538	-0.509896	-0.027476
H	4.448023	-3.760849	1.656787
H	6.606003	-2.862649	0.789450

37A-TS

B3LYP SCF energy: -1201.88250186 a.u.
B3LYP enthalpy: -1201.509824 a.u.
B3LYP free energy: -1201.601116 a.u.
M06 SCF energy in solution: -1201.43262889 a.u.
M06 enthalpy in solution: -1201.059951 a.u.
M06 free energy in solution: -1201.151243 a.u.
Imaginary frequency: -233.2913 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	3.638908	-1.552451	-1.289247
O	3.505964	-1.874804	-0.071399
O	2.790897	-0.731228	-1.812250
C	4.771550	-2.074372	-2.126398
H	5.664503	-1.465230	-1.933583
H	5.003826	-3.107999	-1.852409
H	4.535634	-2.012755	-3.192311
Pd	1.695391	-0.469156	-0.066391
C	1.360345	0.039066	2.756878
O	2.460041	0.608063	2.714161
O	0.749155	-0.493315	1.732538
C	0.571645	-0.072177	4.053963
H	0.076178	-1.044719	4.139219
H	1.226760	0.087232	4.914733
H	-0.209397	0.699484	4.064508
C	-1.291775	0.236450	-0.514518

H	-1.364170	0.322624	0.574768
H	-1.989645	0.974423	-0.940812
C	0.097451	0.612165	-0.979260
H	0.285381	0.407859	-2.036086
C	0.786850	1.716117	-0.431715
H	0.570034	2.065968	0.568926
H	1.666706	2.115288	-0.919996
C	-0.861066	4.177517	-0.343606
O	-0.208008	3.478697	-1.200372
O	-0.885070	3.992559	0.895422
C	-1.694293	5.318031	-0.944124
H	-1.143829	5.832915	-1.739475
H	-2.605014	4.900120	-1.394345
H	-1.989626	6.038949	-0.175347
C	-1.723251	-1.174555	-0.966527
H	-1.040366	-1.912728	-0.528157
H	-1.612889	-1.243725	-2.057175
C	-3.148956	-1.508214	-0.579838
C	-4.227346	-1.112057	-1.389527
C	-3.431656	-2.200693	0.609173
C	-5.547158	-1.395918	-1.022500
H	-4.030757	-0.580212	-2.318887
C	-4.749966	-2.488234	0.981107
H	-2.610283	-2.522125	1.247103
C	-5.813856	-2.085840	0.166033
H	-6.366071	-1.082762	-1.666469
H	-4.944444	-3.029298	1.904570
H	-6.838905	-2.310921	0.451045

38M-TS

B3LYP SCF energy: -1499.62312437 a.u.
B3LYP enthalpy: -1499.271850 a.u.
B3LYP free energy: -1499.369825 a.u.
M06 SCF energy in solution: -1499.17364220 a.u.
M06 enthalpy in solution: -1498.822368 a.u.
M06 free energy in solution: -1498.920343 a.u.
Imaginary frequency: -211.2651 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-3.716140	-1.325029	-1.782634
O	-4.106838	-0.190020	-1.374514
O	-2.647217	-1.835785	-1.272015
C	-4.481249	-2.103022	-2.814993
H	-5.170340	-2.788376	-2.303775
H	-5.070566	-1.432175	-3.446110
H	-3.805257	-2.702820	-3.431698
Pd	-2.318806	-0.245939	0.033138
C	-2.945328	1.612616	2.154368
O	-3.713088	0.743118	2.591848
O	-2.191364	1.484009	1.096814
C	-2.787786	2.950743	2.862006
H	-3.712954	3.215999	3.382225
H	-1.989957	2.863932	3.611842
H	-2.509782	3.749122	2.167523

C	0.905611	0.854417	0.151682
H	1.448327	0.959929	1.099165
C	0.302753	-0.522351	0.091704
H	0.329523	-1.033892	-0.864969
C	-0.657128	-0.978483	1.048992
H	-0.602706	-0.528986	2.041302
H	-0.834360	-2.055425	1.064959
H	0.079121	1.575162	0.199502
C	2.361868	-2.502873	-0.067589
O	2.012700	-1.517645	0.656211
O	1.901984	-2.926027	-1.131571
C	3.571047	-3.280870	0.558168
C	1.823520	1.186875	-1.039838
H	2.635482	0.451484	-1.081028
H	1.246846	1.087645	-1.968408
C	2.405719	2.582475	-0.951081
C	3.606055	2.817963	-0.259732
C	1.748060	3.678676	-1.533459
C	4.133204	4.109349	-0.149962
H	4.134389	1.980864	0.193233
C	2.271270	4.972277	-1.427731
H	0.819778	3.516850	-2.078737
C	3.466648	5.192708	-0.734110
H	5.065577	4.268048	0.387424
H	1.747538	5.805944	-1.890293
H	3.876227	6.196839	-0.653094
F	4.061815	-4.239194	-0.257722
F	3.206919	-3.899131	1.715372
F	4.606823	-2.456229	0.862087

38A-TS

B3LYP SCF energy: -1499.62089435 a.u.
B3LYP enthalpy: -1499.269218 a.u.
B3LYP free energy: -1499.365760 a.u.
M06 SCF energy in solution: -1499.17235668 a.u.
M06 enthalpy in solution: -1498.820680 a.u.
M06 free energy in solution: -1498.917222 a.u.
Imaginary frequency: -309.8791 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-4.257385	-0.482911	-1.529451
O	-4.446847	-0.067508	-0.348523
O	-3.051485	-0.716354	-1.926365
C	-5.399603	-0.744992	-2.470855
H	-5.636126	-1.817119	-2.454538
H	-6.289486	-0.189673	-2.162624
H	-5.127941	-0.478347	-3.496960
Pd	-2.163468	-0.209521	-0.111915
C	-1.877208	-0.234897	2.779143
O	-2.444263	-1.337348	2.774569
O	-1.567567	0.460044	1.719401
C	-1.441938	0.424729	4.081010
H	-1.981395	-0.007631	4.928254
H	-0.367668	0.253171	4.230275

H	-1.602486	1.507326	4.052969
C	0.742020	0.766767	-0.354436
H	0.737946	0.874538	0.735535
H	1.770844	0.501008	-0.645857
C	-0.170737	-0.371921	-0.770542
H	-0.303826	-0.445167	-1.853915
C	-0.072674	-1.636375	-0.106395
H	0.117840	-1.665777	0.959629
H	-0.586622	-2.494672	-0.522929
C	2.549972	-2.441690	0.306081
O	1.642169	-2.420784	-0.592322
O	2.508990	-2.140996	1.498212
C	3.915014	-2.937167	-0.281403
C	0.377832	2.112085	-1.016998
H	-0.639535	2.392289	-0.716210
H	0.364758	1.978067	-2.106971
C	1.341141	3.223541	-0.655943
C	2.483107	3.472705	-1.435773
C	1.132000	4.014925	0.486218
C	3.390600	4.478801	-1.085501
H	2.660728	2.875081	-2.328218
C	2.035555	5.022531	0.841176
H	0.250074	3.842174	1.100381
C	3.170175	5.258036	0.056075
H	4.266431	4.656080	-1.705857
H	1.851390	5.625053	1.727969
H	3.872165	6.042734	0.328258
F	4.882999	-3.028929	0.654866
F	3.800908	-4.163763	-0.853668
F	4.374674	-2.093153	-1.242896

39M-TS

B3LYP SCF energy: -1069.06956013 a.u.
B3LYP enthalpy: -1068.680120 a.u.
B3LYP free energy: -1068.768787 a.u.
M06 SCF energy in solution: -1068.69322572 a.u.
M06 enthalpy in solution: -1068.303786 a.u.
M06 free energy in solution: -1068.392453 a.u.
Imaginary frequency: -262.5975 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-3.021491	0.582375	-2.069376
O	-2.420025	1.633551	-1.711614
O	-2.818298	-0.512942	-1.414830
C	-3.994652	0.581736	-3.219765
H	-3.721450	1.352387	-3.945234
H	-4.029040	-0.401339	-3.697401
H	-4.997084	0.811560	-2.837695
Pd	-1.537074	0.396724	-0.048557
C	-0.597932	1.973442	2.199760
O	-1.598938	1.620256	2.824087
O	-0.242758	1.536412	1.013648
C	0.374109	3.008610	2.761034
H	0.134339	3.216972	3.806247

H	1.409727	2.661665	2.675468
H	0.291226	3.935900	2.181622
C	4.153191	-0.960159	-1.354832
C	3.052771	-0.228317	-0.886021
C	3.272578	1.057194	-0.364549
C	4.562133	1.591982	-0.311475
C	5.653318	0.851349	-0.779064
C	5.445528	-0.427524	-1.302687
H	3.997915	-1.952154	-1.776876
H	2.423332	1.635930	-0.006709
H	4.714392	2.591445	0.088698
H	6.655649	1.270608	-0.741469
H	6.285587	-1.007618	-1.677277
C	1.653547	-0.806357	-0.916980
H	0.933166	-0.029567	-1.195515
H	1.590944	-1.593385	-1.681127
C	1.234762	-1.390844	0.454404
H	1.339464	-0.619015	1.223175
H	1.943622	-2.193166	0.702797
C	-0.200975	-1.906166	0.465533
H	-0.534691	-2.352180	-0.472625
C	-1.218737	-1.210060	1.216649
H	-0.918029	-0.813240	2.186931
H	-2.204590	-1.680106	1.233146
N	0.044680	-3.644953	1.308981
H	0.762378	-4.149155	0.786907
C	-1.192283	-4.439583	1.430346
H	0.432881	-3.419148	2.225553
H	-1.925728	-3.861438	1.995724
H	-1.590531	-4.629794	0.430089
H	-1.015887	-5.394067	1.938165

39A-TS

B3LYP SCF energy: -1069.07534837 a.u.
B3LYP enthalpy: -1068.685790 a.u.
B3LYP free energy: -1068.773600 a.u.
M06 SCF energy in solution: -1068.68973376 a.u.
M06 enthalpy in solution: -1068.300175 a.u.
M06 free energy in solution: -1068.387985 a.u.
Imaginary frequency: -280.9506 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	3.716720	-1.375186	-1.009130
O	3.369806	-1.900447	0.082948
O	2.990385	-0.430475	-1.515091
C	4.938120	-1.836114	-1.761390
H	5.677810	-2.241351	-1.066203
H	4.648512	-2.633602	-2.456992
H	5.366622	-1.015900	-2.343984
Pd	1.583128	-0.487432	0.001518
C	0.175096	-0.132080	2.611493
O	0.411548	1.082860	2.670836
O	0.412065	-0.916692	1.598014
C	-0.438275	-0.861280	3.803129

H	-1.011460	-1.737413	3.488113
H	0.374566	-1.208035	4.453476
H	-1.065632	-0.175742	4.379241
C	-4.172935	-0.297652	-1.871385
C	-3.283887	-0.636681	-0.840089
C	-3.820584	-1.021388	0.399017
C	-5.202390	-1.060889	0.603144
C	-6.076624	-0.716731	-0.433036
C	-5.556751	-0.335807	-1.673453
H	-3.777003	-0.010101	-2.844217
H	-3.146298	-1.299220	1.206535
H	-5.596603	-1.366748	1.569365
H	-7.151953	-0.751866	-0.277024
H	-6.227205	-0.075441	-2.489229
C	-1.784939	-0.562944	-1.042232
H	-1.289644	-1.374656	-0.498286
H	-1.549008	-0.698305	-2.106626
C	-1.186362	0.776415	-0.561357
H	-1.370057	0.901544	0.510930
H	-1.733394	1.590396	-1.071543
C	0.297547	0.925914	-0.860268
H	0.530591	0.817830	-1.925590
C	1.048028	1.952119	-0.184483
H	0.888920	2.070092	0.884807
H	2.047612	2.176448	-0.548408
N	0.335118	3.743011	-0.606985
H	-0.644120	3.700086	-0.327738
C	1.058234	4.813840	0.103047
H	0.365161	3.861836	-1.619141
H	1.024220	4.605732	1.175525
H	2.103069	4.809248	-0.219181
H	0.629160	5.804754	-0.086465

