DFT investigation of the palladium-catalyzed ene-yne coupling

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Abstract

The mechanism of the recently developed palladium-catalyzed ene-yne coupling has been evaluated by DFT methods. The calculations validate the previously proposed reaction mechanism and explain the stereoselectivity of the reaction (exclusive formation of the E-isomer of the disubstituted alkene). Concerning chemoselectivity, the calculations also clarify why the ene-yne coupling is able to dominate over plausible alternative reaction pathways such as alkene homocoupling and alkyne polymerization. The role of the phosphine ligand at various stages of the catalytic cycle has also been delineated.

Introduction

Transition metal-catalyzed cross-coupling reactions are powerful tools for carbon-carbon and carbon-heteroatom bond formation. The advent of such processes has changed, in a fundamental sense, the way organic chemists approach synthetic planning, including the total synthesis of highly complex molecules.[1] Many of the most commonly used catalytic organometallic reactions (e.g. Suzuki, Stille, Negishi etc.) involve the coupling of two functionalized reactants, meaning that the starting materials are often expensive and, since the functionalities are lost in the coupling reactions, the atom economy of the reactions is less than ideal. The recently developed palladium-catalyzed cross-coupling between an alkene and an alkyne, the ene-yne coupling[2] (Scheme 1), has the advantages of perfect atom economy, since no atoms are lost in the reaction, and of cheap, unfunctionalized starting materials.

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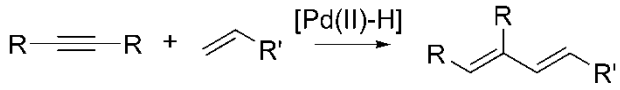


Scheme 1. General ene-yne reaction

The intermolecular palladium-catalyzed ene-yne coupling (Scheme 1) is based on the intramolecular enyne cycloisomerization developed by Trost *et al.*[3] Like the enyne cycloisomerization, the intermolecular ene-yne coupling is expected to be catalyzed by a Pd(II)-H species. The postulated mechanism[2] (Figure 1) starts with coordination of the alkyne to a hydridopalladium complex (step I), and the alkyne is then inserted into the Pd-H bond (step II). The subsequent mechanism is analogous to the well known Heck reaction.[4,5] Coordination of the alkene to palladium (step III) is followed by carbopalladation (step IV). Subsequent β-hydride elimination (step V) gives the complex between the coupling product and palladium, which dissociates into the product and the active catalyst (step VI). Here, the reaction mechanism is expected to diverge from the Heck mechanism, since the Pd(II) hydride closes the cycle without the more common base-assisted reductive elimination. Thus, the reaction is expected to take place via a Pd(II) cycle without involvement of Pd(0).

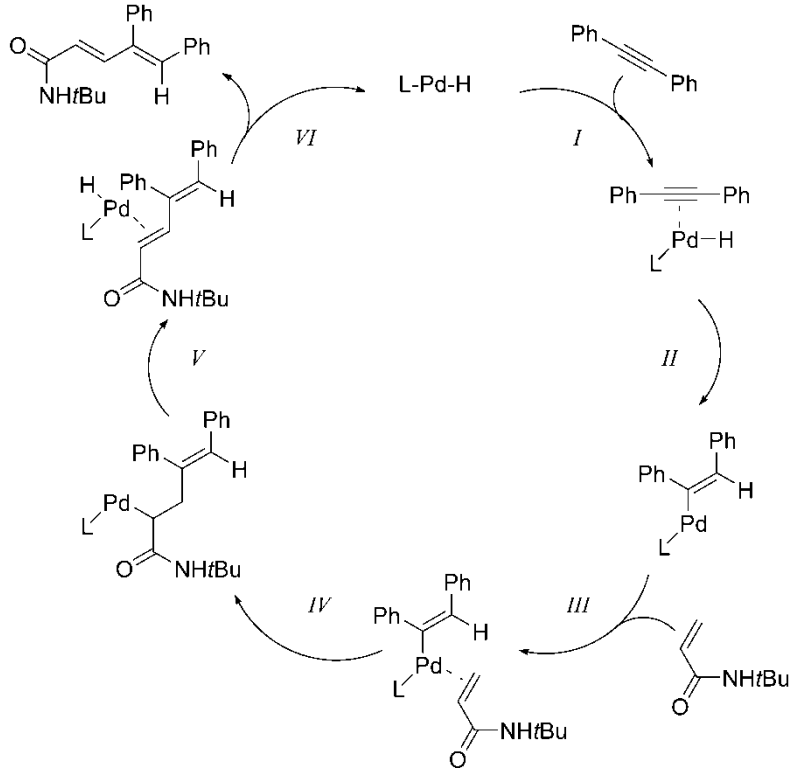
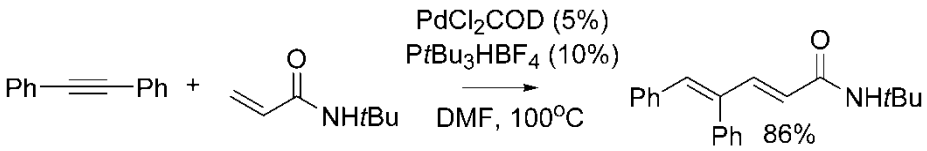


Figure 1 Postulated catalytic cycle for the Pd-catalyzed coupling between diphenyl acetylene and *N-tert*-butyl acrylamide.