40M-TS

B3LYP SCF energy: -1147.70362227 a.u.
B3LYP enthalpy: -1147.255313 a.u.
B3LYP free energy: -1147.349726 a.u.
M06 SCF energy in solution: -1147.28110243 a.u.
M06 enthalpy in solution: -1146.832793 a.u.
M06 free energy in solution: -1146.927206 a.u.
Imaginary frequency: -259.2766 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	3.476014	-0.497315	-1.901553
O	3.090043	-1.662440	-1.607227
O	2.979232	0.511552	-1.264499
C	4.526213	-0.255329	-2.955187
H	4.392162	0.726276	-3.418083
H	5.516009	-0.278277	-2.482496
H	4.491446	-1.044601	-3.710648
Pd	1.806958	-0.680944	-0.027033
C	0.992782	-2.453901	2.121817
O	1.852750	-1.932407	2.832181
O	0.672600	-2.071869	0.906522

C	0.184275	-3.659739	2.592690
H	-0.873247	-3.554981	2.328761
H	0.559462	-4.560176	2.091171
H	0.294977	-3.784537	3.672484
C	-4.745274	0.414716	-0.691266
C	-3.506847	-0.208917	-0.897276
C	-3.479155	-1.604241	-1.054089
C	-4.656858	-2.352925	-1.001330
C	-5.886323	-1.718619	-0.792637
C	-5.927786	-0.330817	-0.638489
H	-4.789217	1.497196	-0.579669
H	-2.528490	-2.107463	-1.218305
H	-4.614519	-3.431985	-1.126186
H	-6.803064	-2.301329	-0.754066
H	-6.878260	0.173352	-0.481526
C	-2.220940	0.592354	-0.931572
H	-1.620847	0.295836	-1.802514
H	-2.462848	1.656185	-1.071385
C	-1.360993	0.398301	0.333203
H	-1.094380	-0.658664	0.442782
H	-1.946003	0.643717	1.231835
C	-0.063891	1.191144	0.322883
H	0.220008	1.612764	-0.639006
C	1.030439	0.807337	1.182884
H	0.765440	0.378514	2.150383
H	1.863811	1.511919	1.241891
N	-0.721530	2.922032	0.997446
H	-1.671377	3.102240	0.665253
C	0.164424	4.092308	0.743943
C	-0.078544	5.208426	1.767184
H	-1.097411	5.608134	1.684998
H	0.070601	4.850252	2.793076
H	0.621527	6.034889	1.600094
H	-0.780613	2.719091	1.996477
H	1.186790	3.715125	0.867247
C	-0.022515	4.574300	-0.696132
H	0.174733	3.779734	-1.422601
H	-1.042510	4.948808	-0.857784
H	0.669344	5.395990	-0.907065

40A-TS

B3LYP SCF energy: -1147.70909166 a.u.
B3LYP enthalpy: -1147.260472 a.u.
B3LYP free energy: -1147.353933 a.u.
M06 SCF energy in solution: -1147.27774530 a.u.
M06 enthalpy in solution: -1146.829126 a.u.
M06 free energy in solution: -1146.922587 a.u.
Imaginary frequency: -267.8220 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	3.491694	-2.147183	-0.960459
O	3.121714	-2.577021	0.165221
O	2.833721	-1.180379	-1.515855
C	4.662198	-2.747657	-1.695119

H	5.402878	-3.119247	-0.982093
H	4.309489	-3.597238	-2.293008
H	5.112753	-2.016415	-2.371649
Pd	1.448951	-1.031496	0.012921
C	0.129048	-0.396544	2.613594
O	0.490872	0.788380	2.602528
O	0.263954	-1.254435	1.641410
C	-0.532239	-0.995340	3.851422
H	-1.238049	-1.787536	3.586549
H	0.247924	-1.441317	4.480967
H	-1.030648	-0.211081	4.427195
C	-4.290266	-0.476740	-1.827983
C	-3.418008	-0.845396	-0.792406
C	-3.968108	-1.138502	0.465648
C	-5.346235	-1.061414	0.683700
C	-6.203351	-0.689509	-0.357129
C	-5.670240	-0.398061	-1.616082
H	-3.885041	-0.259435	-2.815128
H	-3.307720	-1.437269	1.277147
H	-5.751410	-1.298044	1.664709
H	-7.276207	-0.634479	-0.190237
H	-6.328084	-0.117131	-2.435300
C	-1.920672	-0.899405	-1.011806
H	-1.483152	-1.717456	-0.429293
H	-1.710241	-1.109488	-2.069398
C	-1.213644	0.412959	-0.609933
H	-1.373021	0.609612	0.455503
H	-1.705603	1.236979	-1.158861
C	0.273061	0.428216	-0.930248
H	0.484414	0.233690	-1.987508
C	1.116345	1.423161	-0.320940
H	0.976308	1.623004	0.738135
H	2.126342	1.533725	-0.703409
N	0.537471	3.252639	-0.857378
H	-0.473225	3.153407	-0.952717
C	0.876731	4.334755	0.107464
C	2.394939	4.517388	0.154786
H	2.655791	5.293032	0.882126
H	2.903470	3.595336	0.451977
H	2.785874	4.832777	-0.822431
C	0.142572	5.638655	-0.230167
H	0.352994	6.401518	0.528348
H	0.464072	6.033679	-1.202713
H	-0.943893	5.490981	-0.260124
H	0.913156	3.448826	-1.786873
H	0.531746	3.971284	1.082884

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B3LYP SCF energy: -1187.01687858 a.u.
B3LYP enthalpy: -1186.539169 a.u.
B3LYP free energy: -1186.635765 a.u.
M06 SCF energy in solution: -1186.57712751 a.u.
M06 enthalpy in solution: -1186.099418 a.u.
M06 free energy in solution: -1186.196014 a.u.
Imaginary frequency: -236.1503 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-3.003807	-0.984306	2.145583
O	-2.565371	-2.109690	1.782265
O	-2.672722	0.070494	1.474905
C	-3.932465	-0.841478	3.324521
H	-3.734687	-1.627944	4.057580
H	-3.829274	0.145828	3.783210
H	-4.967394	-0.951376	2.977352
Pd	-1.563750	-1.005042	0.075835
C	-0.875768	-2.653354	-2.212659
O	-1.820428	-2.151784	-2.823885
O	-0.458528	-2.296176	-1.020939
C	-0.067612	-3.808735	-2.798718
H	-0.256279	-3.889123	-3.871979
H	1.003292	-3.681743	-2.609672
H	-0.377675	-4.742816	-2.314490
C	4.063542	0.189121	1.543528
C	3.146820	-0.565145	0.795529
C	3.628566	-1.647517	0.043072
C	4.990185	-1.962773	0.033068
C	5.894439	-1.199947	0.778740
C	5.426358	-0.122719	1.537317
H	3.705847	1.021408	2.148195
H	2.925609	-2.251374	-0.526974
H	5.343397	-2.809270	-0.550827
H	6.952877	-1.447853	0.775524
H	6.119635	0.469122	2.130329
C	1.673020	-0.213944	0.772369
H	1.074698	-1.115284	0.617374
H	1.372648	0.214871	1.737370
C	1.356040	0.805908	-0.353809
H	1.635074	0.369508	-1.320812
H	2.001052	1.676740	-0.184364
C	-0.097714	1.249705	-0.397999
H	-0.467019	1.680099	0.530531
C	-1.076614	0.545077	-1.193669
H	-0.719252	0.134944	-2.138784
H	-2.046038	1.042350	-1.290563
N	0.089788	3.007237	-1.304218
H	1.045093	3.041175	-1.666263
C	-0.252343	4.298641	-0.616686
C	0.668828	4.451457	0.602774
H	0.460410	5.399462	1.109739
H	0.520125	3.644886	1.327652
H	1.725639	4.459327	0.307260
C	-0.027355	5.461605	-1.602087
H	-0.278796	6.417159	-1.127598
H	1.019923	5.514600	-1.925157
H	-0.657764	5.355103	-2.493349
C	-1.728413	4.238435	-0.195041
H	-2.384726	4.110820	-1.064837
H	-1.925456	3.417833	0.501318
H	-2.010604	5.174728	0.297910
H	-0.524214	2.865172	-2.108337

41A-TS

B3LYP SCF energy: -1187.02465145 a.u.
B3LYP enthalpy: -1186.546928 a.u.
B3LYP free energy: -1186.642481 a.u.
M06 SCF energy in solution: -1186.57413397 a.u.
M06 enthalpy in solution: -1186.096411 a.u.
M06 free energy in solution: -1186.191964 a.u.
Imaginary frequency: -263.8689 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-3.362282	2.487417	-0.924814
O	-2.987823	2.847579	0.223837
O	-2.741915	1.517693	-1.517024
C	-4.494367	3.174396	-1.643620
H	-5.226355	3.547103	-0.922248
H	-4.095500	4.032954	-2.198092
H	-4.969128	2.496141	-2.357714
Pd	-1.388731	1.234051	0.020699
C	-0.138531	0.438370	2.617087
O	-0.565752	-0.724493	2.567772
O	-0.212730	1.329543	1.669901
C	0.538609	0.961332	3.880296
H	1.276553	1.734705	3.650257
H	-0.227677	1.411509	4.523755
H	1.002197	0.135911	4.427027
C	4.325846	0.538480	-1.828431
C	3.458544	0.918131	-0.792664
C	4.009457	1.178009	0.472301
C	5.383505	1.058175	0.696866
C	6.235628	0.675812	-0.344258
C	5.701696	0.416994	-1.609978
H	3.920488	0.346663	-2.820784
H	3.353118	1.484705	1.284148
H	5.789514	1.269593	1.683272
H	7.305453	0.587503	-0.172300
H	6.355964	0.128277	-2.429351
C	1.964787	1.019249	-1.019257
H	1.547972	1.838141	-0.422747
H	1.766501	1.256945	-2.073329
C	1.217590	-0.279731	-0.647862
H	1.370676	-0.504638	0.412846
H	1.684221	-1.106399	-1.214275
C	-0.268389	-0.239085	-0.969537
H	-0.471442	-0.007562	-2.021072
C	-1.147420	-1.218742	-0.386508
H	-1.017492	-1.447475	0.665244
H	-2.160722	-1.285637	-0.770417
N	-0.639166	-3.050119	-1.013822
H	0.374027	-2.990441	-1.122617
C	-1.005887	-4.252046	-0.192164
C	-2.519815	-4.205925	0.064478
H	-2.832043	-5.099262	0.615719
H	-2.799357	-3.329842	0.657324
H	-3.083382	-4.183624	-0.877527

C	-0.633864	-5.526077	-0.974843
H	-0.883238	-6.420214	-0.391761
H	-1.180296	-5.584222	-1.925029
H	0.440886	-5.558258	-1.192894
C	-0.220039	-4.187509	1.126678
H	0.862114	-4.209273	0.942442
H	-0.449629	-3.287605	1.705246
H	-0.465693	-5.058936	1.743215
H	-1.036607	-3.118337	-1.952224

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B3LYP SCF energy: -1555.65129460 a.u.
B3LYP enthalpy: -1555.010925 a.u.
B3LYP free energy: -1555.128214 a.u.
M06 SCF energy in solution: -1555.09782009 a.u.
M06 enthalpy in solution: -1554.457450 a.u.
M06 free energy in solution: -1554.574739 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.956635	-2.568278	-0.101186
O	-0.987051	-2.875151	-0.802092
O	-2.034672	-1.548577	0.703703
C	-3.255159	-3.430925	-0.093846
Pd	-0.626213	-0.074405	0.781203
C	1.391239	2.053377	0.255185
O	1.773016	1.516461	-0.789022
O	0.556661	1.556300	1.119607
C	1.910821	3.462705	0.675556
C	-2.708193	1.683769	-0.231365
O	-3.088611	1.815985	0.937115
O	-1.689434	0.985213	-0.632664
C	-3.451496	2.390609	-1.407216
C	4.791603	-2.755074	-0.618717
C	3.952640	-1.634465	-0.729467
C	4.510061	-0.429069	-1.189609
C	5.865640	-0.351119	-1.523724
C	6.691489	-1.474547	-1.405750
C	6.147982	-2.680511	-0.951573
H	4.372931	-3.700532	-0.276164
H	3.864207	0.441248	-1.284480
H	6.276653	0.590315	-1.883059
H	7.745130	-1.412783	-1.670438
H	6.777035	-3.564320	-0.862751
C	2.489734	-1.709816	-0.346805
H	1.909167	-1.000903	-0.943631
H	2.096269	-2.711875	-0.559155
C	2.255686	-1.387014	1.146413
H	2.582316	-0.366268	1.370847
H	2.881431	-2.061310	1.756574
C	0.828656	-1.599515	1.586065
H	0.372265	-2.515726	1.217649
C	0.193493	-0.917111	2.609944
H	0.688246	-0.096593	3.124787
H	-0.693562	-1.330243	3.083614

C	0.714101	4.438490	0.677328
H	-0.067317	4.097513	1.362990
H	1.042865	5.441719	0.984704
H	0.272622	4.519222	-0.323465
C	2.513739	3.386893	2.094261
H	3.358290	2.685760	2.129485
H	2.885702	4.374723	2.401577
H	1.764646	3.055243	2.819431
C	2.979220	3.950628	-0.315710
H	3.323110	4.955251	-0.031053
H	3.846836	3.281189	-0.328199
H	2.582972	3.992413	-1.335201
C	-3.081529	-4.649582	-1.014114
H	-4.001794	-5.251234	-1.017951
H	-2.862210	-4.340694	-2.041322
H	-2.252883	-5.284954	-0.682105
C	-4.428084	-2.559659	-0.591718
H	-5.359994	-3.143260	-0.592301
H	-4.561017	-1.683551	0.049677
H	-4.249076	-2.206452	-1.614720
C	-3.542677	-3.900351	1.348350
H	-4.454906	-4.513414	1.373678
H	-2.717531	-4.511506	1.738274
H	-3.678514	-3.044182	2.015949
C	-3.926371	1.322928	-2.415188
H	-4.454187	1.799461	-3.254403
H	-3.077877	0.756026	-2.809504
H	-4.616838	0.613466	-1.941656
C	-4.659438	3.176556	-0.873128
H	-4.348710	3.935979	-0.147695
H	-5.179221	3.676725	-1.703391
H	-5.369896	2.514900	-0.365710
C	-2.468980	3.353315	-2.107445
H	-2.966345	3.861584	-2.946583
H	-2.110549	4.123464	-1.412461
H	-1.598992	2.810972	-2.489617

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B3LYP SCF energy: -2068.12854280 a.u.
B3LYP enthalpy: -2067.376924 a.u.
B3LYP free energy: -2067.518105 a.u.
M06 SCF energy in solution: -2067.51400125 a.u.
M06 enthalpy in solution: -2066.762382 a.u.
M06 free energy in solution: -2066.903563 a.u.
Imaginary frequency: -231.5960 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.331403	-2.591903	1.479134
O	0.302734	-1.789952	2.422613
O	0.538201	-2.331036	0.230979
C	0.093456	-4.118257	1.732684
Pd	1.087701	-0.518519	-0.566298
C	2.055946	2.256200	-1.323036
O	2.045746	2.716097	-0.170292

O	1.648028	1.101230	-1.714940
C	2.618290	3.119630	-2.503999
C	3.933457	-1.583655	-0.864264
O	3.706870	-2.097544	-1.972549
O	3.126997	-0.920716	-0.117058
C	5.366344	-1.715162	-0.229428
C	-1.294759	2.924119	3.856186
C	-0.439965	2.804270	2.746972
C	0.338417	3.919233	2.387369
C	0.255511	5.112740	3.112288
C	-0.603005	5.219741	4.212809
C	-1.379289	4.115894	4.583425
H	-1.896570	2.066456	4.153514
H	1.011727	3.828281	1.537567
H	0.869787	5.962347	2.817291
H	-0.663816	6.149385	4.777129
H	-2.047479	4.180833	5.441395
C	-0.366126	1.520164	1.948118
H	0.616479	1.434368	1.476746
H	-0.481456	0.652457	2.606960
C	-1.460677	1.476166	0.846957
H	-1.275844	2.259280	0.103397
H	-2.428360	1.689093	1.311723
C	-1.552428	0.126281	0.162969
H	-1.672600	-0.715323	0.837635
C	-0.921268	-0.143975	-1.092273
H	-0.905612	0.687909	-1.797316
H	-1.200556	-1.096689	-1.547753
C	-5.522388	0.142650	-1.529877
C	-5.592498	-1.016974	-0.762674
C	-6.679872	-1.877050	-0.843717
C	-7.714287	-1.537840	-1.732343
C	-7.643841	-0.369251	-2.505764
C	-6.537174	0.491683	-2.411531
C	-4.212788	0.822175	-1.173639
C	-4.327658	-1.061055	0.073695
H	-6.719970	-2.780488	-0.240035
H	-8.581837	-2.188966	-1.825595
H	-8.457803	-0.130058	-3.188139
H	-6.468833	1.399462	-3.006173
N	-3.579229	0.058207	-0.216893
O	-4.055305	-1.954947	0.874468
O	-3.824798	1.880038	-1.666314
C	1.540540	3.243508	-3.600565
H	1.923489	3.829584	-4.450846
H	1.241751	2.254332	-3.959521
H	0.643462	3.748351	-3.218550
C	3.015944	4.518604	-2.007510
H	3.769502	4.455460	-1.215174
H	3.427741	5.112245	-2.838667
H	2.153046	5.052918	-1.593770
C	3.855776	2.400355	-3.081787
H	4.264400	2.965270	-3.934578
H	4.645804	2.309873	-2.325197
H	3.596417	1.390910	-3.414517
C	5.945652	-0.300695	-0.022251
H	5.283835	0.295659	0.612827

H	6.940985	-0.353779	0.448111
H	6.053146	0.223607	-0.981322
C	6.294685	-2.526584	-1.146733
H	7.295604	-2.615624	-0.694297
H	5.897538	-3.533475	-1.317882
H	6.395072	-2.048795	-2.127695
C	5.240416	-2.418290	1.137631
H	4.834979	-3.432328	1.022254
H	6.225921	-2.500380	1.624055
H	4.565247	-1.861215	1.793900
C	1.384224	-4.878992	1.362118
H	1.244997	-5.962503	1.504050
H	1.657152	-4.689983	0.319370
H	2.224358	-4.559556	1.992657
C	-0.251042	-4.365303	3.210107
H	-1.166117	-3.834389	3.494756
H	-0.401910	-5.441759	3.387361
H	0.550405	-4.010099	3.867017
C	-1.067248	-4.605648	0.840380
H	-1.258277	-5.676433	1.015505
H	-1.990882	-4.053213	1.052626
H	-0.824848	-4.460658	-0.216816

42A-TS

B3LYP SCF energy: -2068.13117304 a.u.
B3LYP enthalpy: -2067.379626 a.u.
B3LYP free energy: -2067.521823 a.u.
M06 SCF energy in solution: -2067.51956537 a.u.
M06 enthalpy in solution: -2066.768018 a.u.
M06 free energy in solution: -2066.910215 a.u.
Imaginary frequency: -305.0689 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.536473	-2.596850	1.718284
O	1.311710	-1.902314	2.718331
O	1.523539	-2.224274	0.481335
C	1.886255	-4.116034	1.871776
Pd	1.267233	-0.290582	-0.161769
C	1.224543	2.689986	-0.661364
O	1.357836	3.010383	0.530050
O	1.028374	1.509634	-1.140534
C	1.274043	3.785018	-1.779504
C	4.122089	-0.439396	-1.253111
O	3.762771	-0.947791	-2.328115
O	3.387475	-0.062529	-0.269648
C	5.653163	-0.194790	-0.988353
C	-2.762200	2.070213	3.726098
C	-1.628597	2.239186	2.913505
C	-1.159725	3.548318	2.697318
C	-1.807404	4.645033	3.273953
C	-2.937482	4.461706	4.080445
C	-3.413430	3.165450	4.304265
H	-3.135065	1.063214	3.908315
H	-0.279801	3.686300	2.071284

H	-1.425026	5.648776	3.094229
H	-3.439640	5.317502	4.529462
H	-4.290087	3.005672	4.930907
C	-0.933439	1.059721	2.270790
H	0.139041	1.260201	2.189362
H	-1.044057	0.169294	2.903017
C	-1.469596	0.739979	0.857000
H	-1.330500	1.608829	0.203856
H	-2.559630	0.568068	0.919756
C	-0.816725	-0.491454	0.250575
H	-0.857405	-1.356954	0.913529
C	-1.048697	-0.801183	-1.125533
H	-1.047115	0.002808	-1.853143
H	-0.734323	-1.770886	-1.491822
C	-5.250938	-0.793650	-1.912086
C	-5.161023	-1.981885	-1.192008
C	-6.291890	-2.716233	-0.859145
C	-7.538307	-2.217054	-1.273101
C	-7.628850	-1.019033	-1.998096
C	-6.475467	-0.288107	-2.328970
C	-3.833046	-0.287495	-2.096531
C	-3.686204	-2.220660	-0.925157
H	-6.206937	-3.642279	-0.295763
H	-8.447515	-2.763599	-1.028411
H	-8.606975	-0.652850	-2.305358
H	-6.531085	0.641998	-2.889267
N	-2.978595	-1.181650	-1.489454
O	-3.237153	-3.192537	-0.321653
O	-3.533223	0.738305	-2.704768
C	-0.050741	3.760178	-2.569530
H	-0.034971	4.520207	-3.366180
H	-0.216365	2.779236	-3.023546
H	-0.907033	3.974192	-1.916873
C	2.445043	3.458174	-2.730083
H	2.489948	4.191910	-3.550405
H	3.403736	3.486555	-2.196373
H	2.330565	2.456427	-3.154172
C	1.480742	5.176715	-1.160408
H	0.661533	5.433123	-0.479072
H	2.410213	5.218039	-0.581976
H	1.525486	5.939435	-1.953350
C	6.069556	-0.992572	0.264506
H	7.135987	-0.830623	0.490982
H	5.472682	-0.686106	1.128801
H	5.914719	-2.069201	0.114348
C	6.492702	-0.647243	-2.193346
H	6.206392	-0.101734	-3.099559
H	7.563320	-0.471226	-1.999981
H	6.344317	-1.713284	-2.398748
C	5.879749	1.308798	-0.731042
H	6.939747	1.508736	-0.504532
H	5.605179	1.903724	-1.612421
H	5.266172	1.650157	0.108066
C	3.304989	-4.349018	1.310765
H	3.576177	-5.414335	1.380915
H	3.360246	-4.037018	0.263539
H	4.050283	-3.771159	1.872770

C	1.837750	-4.528374	3.351440
H	0.839162	-4.368230	3.773185
H	2.095457	-5.594058	3.455837
H	2.540533	-3.937346	3.948849
C	0.872936	-4.952721	1.063802
H	1.104379	-6.025954	1.153676
H	-0.151328	-4.794550	1.424455
H	0.898746	-4.674059	0.006428

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B3LYP SCF energy: -2095.04298021 a.u.
B3LYP enthalpy: -2094.732391 a.u.
B3LYP free energy: -2094.841288 a.u.
M06 SCF energy in solution: -2094.67251138 a.u.
M06 enthalpy in solution: -2094.361922 a.u.
M06 free energy in solution: -2094.470819 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.927107	-2.532871	0.185022
O	1.011288	-2.819892	0.943072
O	2.049687	-1.558423	-0.648272
C	3.165255	-3.483342	0.098505
Pd	0.672038	-0.060086	-0.742085
C	-1.310633	2.039759	-0.181330
O	-1.669214	1.578472	0.892123
O	-0.499528	1.576293	-1.067087
C	-1.940343	3.383762	-0.674179
C	2.775836	1.671983	0.185225
O	3.183566	1.802783	-0.960849
O	1.772582	1.008301	0.641812
C	3.521729	2.408642	1.344959
C	-4.817087	-2.669095	0.574082
C	-3.968239	-1.560693	0.722918
C	-4.519680	-0.357043	1.191950
C	-5.881273	-0.266398	1.496838
C	-6.717087	-1.376994	1.340564
C	-6.179016	-2.582294	0.878285
H	-4.403121	-3.614232	0.225218
H	-3.870211	0.505573	1.321231
H	-6.287563	0.674399	1.861784
H	-7.775433	-1.306079	1.581974
H	-6.816785	-3.456089	0.760804
C	-2.498951	-1.650772	0.365931
H	-1.920386	-0.952553	0.977653
H	-2.121348	-2.657807	0.583933
C	-2.239789	-1.332799	-1.124607
H	-2.557153	-0.312189	-1.363513
H	-2.862966	-2.003346	-1.740623
C	-0.814739	-1.567248	-1.554957
H	-0.377251	-2.495166	-1.191570
C	-0.158099	-0.893741	-2.571613
H	-0.633660	-0.062440	-3.087379
H	0.725087	-1.322012	-3.039242
F	3.165489	-4.403595	1.082835