The ruthenium-catalyzed version of the intramolecular reaction has been proposed to take place by a different mechanism.[6] It is assumed to take place via a Ru(0/II) catalytic cycle involving the formation of a ruthenacyclopentene complex by a [2+2+1] cycloaddition. However, in the case of

the palladium-catalyzed reaction, the importance of the Pd(II)-H complex has been verified by an experiment in which $HPdCl(PtBu_3)_2$ was synthesized separately and shown to be an active catalyst for the ene-yne coupling.[2] This renders the [2+2+1] cycloaddition mechanism less likely in this case, since this would involve a Pd(0) catalyst instead of the Pd(II)-H catalyst.

The type of phosphine ligand employed in the reaction has been found to be crucial for the reaction efficiency. Only the two bulky, aliphatic phosphines tris(*tert*-butyl)phosphine and CataCXium A (di(1-adamantyl)-*n*-butylphosphine) were found to be efficient out of several investigated ligands including common aromatic phosphines. DMF was found to be the best solvent for the reaction, and a high reaction temperature of 100°C was typically used. The optimized reaction conditions are given in Scheme 2,[2] yielding only the double bond isomer shown.



Scheme 2 Reaction conditions for the coupling between diphenylacetylene and *N*-*tert*-butyl acrylamide.

The present DFT study of the ene-yne coupling was performed in order to verify the proposed reaction mechanism (Figure 1). Furthermore, we aim to explain the selectivity of the reaction: why coupling between one alkyne and one alkene is favored over homo-coupling of two alkenes and over alkyne polymerization. Coupling of the alkene with the alkyne in reverse order cannot take place due to the lack of β-hydrogens after the coupling step, which means that the reaction cannot proceed through β-hydride elimination. However, alkene homo-coupling could in theory take place, and a conceivable mechanism for this is depicted in Figure 2. First, the alkene could coordinate to the hydridopalladium complex (step Ia) followed by insertion of the alkene into the Pd-H bond (step IIa). Subsequent coordination of a second alkene to the complex (step IIIa), followed by insertion of the second alkene into the Pd-C bond (step IVa), β-hydride elimination (step Va) and dissociation of the homo-coupling product (step VIa) would close the catalytic cycle and regenerate the catalyst. Likewise, oligomerization of the alkyne could take place by a number of consecutive alkyne coordination-insertion steps[7] IIIb and IVb in Figure 2, initiated by a hydride addition (R=H). This alternative cycle could be terminated by coordination of an alkene and re-entry into the "normal" cycle, forming heavier products composed of one alkene and at least two alkyne monomers, or by hydride transfer from another complex followed by reductive elimination to form reduced alkyne oligomers. An important part of the current study is to rationalize why these plausible alternatives are less favorable than the desired coupling reaction (Figure 1).

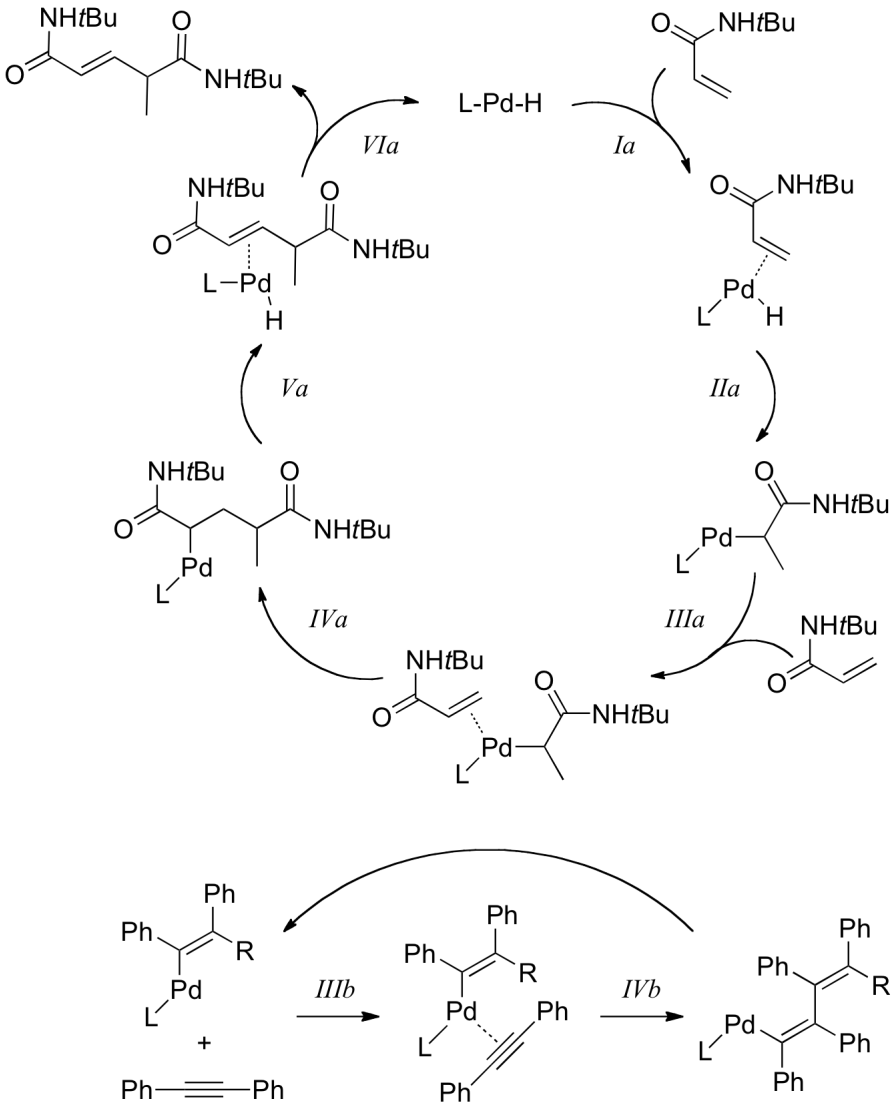


Figure 2 Plausible alternative Pd-catalyzed reactions of the substrates.

Results and Discussion

The catalytic cycle for the title reaction (Figure 1) has been thoroughly investigated by DFT methods and compared to the plausible alternatives in Figure 2. All important isomeric forms have been investigated, but only the most relevant are shown. Acrylamide has been used as a model for the experimentally employed *N-tert*-butyl acrylamide. All free energies are given relative to the energy of the assumed resting state of the catalyst, **1c**.

The Pd-H catalyst complexes. Based on the experimental observation that $HPdCl(PtBu_3)_2$[8] is an excellent catalyst for the title reaction,[2] and earlier studies of Pd(II)-alkyne coordination,[9] the reaction is assumed to take place via a neutral catalytic cycle, with one chloride ligand coordinating to palladium at all times. The energy of the different possible L_n-Pd(H)Cl complexes has been evaluated, where L can be either $PtBu_3$ or a solvent molecule (DMF). For the tricoordinated

complexes there are three different isomeric complexes. For the different ligand combinations, the isomer of lowest free energy as well as the assumed active catalyst is shown in Figure 3.

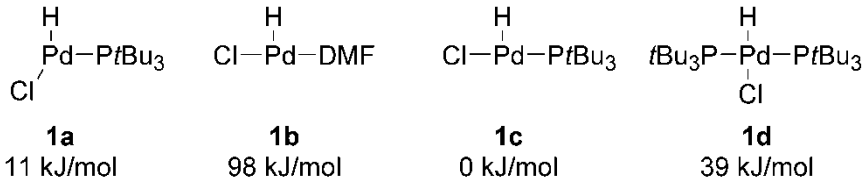


Figure 3 Free energy of different L_n-Pd(H)Cl complexes.

For steric reasons only one complex with two phosphine ligands is possible, namely **1d** (Figure 3) where the bulky ligands are positioned *trans* to each other. As can be seen from Figure 3, the coordination of a second phosphine ligand to **1a** forming **1d** is endergonic by 28 kJ/mol. This energy difference might, however, be exaggerated, due to the method of computing the solution phase free energies, as discussed in the methods section. Since we cannot at this time be certain of the magnitude of this specific systematic error, we cannot exclude the possibility that **1d** is in fact the resting state of the catalyst. Excluding entropic and solvation contributions, that is, comparing only the enthalpies, **1d** is favored, as evidenced also by the fact that this is the preferred form in the crystal phase.[8] However, even should **1d** be favored also in solution, it does not have an empty coordination site, and must dissociate a phosphine to form **1a** before catalysis can take place.

The active catalyst complex **1a** has a distorted T-shape (almost a Y-shape) due to the steric repulsion from the phosphine and the electronic repulsion from the hydride. Since chloride is site labile,[10] the chloride in **1a** is expected to easily switch position, and to be in rapid equilibrium with the slightly more stable **1c** where the empty coordination site is *trans* to the very strongly *trans*-influencing[11] hydride. This complex is in itself not a catalyst since the bulky phosphine ligand in *cis* position to the vacant site on palladium renders coordination of the alkyne impossible, and since the alkyne and the hydrogen need to be positioned *cis* to each other in order for hydropalladation to occur. Complex **1c** is expected to first pay the energy penalty of switching the position of chloride to form **1a** before the alkyne coordination can take place. Substitution of the phosphine ligand with a solvent molecule (**1b**) is associated with an energy penalty of 98 kJ/mol (compare **1b** and **c**). Thus, it is likely that one equivalent of the phosphine ligand is necessary in order to stabilize the 'free catalyst'.