F	3.152531	-4.165138	-1.082422
F	4.339103	-2.820238	0.165340
F	4.640954	3.029609	0.916824
F	2.732739	3.358460	1.910409
F	3.893984	1.556423	2.331644
F	-1.018027	4.257441	-1.131555
F	-2.634718	4.004315	0.299566
F	-2.813161	3.147219	-1.695566

43M-TS

B3LYP SCF energy: -2607.53878467 a.u.
B3LYP enthalpy: -2607.116454 a.u.
B3LYP free energy: -2607.251148 a.u.
M06 SCF energy in solution: -2607.10042809 a.u.
M06 enthalpy in solution: -2606.678097 a.u.
M06 free energy in solution: -2606.812791 a.u.
Imaginary frequency: -208.6850 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.374155	-2.514049	1.507197
O	0.315895	-1.722732	2.440597
O	0.599727	-2.344044	0.258594
C	0.109513	-4.030227	1.806582
Pd	1.224046	-0.557781	-0.548508
C	2.242821	2.185633	-1.172629
O	2.174491	2.659117	-0.040367
O	1.893389	1.056515	-1.646757
C	2.813413	3.140784	-2.277228
C	4.045089	-1.610835	-0.545083
O	3.960495	-2.146974	-1.649611
O	3.214042	-0.936924	0.141822
C	5.444036	-1.728765	0.160868
C	-2.000803	3.301020	3.141073
C	-0.873258	3.025900	2.348760
C	0.059963	4.055530	2.138615
C	-0.131596	5.319635	2.706224
C	-1.257370	5.581211	3.495101
C	-2.193843	4.563812	3.710162
H	-2.731557	2.512014	3.310806
H	0.934593	3.853307	1.525087
H	0.605063	6.101960	2.531242
H	-1.403209	6.565382	3.937826
H	-3.073946	4.751446	4.323557
C	-0.683471	1.660567	1.721430
H	0.381972	1.436909	1.617531
H	-1.113821	0.891492	2.372721
C	-1.363521	1.569309	0.329929
H	-0.851562	2.223758	-0.384657
H	-2.392491	1.924838	0.426781
C	-1.404870	0.153319	-0.201662
H	-1.628970	-0.604019	0.542345
C	-0.693981	-0.263617	-1.363650
H	-0.580295	0.479954	-2.151316
H	-0.942824	-1.257583	-1.735943

C	-5.465604	-0.604282	-1.810203
C	-5.692854	-0.721470	-0.441568
C	-6.918326	-1.142496	0.058158
C	-7.928972	-1.448944	-0.868625
C	-7.700767	-1.329329	-2.247920
C	-6.455522	-0.900620	-2.737938
C	-4.034384	-0.122095	-1.975626
C	-4.403642	-0.314913	0.245385
H	-7.081005	-1.232500	1.129401
H	-8.901932	-1.785795	-0.515082
H	-8.500088	-1.574875	-2.945029
H	-6.264540	-0.805437	-3.804096
N	-3.483450	0.022013	-0.720745
O	-4.239756	-0.289564	1.465966
O	-3.503390	0.105922	-3.061205
F	-0.101948	-4.270287	3.122029
F	-0.991485	-4.489775	1.148916
F	1.148560	-4.820066	1.431288
F	6.002914	-2.957361	-0.015608
F	6.327403	-0.829234	-0.368144
F	5.427319	-1.508756	1.496404
F	3.145883	2.535093	-3.437840
F	3.923027	3.795211	-1.847327
F	1.894584	4.103174	-2.589828

43A-TS

B3LYP SCF energy: -2607.54171092 a.u.
B3LYP enthalpy: -2607.119411 a.u.
B3LYP free energy: -2607.255102 a.u.
M06 SCF energy in solution: -2607.10270144 a.u.
M06 enthalpy in solution: -2606.680402 a.u.
M06 free energy in solution: -2606.816093 a.u.
Imaginary frequency: -243.7856 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.455444	-2.271895	2.155284
O	1.474985	-1.427686	3.043995
O	1.325493	-2.169263	0.886088
C	1.641727	-3.771297	2.574000
Pd	1.241914	-0.353759	-0.074599
C	1.514767	2.475423	-0.959496
O	1.821771	2.949336	0.131751
O	1.146517	1.303204	-1.303696
C	1.483915	3.470316	-2.170253
C	3.927897	-1.052712	-1.264548
O	3.470272	-1.745966	-2.172083
O	3.370103	-0.391331	-0.332439
C	5.492465	-0.906793	-1.250933
C	-2.488383	3.153931	3.265999
C	-1.316664	3.065686	2.495615
C	-0.712573	4.261896	2.070499
C	-1.264740	5.502454	2.404484
C	-2.432372	5.575558	3.172494
C	-3.043370	4.392693	3.602859

H	-2.968457	2.237029	3.604229
H	0.195751	4.205822	1.474517
H	-0.778957	6.414838	2.062925
H	-2.861020	6.542063	3.432662
H	-3.951736	4.433551	4.202185
C	-0.729074	1.724515	2.112527
H	0.353790	1.816927	1.985040
H	-0.897486	1.001466	2.921320
C	-1.334016	1.155200	0.810190
H	-1.155652	1.845868	-0.022256
H	-2.427362	1.078747	0.927264
C	-0.818774	-0.232241	0.479018
H	-0.892546	-0.920917	1.320333
C	-1.101120	-0.814616	-0.785347
H	-1.117563	-0.204099	-1.680773
H	-0.921990	-1.872365	-0.933342
C	-5.251089	-1.484212	-2.040827
C	-5.425144	-1.707026	-0.677574
C	-6.657870	-2.073747	-0.153538
C	-7.731059	-2.214205	-1.049523
C	-7.555586	-1.989689	-2.423521
C	-6.302096	-1.618667	-2.938664
C	-3.793327	-1.110237	-2.235477
C	-4.075949	-1.470760	-0.021585
H	-6.779709	-2.244814	0.913269
H	-8.712573	-2.500931	-0.675951
H	-8.403466	-2.105390	-3.096480
H	-6.152182	-1.441515	-4.000904
N	-3.178299	-1.121817	-1.004610
O	-3.864782	-1.579293	1.185614
O	-3.280702	-0.848479	-3.323273
F	2.925291	-4.178813	2.370696
F	1.377952	-3.972825	3.888909
F	0.844799	-4.626674	1.886819
F	6.116176	-2.093346	-1.489441
F	5.904164	-0.054622	-2.237226
F	6.012428	-0.431631	-0.094491
F	1.659677	2.890820	-3.377096
F	0.280780	4.117423	-2.215669
F	2.432497	4.433862	-2.057831

44M-TS

B3LYP SCF energy: -1918.81609779 a.u.
B3LYP enthalpy: -1918.325289 a.u.
B3LYP free energy: -1918.450165 a.u.
M06 SCF energy in solution: -1918.35752435 a.u.
M06 enthalpy in solution: -1917.866716 a.u.
M06 free energy in solution: -1917.991592 a.u.
Imaginary frequency: -282.4972 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.441050	-1.769670	2.650242
O	1.839991	-0.651303	3.005644
O	1.360549	-2.241028	1.449652

C	0.910121	-2.756170	3.704780
H	1.340017	-2.524546	4.684843
H	-0.180819	-2.649342	3.770346
H	1.133250	-3.791037	3.424226
Pd	2.110146	-1.377781	-0.257739
C	3.276491	0.244461	-2.538013
O	3.377649	1.309815	-1.905831
O	2.766574	-0.868741	-2.145716
C	3.834048	0.171925	-3.971267
H	3.277043	-0.549685	-4.577906
H	3.811467	1.162915	-4.437290
H	4.878745	-0.163694	-3.923578
C	4.499435	-3.249353	-0.118493
O	3.903480	-4.166250	-0.708770
O	4.060566	-2.084941	0.203721
C	5.973471	-3.459013	0.297767
H	6.620552	-2.837686	-0.336020
H	6.128323	-3.137825	1.334809
H	6.261005	-4.509603	0.181498
C	1.509301	4.256635	1.945478
C	1.973058	3.417399	0.918278
C	2.764495	3.987213	-0.096057
C	3.072660	5.351283	-0.079879
C	2.600884	6.177179	0.947825
C	1.816346	5.621550	1.964346
H	0.905890	3.827797	2.744253
H	3.136207	3.339807	-0.887439
H	3.689813	5.770476	-0.873473
H	2.845377	7.238570	0.959106
H	1.447415	6.248638	2.775205
C	1.620732	1.945595	0.887222
H	2.437959	1.378945	0.433695
H	1.489923	1.559620	1.903714
C	0.326441	1.696896	0.066546
H	0.501750	1.946608	-0.985324
H	-0.454084	2.367374	0.441858
C	-0.176708	0.269244	0.181732
H	-0.321867	-0.071065	1.203242
C	0.167200	-0.743625	-0.778077
H	0.214275	-0.402437	-1.813070
H	-0.383907	-1.680476	-0.659217
C	-4.206186	0.416248	-1.117442
C	-4.393054	-0.080609	0.170404
C	-5.630245	-0.517489	0.613233
C	-6.687468	-0.428684	-0.309918
C	-6.517747	0.068036	-1.611939
C	-5.255057	0.501455	-2.027515
C	-2.747600	0.816609	-1.229128
C	-3.046002	0.004113	0.866707
H	-5.783164	-0.906798	1.613001
H	-7.373967	0.106231	-2.275023
H	-5.092980	0.891250	-3.028514
N	-2.143024	0.556607	-0.018482
O	-2.841158	-0.352411	2.022277
O	-2.245242	1.302370	-2.238232
N	-8.022863	-0.866824	0.096576
O	-8.944248	-0.802470	-0.731599

O	-8.176622	-1.284037	1.250781

44A-TS

B3LYP SCF energy: -1918.81894344 a.u.
B3LYP enthalpy: -1918.328072 a.u.
B3LYP free energy: -1918.452786 a.u.
M06 SCF energy in solution: -1918.36241007 a.u.
M06 enthalpy in solution: -1917.871539 a.u.
M06 free energy in solution: -1917.996253 a.u.
Imaginary frequency: -370.6885 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.925576	-1.557454	2.698803
O	2.786412	-0.419579	3.169617
O	2.866244	-1.919823	1.459760
C	3.168020	-2.750709	3.641247
H	2.237602	-3.325558	3.739681
H	3.928954	-3.422331	3.228068
H	3.471387	-2.395525	4.631408
Pd	2.632352	-0.639570	-0.128900
C	2.644034	1.578472	-2.173296
O	2.894642	2.486711	-1.364373
O	2.369271	0.343835	-1.921530
C	2.643628	1.882198	-3.681326
H	3.561195	1.474156	-4.125049
H	1.795351	1.395454	-4.175329
H	2.613722	2.962858	-3.854154
C	5.323668	-1.648074	-1.131776
O	4.821124	-2.624971	-1.713140
O	4.731786	-0.712988	-0.478163
C	6.861767	-1.490925	-1.134087
H	7.146894	-0.437245	-1.234400
H	7.257622	-1.850416	-0.174191
H	7.307260	-2.084240	-1.940333
C	-0.871786	3.777485	2.102160
C	0.158860	3.382737	1.232755
C	0.622637	4.318918	0.289571
C	0.068582	5.600764	0.222105
C	-0.959983	5.979770	1.093785
C	-1.428923	5.059587	2.037206
H	-1.237965	3.067471	2.842623
H	1.424191	4.021221	-0.384505
H	0.444477	6.309045	-0.514913
H	-1.389427	6.979131	1.039101
H	-2.226824	5.339241	2.724113
C	0.747429	1.990524	1.284136
H	1.810238	2.026895	1.027231
H	0.679470	1.588786	2.303011
C	0.053517	1.011501	0.310154
H	0.159665	1.377174	-0.717485
H	-1.031116	1.008770	0.530098
C	0.588391	-0.407648	0.426527
H	0.565998	-0.777023	1.453244
C	0.187750	-1.384028	-0.548913

H	0.183941	-1.096967	-1.595705
H	0.441911	-2.419692	-0.354904
C	-3.982667	-1.117371	-0.738852
C	-3.837069	-1.767466	0.484637
C	-4.925317	-2.017192	1.314450
C	-6.185656	-1.590580	0.885060
C	-6.313418	-0.939349	-0.351828
C	-5.216700	-0.683059	-1.193250
C	-2.602062	-1.058740	-1.368055
C	-2.370648	-2.128262	0.621534
H	-4.794957	-2.526594	2.265025
H	-7.071786	-1.752535	1.487311
H	-5.338456	-0.175221	-2.142821
N	-1.720780	-1.686619	-0.510574
O	-1.895401	-2.732862	1.577269
O	-2.357589	-0.556907	-2.459262
N	-7.648824	-0.518007	-0.778833
O	-8.605052	-0.722985	-0.016308
O	-7.766199	0.024461	-1.883666