Alkyne coordination and hydropalladation (steps I and II). Despite the observation that the solvato complex **1b** is 87 kJ/mol higher in energy than **1a**, the reactions from both these complexes have been investigated, since **1b** is substantially less encumbered than **1a**. The energy difference between the two paths does indeed decrease to 18 kJ/mol upon alkyne coordination (**2a** vs. **2b**, Figure 4), as a result both of the steric bulk and the *trans* influence of the phosphine. At the hydropalladation transition state, the phosphine-coordinated TS **3a** is favored by only 6 kJ/mol compared to the solvent-complexed TS **3b**. This corresponds to a rate difference of less than an order of magnitude at the standard state (1 M of all species), and since the relative concentrations of phosphine and DMF differ by more than an order of magnitude, it is certainly possible that a

significant proportion of the reactions follow paths where the ligand has been fully dissociated. This is in line with our earlier suggestions of low-ligated states in Pd-catalyzed reactions,[12] and also with recent experimental studies by Hartwig and coworkers.[13]

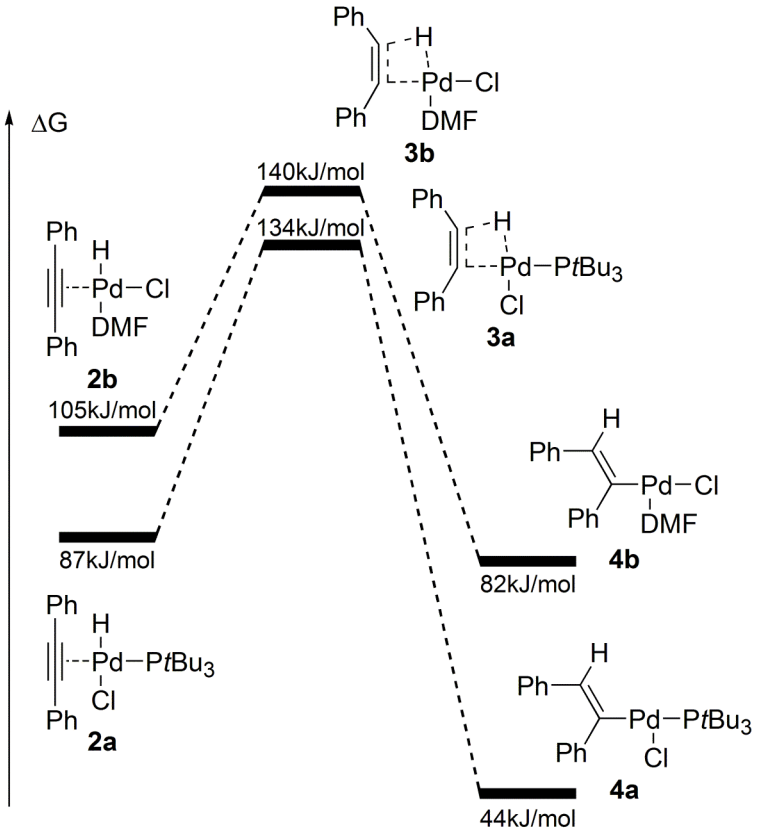


Figure 4 Free energy profile for the hydropalladation step.

The solvato complex **2b** and TS **3b** prefer a geometry where the small, weak DMF ligand is *cis* to the alkyne and *trans* to the very strongly influencing hydride ligand. The alternative geometry (not shown) is higher in energy. The situation is inverted for the bulky, strong phosphine. Steric factors favor a geometry where the phosphine is *trans* to the second most bulky ligand, the alkyne. Electronically, the phosphine has a stronger trans influence than chloride, and therefore prefers a position *cis* to the hydride. The barrier for the hydropalladation step is quite high, 134 kJ/mol, in accordance with a reaction temperature of 100°C. Even so, the calculated barrier is likely to be exaggerated by the systematic errors discussed in the methods section, in particular by the problematic description of non-bonded interactions[14] that lead to exaggerated repulsion with the bulky *t*-butyl groups. As discussed earlier, we can speculate that **1d** is in fact the low energy point, even though it is not formally within the catalytic cycle but must dissociate a phosphine in order to react. It is interesting to note that in a comparison of **3a** with **1d**, we replace a bulky ligand with a bulky substrate, and therefore would expect a partial cancellation of systematic errors in non-bonded interactions. For this comparison, the barrier is more modest, ca. 95 kJ/mol. It should also

be noted that the title reaction runs efficiently at 20°C (87% yield) when the $HPdCl(PtBu_3)_2$ complex is added to the reaction mixture instead of being prepared *in situ*.[2]

The insertion products **4** are tricoordinated T-shaped complexes. These types of complexes are common intermediates in catalytic cycles.[15] Only the insertion product complexes that can be directly reached from the lowest energy transition states are shown in Figure 4. Due to repulsive *trans* interactions between chloride and the vinyl ligand in **4b**, the isomeric complex, where chloride and DMF have switched positions, is 48 kJ/mol lower in energy. Complex **4a** can rearrange to have the vinyl group in a distorted *cis* position relative to the phosphine, yielding a complex that is 12 kJ/mol lower in energy.

Cross-coupling (steps III and IV). In order for cross-coupling to occur, the alkene has to coordinate to the hydropalladation product complexes **4** (Figure 4). Due to steric crowding in the formed Pd-π-alkene complexes **5** (Figure 5) it is no longer advantageous to have a phosphine ligand coordinating to palladium. In the real complexes this tendency should be even more pronounced due to the steric demands of the amide *tert*-butyl group, which has been excluded from this model study.

Attempts to optimize the complex with a phosphine ligand in *trans* position to the alkene always led to *in silico* dissociation of the alkene from the complex. It is therefore assumed that the alkene cannot coordinate *trans* to the phosphine, due to the high *trans* influence of the latter. This effect would be even more important in the transition state and in the product complex, where a Pd-C σ-bond would be formed *trans* to the destabilizing phosphine ligand. Complex **5a** with the phosphine ligand *cis* to the alkene is disfavored by 83 kJ/mol compared to complex **5e** with no phosphine ligand. Even the coordination of a solvent molecule (**5b**) to this complex has an energy cost of 29 kJ/mol. The cross-coupling from complex **5e** through transition state **6e** has an energy barrier of 55 kJ/mol. Since the barrier from **5e** is lower than the energy of complex **5a** itself, the latter can be excluded from further consideration, even when accounting for expected systematic errors in the comparison. In the transition state **6e** the chloride has switched position in order to avoid the *trans* influence from the forming Pd-C bond. In the cross-coupling product **7e** an intramolecular Pd-π-alkene coordination is more favorable than having external ligands coordinating to palladium.

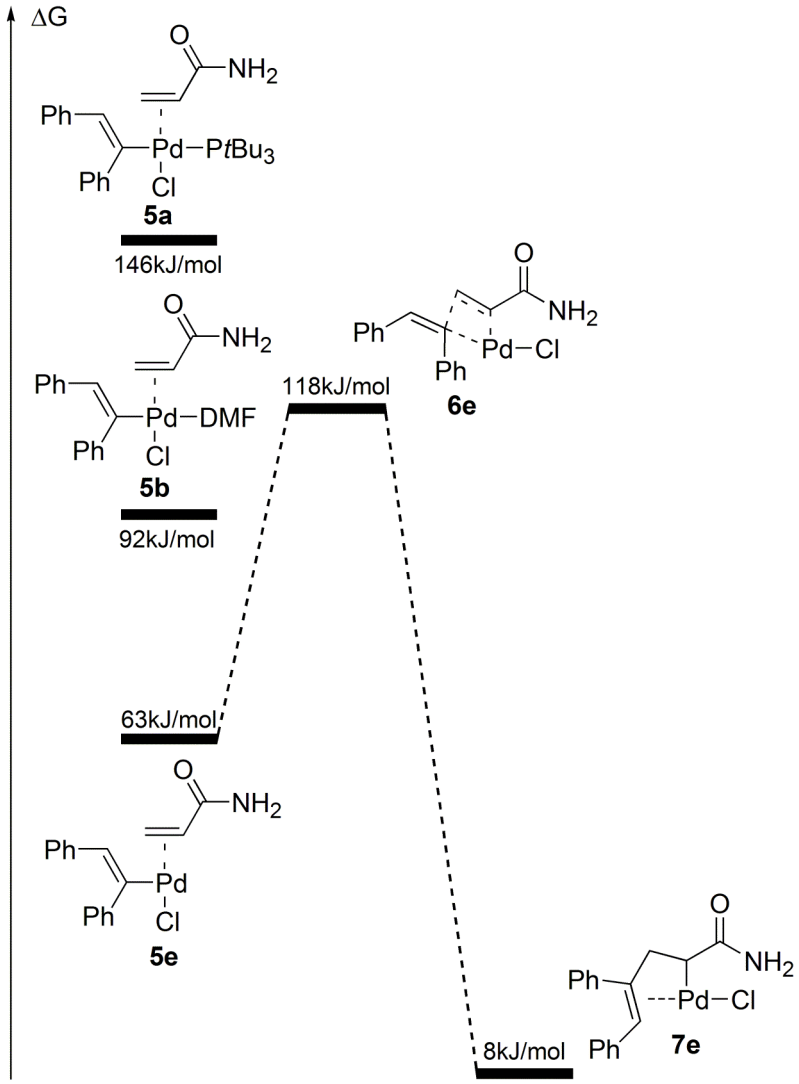


Figure 5 Free energy profile for the cross-coupling step.

β-hydride elimination (step V). In order for β-hydride elimination to take place the stable cross-coupling product **7c** has to rearrange to an agostic complex **8** from which a β-hydrogen can be eliminated.