45M-TS

B3LYP SCF energy: -2149.52169260 a.u.
B3LYP enthalpy: -2149.033904 a.u.
B3LYP free energy: -2149.155450 a.u.
M06 SCF energy in solution: -2149.12333240 a.u.
M06 enthalpy in solution: -2148.635544 a.u.
M06 free energy in solution: -2148.757090 a.u.
Imaginary frequency: -257.0187 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.194785	-1.786524	-2.623139
O	-1.035880	-0.603401	-2.970842
O	-1.448492	-2.245108	-1.447999
C	-1.032826	-2.895565	-3.678822
H	-1.450492	-2.561048	-4.635294
H	0.038919	-3.084070	-3.826561
H	-1.511198	-3.826571	-3.358765
Pd	-1.896689	-1.217477	0.282676
C	-2.781304	0.582385	2.567126
O	-2.890564	1.624790	1.898232
O	-2.341710	-0.565062	2.192090
C	-3.229191	0.588982	4.041471
H	-2.543608	-0.000479	4.660531
H	-3.293849	1.615589	4.417318
H	-4.220983	0.122717	4.110861
C	-4.664580	-2.555616	0.202635
O	-4.303456	-3.578810	0.811515
O	-3.975699	-1.519075	-0.108848
C	-6.127054	-2.468571	-0.297410
H	-6.753638	-3.209585	0.211777
H	-6.530385	-1.460569	-0.144163
H	-6.148291	-2.670563	-1.377282
C	-0.440839	4.247873	-1.874121
C	-1.059638	3.476938	-0.874729

C	-1.813133	4.146186	0.107018
C	-1.936462	5.539575	0.085644
C	-1.313132	6.295814	-0.914276
C	-0.563051	5.641162	-1.897987
H	0.138429	3.742685	-2.645610
H	-2.303177	3.552945	0.876282
H	-2.528154	6.036692	0.853367
H	-1.413575	7.380484	-0.929849
H	-0.076434	6.214248	-2.686572
C	-0.911865	1.970336	-0.843996
H	-1.783940	1.523378	-0.359439
H	-0.865266	1.567420	-1.861080
C	0.363707	1.546096	-0.068225
H	0.256324	1.796629	0.992438
H	1.211805	2.118432	-0.460233
C	0.676110	0.061512	-0.218596
H	0.713149	-0.256896	-1.258665
C	0.132717	-0.927377	0.701491
H	0.182173	-0.624673	1.749180
H	0.548597	-1.926080	0.538374
C	4.561804	-0.257817	1.257590
C	4.962682	-0.765464	0.030431
C	6.237520	-1.271411	-0.191862
C	7.131630	-1.257203	0.886866
C	6.741483	-0.746052	2.134917
C	5.451387	-0.239827	2.330626
C	3.132135	0.235923	1.253017
H	6.527090	-1.664582	-1.162393
H	7.452245	-0.746432	2.958721
H	5.127724	0.158763	3.288017
N	2.542781	0.065145	0.025481
O	2.606932	0.726350	2.250012
H	8.138722	-1.647315	0.755171
S	3.577581	-0.607591	-1.114610
O	3.127071	-1.937827	-1.553555
O	3.931155	0.366911	-2.164083

45A-TS

B3LYP SCF energy: -2149.52403263 a.u.
B3LYP enthalpy: -2149.036193 a.u.
B3LYP free energy: -2149.157453 a.u.
M06 SCF energy in solution: -2149.12769220 a.u.
M06 enthalpy in solution: -2148.639853 a.u.
M06 free energy in solution: -2148.761113 a.u.
Imaginary frequency: -321.5280 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.213911	-1.504317	2.924774
O	2.216733	-0.323434	3.304355
O	2.135609	-1.958223	1.719776
C	2.279154	-2.638318	3.966992
H	2.568715	-2.239904	4.945007
H	1.290042	-3.107850	4.050902
H	2.985505	-3.413672	3.648599

Pd	2.089553	-0.833204	-0.004426
C	2.439246	1.127507	-2.279345
O	2.872619	2.056245	-1.577482
O	1.952792	-0.002080	-1.893871
C	2.454802	1.266827	-3.812416
H	3.272069	0.654096	-4.215106
H	1.520281	0.893648	-4.246379
H	2.615704	2.310742	-4.101089
C	4.604963	-2.365540	-0.883088
O	3.972425	-3.318520	-1.372979
O	4.152562	-1.294066	-0.341506
C	6.151512	-2.431095	-0.872656
H	6.510923	-3.185127	-1.582095
H	6.583690	-1.451241	-1.108028
H	6.490102	-2.706513	0.135837
C	-0.452284	4.290647	1.907782
C	0.445691	3.621127	1.059766
C	1.074569	4.365820	0.043789
C	0.808135	5.729140	-0.113028
C	-0.090834	6.383349	0.739174
C	-0.722109	5.655278	1.753128
H	-0.942713	3.730157	2.702627
H	1.774401	3.854240	-0.615323
H	1.308199	6.285049	-0.905097
H	-0.295735	7.446006	0.614816
H	-1.423019	6.149056	2.425594
C	0.728731	2.143638	1.212712
H	1.779432	1.941671	0.982935
H	0.570860	1.834371	2.253382
C	-0.139710	1.263792	0.285285
H	0.038788	1.548361	-0.758246
H	-1.205189	1.477910	0.484413
C	0.123866	-0.223774	0.484392
H	0.007560	-0.520785	1.528697
C	-0.510476	-1.154452	-0.432433
H	-0.406642	-0.945120	-1.494675
H	-0.418699	-2.208379	-0.187493
C	-4.852364	-0.842376	-0.695353
C	-4.524777	-1.418593	0.523541
C	-5.529393	-1.769803	1.423450
C	-6.859852	-1.522803	1.066090
C	-7.175079	-0.936908	-0.170141
C	-6.164431	-0.586253	-1.074780
C	-3.034508	-1.603423	0.707680
H	-5.262508	-2.220796	2.375045
H	-7.661381	-1.785496	1.753226
H	-6.395809	-0.131042	-2.033676
N	-2.334568	-1.115166	-0.366348
O	-2.555179	-2.135731	1.705059
H	-8.215424	-0.751733	-0.429101
S	-3.321244	-0.536368	-1.599005
O	-3.265544	-1.411938	-2.784582
O	-3.149429	0.907866	-1.816837

46

B3LYP SCF energy: -1513.15433227 a.u.
B3LYP enthalpy: -1512.916024 a.u.
B3LYP free energy: -1512.982304 a.u.
M06 SCF energy in solution: -1512.88944801 a.u.
M06 enthalpy in solution: -1512.651140 a.u.
M06 free energy in solution: -1512.717420 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Pd	2.134895	0.144093	0.015229
C	-1.004238	-0.283352	-0.206886
H	-1.099563	0.740014	-0.579252
C	0.276511	-0.910255	-0.675604
H	0.456489	-1.920811	-0.311608
C	1.049853	-0.464051	-1.747910
H	0.768860	0.433729	-2.293445
H	1.739346	-1.140296	-2.247230
H	-1.025121	-0.253404	0.889255
C	-2.205075	-1.140576	-0.702066
H	-2.187245	-1.172972	-1.798039
H	-2.081767	-2.169172	-0.341569
C	-3.530690	-0.585546	-0.225135
C	-4.251175	0.331703	-1.007367
C	-4.056992	-0.957541	1.023017
C	-5.463879	0.864458	-0.555856
H	-3.861745	0.627680	-1.979831
C	-5.268821	-0.427622	1.478619
H	-3.516009	-1.672462	1.640366
C	-5.976827	0.486961	0.690176
H	-6.008187	1.570597	-1.178866
H	-5.661365	-0.732300	2.446183
H	-6.920520	0.897495	1.041441
Cl	1.319755	2.340428	-0.147857
Cl	3.210619	-1.931239	0.229441
O	3.572898	0.924462	1.442520
H	3.751346	1.871378	1.275700
H	4.428800	0.455272	1.383362

47M-TS

B3LYP SCF energy: -1628.86420218 a.u.
B3LYP enthalpy: -1628.568692 a.u.
B3LYP free energy: -1628.645162 a.u.
M06 SCF energy in solution: -1628.56937358 a.u.
M06 enthalpy in solution: -1628.273863 a.u.
M06 free energy in solution: -1628.350333 a.u.
Imaginary frequency: -208.3989 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Pd	2.175698	-0.523851	0.070711
C	-1.136886	0.567786	0.344592
H	-1.470826	0.571068	1.390314
C	0.131570	1.369357	0.215677
H	0.342135	1.752965	-0.780914
C	1.302160	1.070370	1.034497

H	1.063536	0.763781	2.055233
H	2.065234	1.852045	1.003868
H	-0.857866	-0.470048	0.121845
O	-0.477095	3.006598	0.836837
C	-2.269645	1.004666	-0.604698
H	-2.539586	2.045378	-0.395808
H	-1.895884	0.964876	-1.635885
C	-3.498370	0.127621	-0.474076
C	-4.563030	0.498971	0.362987
C	-3.590561	-1.089218	-1.170271
C	-5.687810	-0.321925	0.504046
H	-4.512654	1.441031	0.906022
C	-4.712778	-1.912999	-1.033272
H	-2.778329	-1.391136	-1.829106
C	-5.766467	-1.532030	-0.193987
H	-6.502783	-0.013772	1.155177
H	-4.766132	-2.848988	-1.584737
H	-6.641002	-2.169570	-0.088314
H	-0.222551	3.011033	1.783739
Cl	1.510440	-2.035612	1.772956
Cl	3.019396	0.877888	-1.645859
O	3.161464	-2.244805	-0.952780
H	3.438849	-2.899930	-0.284431
H	3.975243	-1.939814	-1.396990
C	0.123249	4.166027	0.184195
H	-0.217862	5.060900	0.709803
H	1.213889	4.095930	0.207177
H	-0.246282	4.166624	-0.840945

47A-TS

B3LYP SCF energy: -1628.85922750 a.u.
B3LYP enthalpy: -1628.563393 a.u.
B3LYP free energy: -1628.639581 a.u.
M06 SCF energy in solution: -1628.56533885 a.u.
M06 enthalpy in solution: -1628.269504 a.u.
M06 free energy in solution: -1628.345692 a.u.
Imaginary frequency: -219.2659 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.924081	0.819600	-0.016148
H	-1.022525	0.673105	1.065075
H	-1.439838	1.762947	-0.256557
C	0.543453	0.969782	-0.403584
H	0.663802	1.115412	-1.481277
C	1.348062	1.915078	0.367681
H	1.262537	1.878576	1.450305
H	2.354527	2.118645	0.008427
O	0.668674	3.508238	0.180494
C	-1.642635	-0.321357	-0.767115
H	-1.172881	-1.275653	-0.498468
H	-1.494921	-0.183521	-1.846360
C	-3.125452	-0.374957	-0.462811
C	-4.048365	0.342684	-1.242341
C	-3.612756	-1.119098	0.624877

C	-5.415391	0.321859	-0.944253
H	-3.692780	0.919598	-2.094431
C	-4.978646	-1.143867	0.927661
H	-2.915727	-1.688146	1.237382
C	-5.886193	-0.421842	0.143940
H	-6.111922	0.882312	-1.564001
H	-5.333536	-1.729961	1.772573
H	-6.948455	-0.442154	0.375817
H	0.635288	3.685105	-0.784770
Cl	1.058615	-0.926717	2.258471
Cl	2.656245	-0.588207	-2.198347
Pd	1.727536	-0.697994	-0.014982
O	2.925835	-2.572637	0.295653
H	3.166945	-2.637599	1.239169
H	3.762658	-2.510602	-0.202358
C	1.430677	4.572361	0.842706
H	2.455540	4.589830	0.464595
H	0.916774	5.513994	0.641457
H	1.407145	4.343280	1.907636

48M-TS

B3LYP SCF energy: -1746.81974136 a.u.
B3LYP enthalpy: -1746.436729 a.u.
B3LYP free energy: -1746.520762 a.u.
M06 SCF energy in solution: -1746.46310606 a.u.
M06 enthalpy in solution: -1746.080094 a.u.
M06 free energy in solution: -1746.164127 a.u.
Imaginary frequency: -222.3533 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Pd	-2.179497	-1.046158	-0.088513
C	1.065426	0.040714	-0.317695
H	1.326296	0.001852	-1.382827
C	-0.171616	0.877227	-0.124045
H	-0.343263	1.237629	0.886234
C	-1.360411	0.647816	-0.932108
H	-1.152213	0.419381	-1.979281
H	-2.129085	1.413014	-0.817405
H	0.761331	-0.979182	-0.045477
O	0.504070	2.542252	-0.759919
C	2.281244	0.439748	0.539444
H	2.637578	1.426515	0.229482
H	1.964667	0.519770	1.586922
C	3.409718	-0.565853	0.425877
C	4.421453	-0.408697	-0.535430
C	3.455408	-1.693173	1.263127
C	5.448321	-1.351407	-0.660553
H	4.407053	0.461323	-1.189569
C	4.480041	-2.637948	1.142996
H	2.683490	-1.829620	2.018571
C	5.480740	-2.470590	0.178637
H	6.223794	-1.209320	-1.409932
H	4.498481	-3.501512	1.804076
H	6.279261	-3.202836	0.085277

H	0.141745	2.572980	-1.669371
C	0.261536	3.883641	-0.125136
C	-1.240041	4.111045	0.035183
H	-1.755327	4.070420	-0.931694
H	-1.689141	3.373885	0.707761
H	-1.408693	5.105900	0.463384
C	0.890604	4.896808	-1.082115
H	0.397334	4.879627	-2.062374
H	0.777947	5.905876	-0.669694
H	1.958789	4.697289	-1.219995
C	0.985867	3.851827	1.215100
H	0.563694	3.098924	1.888763
H	2.054202	3.653058	1.083520
H	0.876840	4.829310	1.697858
Cl	-1.601522	-2.361873	-1.978101
Cl	-2.938780	0.141489	1.820118
O	-3.101731	-2.880270	0.783425
H	-3.405499	-3.458993	0.058377
H	-3.895733	-2.638284	1.296986

48A-TS

B3LYP SCF energy: -1746.81714394 a.u.
B3LYP enthalpy: -1746.433723 a.u.
B3LYP free energy: -1746.518243 a.u.
M06 SCF energy in solution: -1746.45839104 a.u.
M06 enthalpy in solution: -1746.074970 a.u.
M06 free energy in solution: -1746.159490 a.u.
Imaginary frequency: -294.6654 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.957583	0.607864	-0.092327
H	-1.062704	0.578564	0.997649
H	-1.078264	1.660189	-0.395059
C	0.436723	0.154253	-0.506133
H	0.562900	0.160072	-1.592371
C	1.580934	0.721818	0.189631
H	1.518520	0.821875	1.267366
H	2.568103	0.487735	-0.193970
O	1.582227	2.493552	-0.151920
C	-2.086207	-0.211723	-0.753286
H	-2.012664	-1.253505	-0.417778
H	-1.931456	-0.213360	-1.840347
C	-3.465066	0.330889	-0.439907
C	-4.063145	1.299851	-1.263319
C	-4.169503	-0.100349	0.696867
C	-5.323721	1.826077	-0.960027
H	-3.537986	1.641482	-2.153669
C	-5.430510	0.422075	1.005011
H	-3.727520	-0.856044	1.343770
C	-6.012651	1.389072	0.177228
H	-5.768939	2.572694	-1.613972
H	-5.959203	0.070699	1.888326
H	-6.993993	1.793771	0.413324
H	1.419472	2.559252	-1.116840

C	2.744928	3.397596	0.193033
C	3.966476	2.973772	-0.617976
H	4.790171	3.666929	-0.412886
H	4.303269	1.966606	-0.352752
H	3.761033	3.007608	-1.695066
C	2.268338	4.799646	-0.180875
H	3.054898	5.523734	0.059694
H	2.059515	4.876555	-1.255368
H	1.365316	5.071495	0.375902
C	2.953955	3.244848	1.694102
H	2.031722	3.456420	2.246277
H	3.305355	2.241563	1.956462
H	3.716746	3.961430	2.017360
Cl	0.290411	-1.619417	2.291565
Cl	1.719374	-2.215472	-2.192506
Pd	0.913670	-1.814869	0.004902
O	1.309573	-3.980848	0.449424
H	1.544214	-4.069538	1.392651
H	2.084114	-4.284940	-0.060351

49M-TS

B3LYP SCF energy: -1608.97233884 a.u.
B3LYP enthalpy: -1608.662563 a.u.
B3LYP free energy: -1608.738222 a.u.
M06 SCF energy in solution: -1608.71860707 a.u.
M06 enthalpy in solution: -1608.408831 a.u.
M06 free energy in solution: -1608.484490 a.u.
Imaginary frequency: -250.6365 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.720774	-0.805660	-0.032091
C	3.946464	0.818200	1.186326
C	2.953547	0.079548	0.526461
C	3.349613	-0.933117	-0.362587
C	4.703693	-1.193981	-0.587523
C	5.685421	-0.448197	0.073957
C	5.302890	0.558867	0.964207
H	3.656978	1.595955	1.891577
H	2.589019	-1.520464	-0.873246
H	4.992090	-1.985044	-1.275475
H	6.738776	-0.655032	-0.098055
H	6.057647	1.137810	1.491241
C	1.483594	0.374406	0.741788
H	0.915525	-0.559785	0.796724
H	1.340953	0.894649	1.697996
C	0.899717	1.240951	-0.404246
H	1.032538	0.721027	-1.358754
H	1.496560	2.161576	-0.449408
C	-0.568855	1.578626	-0.212465
H	-0.870424	1.840577	0.799684
C	-1.593306	0.997181	-1.037873
H	-1.315770	0.784953	-2.071193
H	-2.594998	1.410071	-0.918952
N	-0.529882	3.571241	-0.707989

H	0.149810	4.013716	-0.089592
C	-1.844211	4.231350	-0.626824
H	-0.150523	3.599839	-1.654275
H	-2.531692	3.734472	-1.314797
H	-2.234324	4.122340	0.388775
H	-1.791294	5.296350	-0.882391
Cl	-3.026737	0.169881	1.661863
Cl	-0.515327	-1.939784	-1.700752
O	-1.946297	-2.756867	0.974763
H	-2.830397	-2.784899	1.379864
H	-1.911635	-3.426138	0.268082

49A-TS

B3LYP SCF energy: -1608.97220308 a.u.
B3LYP enthalpy: -1608.662092 a.u.
B3LYP free energy: -1608.737765 a.u.
M06 SCF energy in solution: -1608.71943823 a.u.
M06 enthalpy in solution: -1608.409327 a.u.
M06 free energy in solution: -1608.485000 a.u.
Imaginary frequency: -290.6244 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.699397	-0.755231	0.030857
C	4.100690	0.238027	1.413336
C	3.173662	-0.299992	0.508288
C	3.651663	-0.811889	-0.709346
C	5.015086	-0.782818	-1.013346
C	5.928503	-0.240479	-0.102767
C	5.466646	0.269424	1.113750
H	3.750758	0.627105	2.368171
H	2.946876	-1.241961	-1.418235
H	5.365523	-1.190228	-1.958767
H	6.990162	-0.222588	-0.336492
H	6.168570	0.684772	1.833229
C	1.690729	-0.307919	0.814987
H	1.244400	-1.255111	0.491190
H	1.534066	-0.235122	1.899376
C	0.937431	0.842992	0.114898
H	1.054088	0.744558	-0.969805
H	1.424439	1.790404	0.410790
C	-0.537294	0.924835	0.481927
H	-0.706270	1.051415	1.554452
C	-1.417059	1.711582	-0.343200
H	-1.305314	1.646746	-1.422502
H	-2.426269	1.895070	0.013350
N	-0.894929	3.602131	-0.266961
H	0.079519	3.634416	-0.564836
C	-1.749677	4.488134	-1.078305
H	-0.922398	3.845849	0.722859
H	-1.704957	4.163122	-2.121125
H	-2.781923	4.399617	-0.729284
H	-1.439259	5.537583	-1.016667
Cl	-3.020378	-0.357651	1.934024
Cl	-0.685385	-1.192105	-2.054598

O	-2.844276	-2.621096	-0.284429
H	-3.740701	-2.475430	0.064891
H	-2.904629	-2.751263	-1.247425

50M-TS

B3LYP SCF energy: -2025.70070889 a.u.
B3LYP enthalpy: -2025.349574 a.u.
B3LYP free energy: -2025.441427 a.u.
M06 SCF energy in solution: -2025.32606856 a.u.
M06 enthalpy in solution: -2024.974934 a.u.
M06 free energy in solution: -2025.066787 a.u.
Imaginary frequency: -149.8031 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Pd	-2.375449	-1.729389	-0.056656
C	-0.212412	4.041302	-0.525822
C	-1.310726	3.180326	-0.358751
C	-2.513919	3.718363	0.121842
C	-2.623321	5.080120	0.423671
C	-1.525599	5.928241	0.249485
C	-0.318771	5.401973	-0.225811
H	0.727755	3.630841	-0.889707
H	-3.370012	3.061616	0.263241
H	-3.566238	5.476570	0.795068
H	-1.608410	6.987870	0.482387
H	0.542415	6.052650	-0.364087
C	-1.177192	1.705495	-0.672064
H	-2.161608	1.277922	-0.896245
H	-0.549876	1.579862	-1.562551
C	-0.530016	0.914884	0.488960
H	-1.181085	0.918528	1.368966
H	0.407471	1.406917	0.760800
C	-0.187320	-0.500245	0.105116
H	0.129276	-0.670257	-0.917108
C	-0.509188	-1.635386	0.890424
H	-0.689876	-1.480438	1.951895
H	-0.011981	-2.568282	0.639045
C	4.323909	0.154997	-0.331507
C	4.402772	-0.919013	0.552568
C	5.621084	-1.493382	0.889578
C	6.779328	-0.954177	0.304353
C	6.699745	0.126450	-0.586483
C	5.459625	0.698597	-0.917135
C	2.853255	0.502050	-0.451757
C	2.979547	-1.232375	0.978929
H	5.669849	-2.331457	1.580311
H	7.752340	-1.379422	0.542397
H	7.612073	0.524121	-1.026658
H	5.385475	1.535713	-1.606800
N	2.133230	-0.343443	0.354435
O	2.668445	-2.133240	1.759049
O	2.402577	1.407275	-1.163344
O	-4.407968	-2.050515	-0.951535
H	-4.961061	-2.199661	-0.164228

H	-4.296978	-2.897950	-1.418317
Cl	-1.543311	-2.913672	-1.911222
Cl	-3.519084	-0.796130	1.782974

50A-TS

B3LYP SCF energy: -2025.70162363 a.u.
B3LYP enthalpy: -2025.350684 a.u.
B3LYP free energy: -2025.442387 a.u.
M06 SCF energy in solution: -2025.32686426 a.u.
M06 enthalpy in solution: -2024.975925 a.u.
M06 free energy in solution: -2025.067628 a.u.
Imaginary frequency: -68.6629 cm-1

Cartesian coordinates

ATOM	X	Y	Z
Pd	-1.936505	-1.982247	-0.095038
C	-1.999688	4.045113	-1.057192
C	-2.514358	2.930846	-0.376415
C	-3.336334	3.157491	0.739468
C	-3.638151	4.456059	1.159659
C	-3.120929	5.557389	0.469575
C	-2.298033	5.346150	-0.641229
H	-1.352850	3.889138	-1.918424
H	-3.736940	2.304014	1.282822
H	-4.277272	4.607172	2.027193
H	-3.354721	6.568751	0.795112
H	-1.885597	6.193983	-1.184238
C	-2.173769	1.520973	-0.809476
H	-3.022713	0.858786	-0.600620
H	-2.009323	1.498167	-1.895320
C	-0.921658	0.963608	-0.099290
H	-1.067414	0.979800	0.985065
H	-0.051870	1.599204	-0.327926
C	-0.531300	-0.418265	-0.560639
H	-0.410005	-0.524896	-1.638213
C	0.245604	-1.280407	0.234549
H	0.312071	-1.150925	1.306620
H	0.770014	-2.122110	-0.197030
C	4.455592	0.804230	-0.272000
C	4.779469	-0.285080	0.534099
C	6.093638	-0.560524	0.887964
C	7.093263	0.300750	0.403795
C	6.767123	1.397439	-0.407701
C	5.432188	1.663575	-0.757708
C	2.946524	0.779522	-0.439572
C	3.468580	-0.979400	0.858406
H	6.334238	-1.413910	1.517222
H	8.134963	0.116918	0.659938
H	7.560378	2.048616	-0.769981
H	5.166871	2.510069	-1.386304
N	2.443666	-0.287447	0.260746
O	3.371395	-1.999183	1.546729
O	2.310365	1.605064	-1.103601
Cl	-1.429347	-3.099225	-2.093604
Cl	-2.636087	-1.183082	2.016919

O	-3.624607	-3.434611	0.177023
H	-3.266829	-4.290828	-0.114206
H	-3.700833	-3.444186	1.149506

6M′-TS

B3LYP SCF energy: -1714.90905755 a.u.