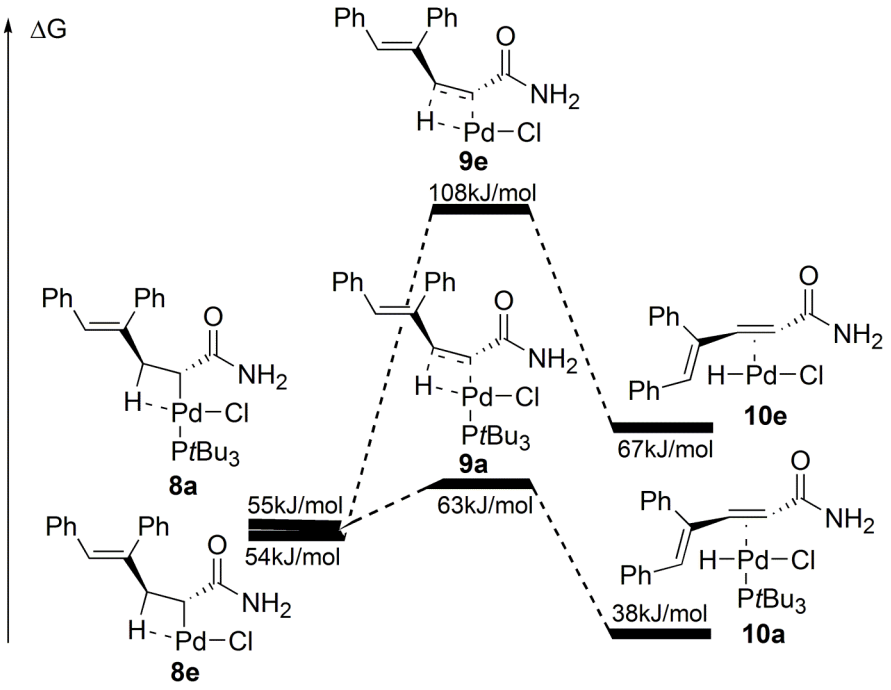


Figure 6 Free energy profile for the β-hydride elimination step.

The agostic complexes with and without a phosphine ligand (**8a** and **8e** respectively, Figure 6) are isoergic. In contrast, there is a decisive energy difference of 45 kJ/mol between having a phosphine ligand present and having a vacant coordination site in the transition state (**9a** and **9e** respectively). This can be explained by the destabilizing effect that the phosphine ligand has on the *trans* Pd-C bond, making this bond easier to break.[16] The phosphine-induced lowering of the barrier for the β-hydride elimination may be one reason why the phosphine ligand was found to be essential for the reaction. On the other hand, the two preceding transition states (**3b** and **6e**) are higher in energy than the β-elimination transition state **9e** without a phosphine ligand, by 26 kJ/mol and 10 kJ/mol respectively, so β-elimination should be able to take place even in the absence of phosphine ligands. The lowest energy β-hydride elimination transition state for the formation of the Z-alkene $\mathbf{9a_z}$ (Figure 7) is 26 kJ/mol higher in energy than transition state **9a**, explaining why only the E-alkene is formed in the reaction.

Full reaction path. Figure 7 shows the lowest energy reaction path for the full ene-yne coupling reaction. The phosphine ligand is stabilizing the hydridopalladium complexes **1a** and **2a**, and it is lowering the energy of the hydropalladation transition state **3a** by 6 kJ/mol compared to the transition state **3b** where a solvent molecule is coordinating to palladium (Figure 4). In the Pd(II)-π-alkene complex **5e** it is no longer favorable to have a phosphine ligand coordinating to palladium, and the subsequent cross-coupling reaction, through transition state **6e**, takes place without any phosphine-assistance. This leads to the stable complex **7e** with an intramolecular Pd-π-alkene coordination. Rearrangement of this complex to the agostic complex **8e** has to occur before further reaction can take place. Coordination of a phosphine molecule *trans* to the Pd-C bond in the agostic complex **8a** weakens the Pd-C bond and makes it more easily breakable in the β-hydride elimination (transition state **9a**). The reaction leads to formation of the E-alkene **J**. In Figure 7 the

Z-alkene product and the β-hydride elimination transition state for its formation are shown in grey. It appears that the E-alkene is both the thermodynamically (**J** is 36 kJ/mol lower in energy than **K**) and the kinetically favored product (**9a** is 26 kJ/mol lower in energy than **9a$_z$**, as expected from the steric repulsion between the substituents of the forming bond). From the free energy profile, the hydropalladation step is expected to be rate-determining. This might explain the importance of the phosphine ligand, since the phosphine ligand lowers the barrier for this step.