B3LYP enthalpy: -1714.409093 a.u.

B3LYP free energy: -1714.528809 a.u.

M06 SCF energy in solution: -1714.35667779 a.u.

M06 enthalpy in solution: -1713.856713 a.u.

M06 free energy in solution: -1713.976429 a.u.

Imaginary frequency: -266.0656 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-3.202812	-2.447458	-2.358445
O	-4.100903	-1.934279	-1.635397
O	-1.970795	-2.398972	-1.989133
C	-3.541960	-3.156138	-3.649938
H	-2.705051	-3.099266	-4.351726
H	-3.737472	-4.214279	-3.434816
H	-4.444677	-2.724887	-4.091794
Pd	-2.372707	-1.422440	-0.195701
C	-3.461177	-1.055430	2.448871
O	-3.442767	-2.282233	2.569395
O	-3.033003	-0.379382	1.414030
C	-4.002506	-0.150604	3.556481
H	-4.425185	-0.756928	4.361615
H	-3.193165	0.472729	3.955264
H	-4.767350	0.524941	3.156845
C	-0.168784	4.528215	-0.287065
C	-1.125440	3.505898	-0.390088
C	-2.450665	3.795411	-0.027667
C	-2.811872	5.069099	0.420868
C	-1.850229	6.080575	0.514941
C	-0.525960	5.803859	0.160462
H	0.862460	4.311980	-0.556902
H	-3.202129	3.011072	-0.093171
H	-3.844802	5.270896	0.696691
H	-2.129711	7.072880	0.862490
H	0.231060	6.582349	0.232157
C	-0.733266	2.119266	-0.854540
H	-1.560849	1.675451	-1.423275
H	0.126402	2.186633	-1.531692

C	-0.383572	1.176654	0.317784
H	-1.235545	1.102375	1.002084
H	0.447473	1.585515	0.899673
C	-0.029682	-0.219317	-0.154519
H	0.124948	-0.356778	-1.221191
C	-0.448090	-1.377736	0.583328
H	-0.519929	-1.267683	1.665015
H	-0.022654	-2.329997	0.261914
C	3.587449	-1.528551	1.217637
C	3.625932	-1.979920	-0.099899
C	4.459750	-3.022030	-0.487848
C	5.264733	-3.608201	0.499532
C	5.225799	-3.153655	1.827688
C	4.381031	-2.100015	2.205470
C	2.588883	-0.404531	1.270524
C	2.648422	-1.145009	-0.879581
H	4.481271	-3.364369	-1.518841
H	5.929863	-4.427652	0.236217
H	5.861135	-3.628397	2.572137
H	4.342132	-1.739560	3.229806
N	2.076581	-0.205320	-0.015858
O	2.384193	-1.266386	-2.070237
O	2.275417	0.229849	2.271341
H	2.550897	1.423104	-0.613506
C	4.093541	2.518345	-1.059881
O	2.769941	2.348930	-0.948377
O	4.921608	1.666701	-0.787970
C	4.438722	3.906453	-1.561549
H	3.932010	4.101236	-2.513262
H	4.089047	4.658336	-0.844526
H	5.519259	3.994863	-1.688573

6A′-TS

B3LYP SCF energy: -1714.91182285 a.u.
B3LYP enthalpy: -1714.411771 a.u.
B3LYP free energy: -1714.532110 a.u.
M06 SCF energy in solution: -1714.35747020 a.u.
M06 enthalpy in solution: -1713.857418 a.u.
M06 free energy in solution: -1713.977757 a.u.
Imaginary frequency: -280.1005 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.311029	-3.715643	-1.683587
O	-2.289357	-3.214223	-2.242304
O	-0.794530	-3.327707	-0.546519
C	-0.561283	-4.900593	-2.293960
H	0.484679	-4.628896	-2.478697
H	-0.559804	-5.744754	-1.594598
H	-1.034764	-5.199066	-3.232657
Pd	-1.759982	-1.853777	0.459271
C	-3.681987	-1.481658	2.086319
O	-3.553056	-2.669247	1.686377
O	-2.867111	-0.569197	1.681204
C	-4.804098	-1.085950	3.020039
H	-5.710103	-0.898313	2.430087
H	-5.018682	-1.902218	3.716019
H	-4.551135	-0.173386	3.566801
C	-2.236576	3.384593	-2.492805
C	-2.695766	2.457410	-1.544374
C	-3.677704	2.877753	-0.631932
C	-4.186362	4.178933	-0.667228
C	-3.720285	5.091465	-1.620022
C	-2.741034	4.688329	-2.533060
H	-1.473146	3.079147	-3.205831
H	-4.040216	2.172488	0.113311
H	-4.948142	4.480456	0.048997
H	-4.115959	6.104420	-1.650323
H	-2.368992	5.388265	-3.278526
C	-2.134185	1.053533	-1.480434
H	-2.929245	0.347804	-1.212391
H	-1.769691	0.753840	-2.471451
C	-0.982139	0.921185	-0.461943
H	-1.322792	1.242960	0.529221
H	-0.165821	1.596046	-0.757866
C	-0.411260	-0.480867	-0.390672
H	-0.164661	-0.912772	-1.361022
C	0.485786	-0.825140	0.668576
H	0.366721	-0.372438	1.645792
H	0.971284	-1.793035	0.651882
C	4.243512	-0.093059	-0.917656
C	4.563857	-0.591018	0.343294
C	5.834850	-1.071428	0.634419
C	6.790685	-1.036646	-0.391884
C	6.467824	-0.534891	-1.662723
C	5.180521	-0.052885	-1.942945

C	2.800700	0.337462	-0.871055
C	3.321258	-0.484201	1.185984
H	6.072887	-1.456371	1.622300
H	7.797603	-1.402363	-0.203201
H	7.229426	-0.520154	-2.439257
H	4.919056	0.339062	-2.922109
N	2.318586	0.113220	0.419581
O	3.200277	-0.870005	2.343352
O	2.166153	0.808041	-1.808182
H	1.805513	1.660266	1.230076
C	2.348324	3.413612	1.855525
O	1.426086	2.455711	1.710002
O	3.499557	3.326975	1.462555
C	1.782206	4.624515	2.569295
H	2.556380	5.386476	2.677253
H	0.936101	5.028477	2.002108
H	1.403525	4.333597	3.555660

CF_3CO_2-
B3LYP SCF energy: -526.37832918 a.u.
B3LYP enthalpy: -526.346890 a.u.
B3LYP free energy: -526.382423 a.u.
M06 SCF energy in solution: -526.31139016 a.u.
M06 enthalpy in solution: -526.279951 a.u.
M06 free energy in solution: -526.315484 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.055209	0.000049	-0.031205
O	1.565907	-1.139512	-0.016086
O	1.566108	1.139512	-0.016080
C	-0.520615	0.000054	-0.011770
F	-1.079290	1.086204	-0.609551
F	-1.079164	-1.084660	-0.612316
F	-0.981955	-0.001612	1.279110

NH_2Me
B3LYP SCF energy: -95.85974078 a.u.
B3LYP enthalpy: -95.791088 a.u.
B3LYP free energy: -95.818354 a.u.
M06 SCF energy in solution: -95.81930299 a.u.
M06 enthalpy in solution: -95.750650 a.u.
M06 free energy in solution: -95.777916 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.750947	-0.000009	-0.120282
H	1.157732	-0.817962	0.328692
C	-0.709641	-0.000009	0.017757

H	1.157683	0.817965	0.328699
H	-1.083356	-0.000901	1.056053
H	-1.115311	0.883004	-0.488195
H	-1.115531	-0.881994	-0.489819

NH_2*i*Pr

B3LYP SCF energy: -174.49461114 a.u.
B3LYP enthalpy: -174.366988 a.u.
B3LYP free energy: -174.400926 a.u.
M06 SCF energy in solution: -174.40974421 a.u.
M06 enthalpy in solution: -174.282121 a.u.
M06 free energy in solution: -174.316059 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	-0.000012	1.386226	-0.204462
H	0.818995	1.907373	0.105870
C	0.000000	0.025957	0.363350
C	1.266895	-0.700941	-0.096090
H	1.304041	-1.717301	0.313843
H	1.295602	-0.761436	-1.190606
H	2.170316	-0.173961	0.238161
C	-1.266881	-0.700964	-0.096088
H	-2.170313	-0.174013	0.238180
H	-1.295597	-0.761445	-1.190604
H	-1.303998	-1.717331	0.313830
H	-0.819053	1.907342	0.105832
H	0.000001	0.042882	1.469695

NH_2*t*Bu

B3LYP SCF energy: -213.81047620 a.u.
B3LYP enthalpy: -213.653761 a.u.
B3LYP free energy: -213.690412 a.u.
M06 SCF energy in solution: -213.70562043 a.u.
M06 enthalpy in solution: -213.548905 a.u.
M06 free energy in solution: -213.585556 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	0.000099	0.133422	1.488156
H	-0.818226	0.659005	1.796081
C	0.000011	-0.004710	0.015691
C	-1.259103	-0.798258	-0.369623
H	-1.304188	-0.961224	-1.452966
H	-1.266250	-1.771577	0.132637
H	-2.169236	-0.257913	-0.076104
C	-0.001057	1.362756	-0.703293
H	-0.001222	1.246758	-1.795218
H	-0.888943	1.947217	-0.428157
H	0.886137	1.948446	-0.428549
C	1.260113	-0.796511	-0.369947
H	2.169592	-0.254960	-0.076625
H	1.268740	-1.769849	0.132254

H	1.305173	-0.959374	-1.453314
H	0.817949	0.659851	1.795898

MeOH

B3LYP SCF energy: -115.72961741 a.u.
B3LYP enthalpy: -115.674176 a.u.
B3LYP free energy: -115.701205 a.u.
M06 SCF energy in solution: -115.69343477 a.u.
M06 enthalpy in solution: -115.637993 a.u.
M06 free energy in solution: -115.665022 a.u.

Cartesian coordinates

ATOM	X	Y	Z
O	-0.753483	0.124229	0.000000
H	-1.146807	-0.764702	0.000000
C	0.672346	-0.019916	0.000000
H	1.090354	0.990376	-0.000002
H	1.025123	-0.550005	0.895384
H	1.025123	-0.550008	-0.895383

***t*BuOH**

B3LYP SCF energy: -233.68836814 a.u.
B3LYP enthalpy: -233.545590 a.u.
B3LYP free energy: -233.582436 a.u.
M06 SCF energy in solution: -233.58547202 a.u.
M06 enthalpy in solution: -233.442694 a.u.
M06 free energy in solution: -233.479540 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.007951	0.000000	0.010692
C	0.673349	1.263701	-0.531191
H	0.195968	2.164113	-0.126079
H	1.736204	1.284072	-0.254104
H	0.613563	1.305308	-1.625825
C	-1.502227	-0.000278	-0.313968
H	-1.661537	-0.000401	-1.398449
H	-1.989967	-0.889339	0.103939
H	-1.990275	0.888690	0.103782
C	0.673846	-1.263389	-0.531293
H	1.736691	-1.283367	-0.254152
H	0.196802	-2.164036	-0.126306
H	0.614143	-1.304897	-1.625936
O	0.065073	-0.000047	1.460639
H	1.005729	0.000034	1.712572

Benzoic-sulfimide-anion

B3LYP SCF energy: -947.79461909 a.u.
B3LYP enthalpy: -947.681813 a.u.
B3LYP free energy: -947.726481 a.u.
M06 SCF energy in solution: -947.67751731 a.u.