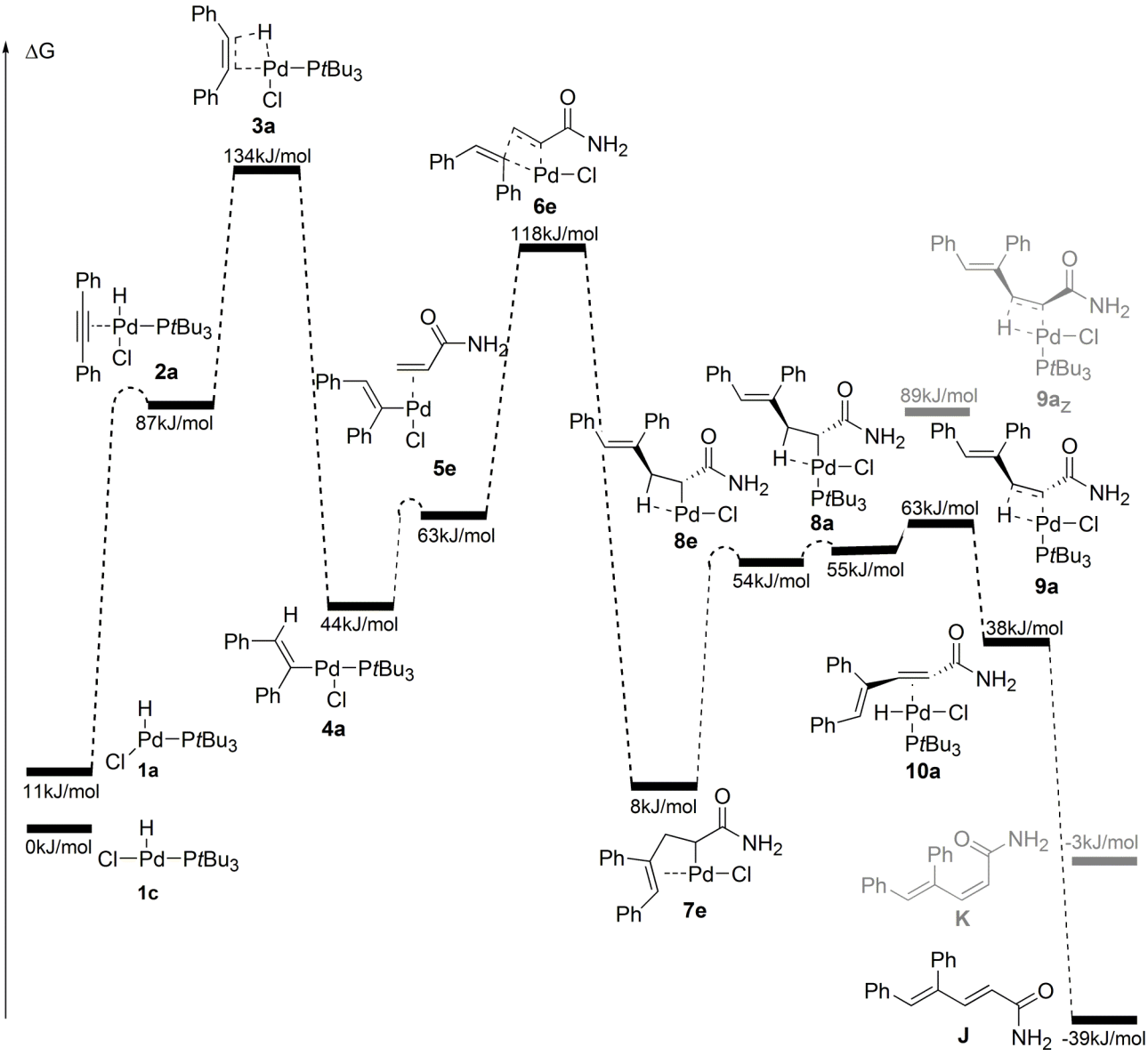


Figure 7 Free energy profile for the full ene-yne coupling reaction.

Alkene homo-coupling. In order to understand why alkene homo-coupling has not been observed, the essential parts of the potential homo-coupling reaction shown in Figure 2 have been evaluated and compared to the reaction path for the ene-yne coupling described above. Figure 8 shows the intermediates and transition states involved in the acrylamide hydropalladation and homo-coupling steps (black) superimposed on the reaction path for the ene-yne coupling (grey). Two regioisomeric insertions are possible in acrylamide, and both have been evaluated, but only the more favorable path is shown.