M06 enthalpy in solution: -947.564711 a.u.
M06 free energy in solution: -947.609379 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.788614	0.692314	-0.000129
C	-0.302955	-0.607960	-0.000150
C	-1.138099	-1.718324	-0.000148
C	-2.521079	-1.487328	-0.000139
C	-3.027763	-0.178093	0.000060
C	-2.163105	0.924363	0.000049
C	0.334728	1.723945	0.000012
H	-0.734537	-2.727528	-0.000180
H	-3.208373	-2.331267	-0.000156
H	-4.104974	-0.021875	0.000145
H	-2.534780	1.945635	0.000083
N	1.572181	1.165482	0.000154
O	0.077061	2.937992	-0.000004
S	1.504883	-0.474494	0.000005
O	2.033121	-1.064132	-1.254024
O	2.032392	-1.064478	1.254232

4-nitrophthalimide-anion
B3LYP SCF energy: -717.07684799 a.u.
B3LYP enthalpy: -716.960976 a.u.
B3LYP free energy: -717.009165 a.u.
M06 SCF energy in solution: -716.90713751 a.u.
M06 enthalpy in solution: -716.791266 a.u.
M06 free energy in solution: -716.839455 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.080145	-0.776025	-0.000036
C	0.671766	0.555661	-0.000085
C	-0.667051	0.908192	0.000014
C	-1.592067	-0.152200	0.000154
C	-1.200161	-1.499995	0.000196
C	0.161761	-1.821331	0.000102
C	2.606800	-0.748151	-0.000133
C	1.954508	1.385285	-0.000291
H	-0.993262	1.941926	-0.000028
H	-1.963038	-2.269838	0.000305
H	0.495342	-2.855684	0.000146
N	3.036383	0.548088	-0.000297
O	1.947151	2.621019	-0.000283
O	3.286753	-1.782112	-0.000233
N	-3.023268	0.154389	0.000244
O	-3.368585	1.341871	0.000250
O	-3.830950	-0.786072	0.000319

iPr2NH

B3LYP SCF energy: -292.43150217 a.u.
B3LYP enthalpy: -292.215151 a.u.
B3LYP free energy: -292.259912 a.u.
B3LYP free energy after quasi-harmonic correction: -292.258539 a.u.
M06 SCF energy in solution: -292.27682768 a.u.

Cartesian coordinates

ATOM	X	Y	Z
N	-0.013711	0.594641	0.088158
H	0.118323	1.337364	-0.598478
C	-1.247964	-0.140929	-0.226599
H	-1.123772	-0.791720	-1.112898
C	1.242666	-0.162185	0.212818
H	1.087670	-0.907702	1.003212
C	-1.669343	-1.028197	0.952278
H	-2.615197	-1.535660	0.726778
H	-0.927254	-1.803780	1.172809
H	-1.804558	-0.419785	1.854783
C	-2.345008	0.878671	-0.555118
H	-3.284244	0.371728	-0.804735
H	-2.522728	1.540451	0.301300
H	-2.065639	1.501948	-1.415248
C	1.680188	-0.902179	-1.067042
H	2.608209	-1.462577	-0.895825
H	0.922493	-1.616398	-1.408671
H	1.864812	-0.189614	-1.883131
C	2.337915	0.800014	0.688653
H	3.283047	0.269808	0.855745
H	2.524587	1.580280	-0.062908
H	2.039517	1.292001	1.620215

$Pd_2(OAc)_4$
B3LYP SCF energy: -1169.91227278 a.u.
B3LYP enthalpy: -1169.682515 a.u.
B3LYP free energy: -1169.751433 a.u.
B3LYP free energy after quasi-harmonic correction: -1169.749588 a.u.
M06 SCF energy in solution: -1169.61643084 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.830406	-1.844423	0.000210
O	-1.388586	-1.493791	1.144283
O	-1.390172	-1.492269	-1.144010
C	-3.052616	-2.734079	0.000428
H	-3.647334	-2.527416	-0.893534
H	-2.827299	-3.806488	-0.001253
H	-3.645234	-2.529774	0.896299
Pd	0.026959	-0.005881	1.309480
C	1.945942	-1.784808	-0.000075
O	1.537426	-1.396842	-1.144400
O	1.539160	-1.395235	1.144302
C	3.021218	-2.850998	0.000018
H	3.638361	-2.769415	0.897572
H	2.536091	-3.834682	0.004678
H	3.633269	-2.775012	-0.901492

C	-1.942213	1.726499	-0.000182
O	-1.504180	1.370509	1.143805
O	-1.503367	1.371253	-1.144077
C	-3.141012	2.653433	-0.000168
H	-3.146512	3.268656	-0.902677
H	-4.057111	2.046871	0.007921
H	-3.138204	3.278840	0.895616
Pd	0.026777	-0.006284	-1.309495
C	1.796547	1.921456	-0.000028
O	1.413071	1.508382	-1.144277
O	1.411807	1.510113	1.144475
C	2.851001	3.008297	-0.000411
H	2.766754	3.620652	0.900142
H	3.840320	2.534784	-0.003393
H	2.762995	3.623378	-0.898769

$[Pd_2(OAc)_5]^-$

B3LYP SCF energy: -1398.50665771 a.u.
B3LYP enthalpy: -1398.218153 a.u.
B3LYP free energy: -1398.315700 a.u.
B3LYP free energy after quasi-harmonic correction: -1398.303784 a.u.
M06 SCF energy in solution: -1398.21269926 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.021676	0.284982	-2.618837
O	-1.166823	0.318852	-2.065530
O	1.131374	0.324182	-2.082887
C	-0.032554	0.160834	-4.136595
H	-0.016400	-0.905334	-4.394756
H	-0.943323	0.600643	-4.551413
H	0.856648	0.629880	-4.566139
Pd	-1.390986	0.308998	0.018029
C	-3.004189	-2.027507	-0.011039
O	-3.984106	-1.279687	0.039596
O	-1.750589	-1.664679	-0.027734
C	-3.167857	-3.546897	-0.094872
H	-3.104505	-3.854298	-1.146566
H	-2.370940	-4.061195	0.451112
H	-4.148198	-3.835860	0.294706
C	-0.002015	2.930104	0.064331
O	-1.134955	2.361323	0.064814
O	1.131583	2.362913	0.050338
C	-0.003859	4.449006	0.049057
H	0.908139	4.836848	0.509941
H	-0.034786	4.789196	-0.993558
H	-0.889990	4.834276	0.560212
Pd	1.390342	0.311180	-0.003419
C	0.020783	0.163700	2.628004
O	1.165839	0.221113	2.076479
O	-1.132236	0.222445	2.094015
C	0.032821	-0.020810	4.139556
H	-0.868153	0.408404	4.585650
H	0.045025	-1.096330	4.355572
H	0.931845	0.425448	4.572919

C	3.007394	-2.021679	-0.064105
O	1.752921	-1.661733	-0.057676
O	3.986465	-1.271017	-0.057929
C	3.174214	-3.542924	-0.046774
H	4.147376	-3.813326	-0.466825
H	3.135167	-3.891653	0.993198
H	2.367538	-4.037458	-0.596347

$[Pd_2(OAc)_6]^{2-}$

B3LYP SCF energy: -1626.97323647 a.u.
B3LYP enthalpy: -1626.630005 a.u.
B3LYP free energy: -1626.746979 a.u.
B3LYP free energy after quasi-harmonic correction: -1626.729326 a.u.
M06 SCF energy in solution: -1626.76986527 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.392646	0.133530	2.581346
O	-0.779823	-0.951371	2.046971
O	0.125731	1.169347	2.063611
C	-0.555844	0.197516	4.101776
H	-0.823918	1.212915	4.410217
H	-1.308378	-0.520913	4.439096
H	0.405992	-0.055544	4.566218
Pd	-0.561879	-1.350450	-0.008395
C	-3.474561	-1.476292	-0.105492
O	-3.469040	-2.612539	0.386531
O	-2.463592	-0.721213	-0.391174
C	-4.813412	-0.786411	-0.426368
H	-5.053153	-0.080431	0.379794
H	-4.745586	-0.212836	-1.357157
H	-5.614113	-1.530719	-0.492555
C	3.474512	1.476412	0.106073
O	3.468969	2.612286	-0.386795
O	2.463550	0.721367	0.391936
C	4.813357	0.786985	0.427958
H	4.745325	0.214249	1.359259
H	5.053417	0.080292	-0.377484
H	5.613940	1.531455	0.493721
Pd	0.561891	1.350435	0.008278
C	0.392620	-0.133585	-2.581478
O	0.780247	0.951119	-2.047048
O	-0.126200	-1.169216	-2.063808
C	0.555731	-0.197538	-4.101926
H	0.824129	-1.212852	-4.410374
H	-0.406238	0.055140	-4.566292
H	1.307981	0.521148	-4.439321
C	-1.689189	3.224128	-0.094100
O	-1.308557	2.026471	-0.402452
O	-1.049689	4.107267	0.491848
C	-3.121047	3.506383	-0.585154
H	-3.551679	4.344129	-0.026232
H	-3.085358	3.777303	-1.649224
H	-3.748917	2.614742	-0.490235
C	1.689258	-3.224142	0.093771

O	1.049305	-4.107749	-0.490984
O	1.308893	-2.026232	0.401431
C	3.121356	-3.506373	0.584145
H	3.747392	-2.612766	0.496132
H	3.085081	-3.785312	1.646141
H	3.554327	-4.339314	0.019837

$Pd(OAc)_2$

B3LYP SCF energy: -584.93555795 a.u.
B3LYP enthalpy: -584.820446 a.u.
B3LYP free energy: -584.871216 a.u.
B3LYP free energy after quasi-harmonic correction: -584.868554 a.u.
M06 SCF energy in solution: -584.78234477 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.442547	0.000006	-0.004219
O	1.766634	-1.087710	-0.010288
O	1.766625	1.087714	-0.010292
C	3.938131	0.000013	0.036295
H	4.329029	0.899525	-0.446125
H	4.266281	-0.000598	1.083042
H	4.329066	-0.898948	-0.447130
Pd	0.000001	-0.000007	-0.009461
C	-2.442553	0.000018	-0.004219
O	-1.766623	1.087717	-0.010290
O	-1.766630	-1.087702	-0.010294
C	-3.938135	-0.000001	0.036297
H	-4.329030	-0.899265	-0.446596
H	-4.266285	0.000029	1.083045
H	-4.329071	0.899207	-0.446663

$[Pd(OAc)_4]^{2-}$

B3LYP SCF energy: -1042.00069132 a.u.
B3LYP enthalpy: -1041.774518 a.u.
B3LYP free energy: -1041.859217 a.u.
B3LYP free energy after quasi-harmonic correction: -1041.848899 a.u.
M06 SCF energy in solution: -1041.96423895 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.249203	2.064324	0.236355
O	2.276057	2.099790	1.475371
O	1.496777	1.370403	-0.544607
C	3.228302	2.952991	-0.566944
H	3.866113	2.323225	-1.200281
H	2.666216	3.620499	-1.232765
H	3.851504	3.546582	0.110858
Pd	0.060381	0.000136	-0.000020
C	2.248528	-2.064677	-0.236381
O	2.275098	-2.100453	-1.475401
O	1.496646	-1.370218	0.544582
C	3.227217	-2.953849	0.566897

H	3.864633	-2.324569	1.201100
H	2.664678	-3.621837	1.231852
H	3.850772	-3.547019	-0.110951
C	-2.305265	-1.876753	-0.166028
O	-2.582902	-1.676297	-1.357430
O	-1.333182	-1.407637	0.537111
C	-3.219310	-2.795952	0.676165
H	-2.622706	-3.455533	1.317716
H	-3.840409	-2.170745	1.331271
H	-3.870403	-3.388874	0.024004
C	-2.305234	1.877015	0.166112
O	-1.333140	1.407956	-0.537079
O	-2.582704	1.676643	1.357557
C	-3.219367	2.796074	-0.676122
H	-3.839569	2.170847	-1.332057
H	-3.871267	3.388244	-0.024088
H	-2.622724	3.456401	-1.316891

PhthN-

B3LYP SCF energy: -512.55578689 a.u.
B3LYP enthalpy: -512.444812 a.u.
B3LYP free energy: -512.486053 a.u.
B3LYP free energy after quasi-harmonic correction: -512.486053 a.u.
M06 SCF energy in solution: -512.43471968 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.142114	-0.696191	-0.000040
C	-0.142128	0.696178	-0.000110
C	-1.326743	1.420472	0.000033
C	-2.536398	0.701124	0.000227
C	-2.536385	-0.701171	0.000291
C	-1.326718	-1.420500	0.000164
C	1.324602	-1.113722	-0.000252
C	1.324555	1.113751	-0.000354
H	-1.313424	2.508280	-0.000013
H	-3.484272	1.237407	0.000325
H	-3.484249	-1.237471	0.000442
H	-1.313387	-2.508308	0.000209
N	2.119318	0.000031	-0.000086
O	1.682964	2.300607	-0.000127
O	1.683046	-2.300579	0.000113