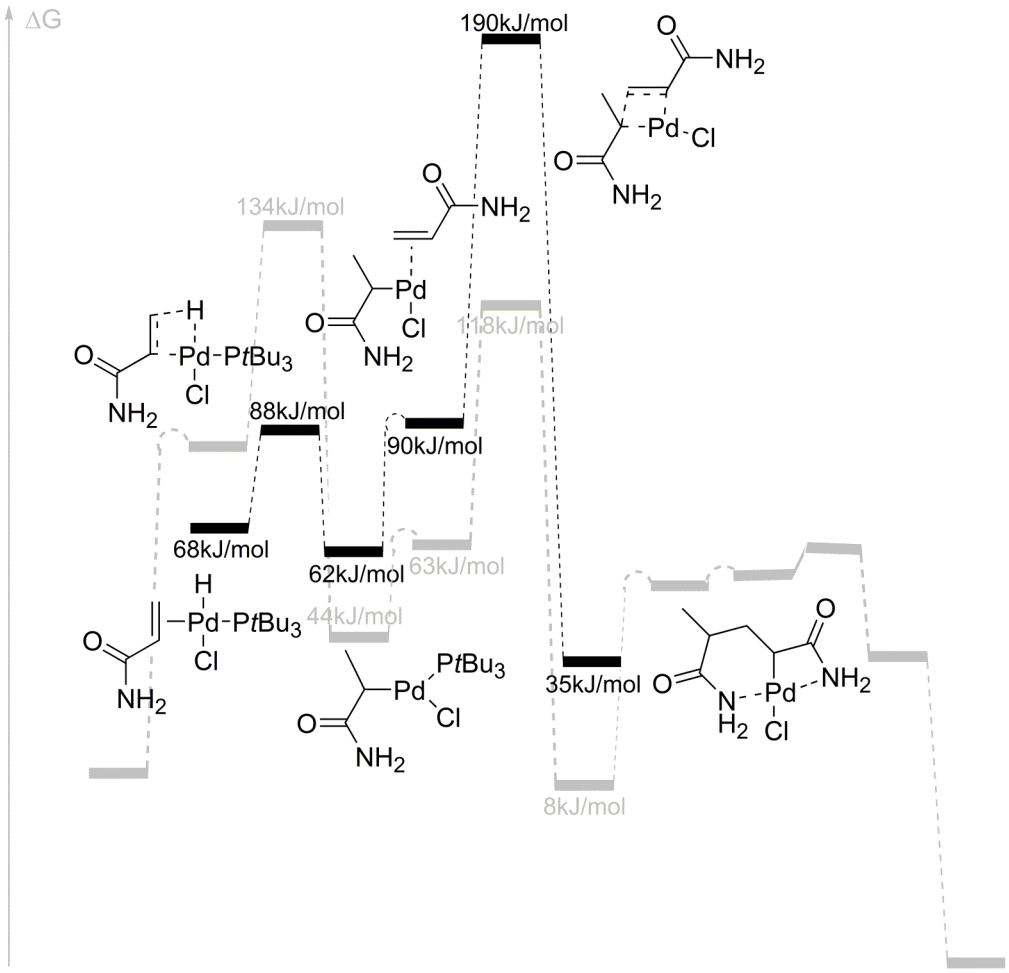


Figure 8 Acrylamide hydropalladation and homo-coupling (black) superimposed on the ene-yne reaction path (grey).

As can be seen from Figure 8 alkene insertion can easily take place, and the transition state for this transformation is even favored over the alkyne insertion by 46 kJ/mol. The product complex has a distorted T-shape due to both steric and electronic repulsion between the alkyl group and the phosphine ligand.

The coordination of a second alkene molecule is endergonic by 28 kJ/mol, and the alkene homo-coupling has a barrier of 100 kJ/mol, which means that it is disfavored by 72 kJ/mol compared to the cross-coupling on the alternative reaction path. The involvement of a phosphine ligand in the homo-coupling step can be ruled out, since coordination of a phosphine ligand to the Pd-π-alkene complex is 90 kJ/mol endergonic which means that the energy of the complex itself is almost as high as the transition state energy for the homo-coupling without a phosphine ligand. Furthermore, from visual inspection of the complex it is obvious that phosphine ligation would lead to an extremely crowded coupling transition state. The product from the alkene homo-coupling is a low-energy intermediate, with two intramolecular coordinations between the amide nitrogens and palladium. However, the reaction barrier is very high, 56 kJ/mol higher than the rate limiting transition state for the ene-yne coupling (the hydropalladation transition state **3a**, Figure 7). Thus alkene homo-coupling cannot compete with the ene-yne reaction.

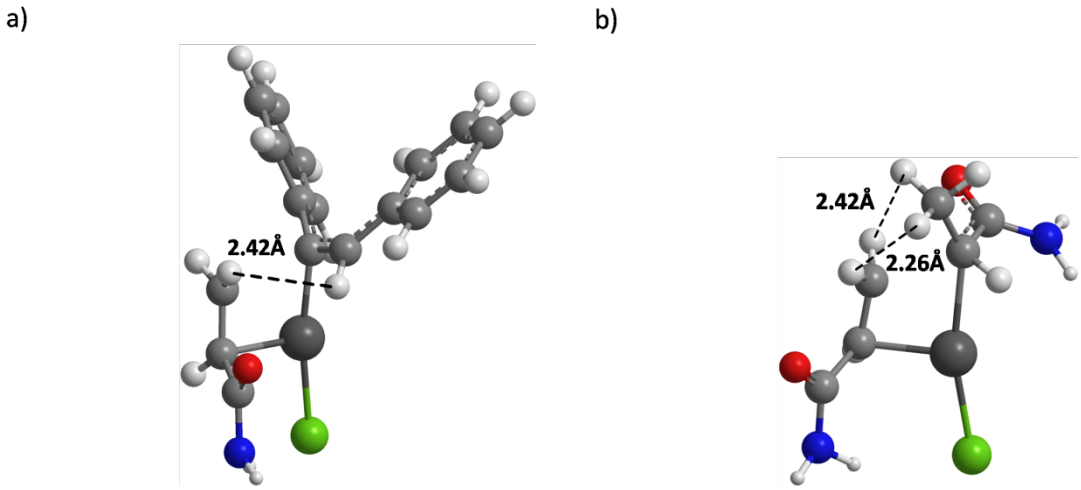


Figure 9 a) Cross-coupling transition state between the alkyne and the alkene. b) Alkene homo-coupling transition state. Distances for close unfavorable contacts are shown. Green: Cl, blue: N, red: O, dark grey: Pd, light grey: C, white: H.

A closer look at the transition state structures for alkene-alkyne cross-coupling (Figure 9a) and for the alkene homo-coupling (Figure 9b) helps explain the large difference in barriers of the two coupling reactions. In the alkene-alkyne cross-coupling transition state an sp^2 carbon is migrating, while it is an sp^3 carbon in the homo-coupling transition state. In general, sp^2 carbons are more efficient in migrations, since the π-face can provide some overlap to support formation of the new bond. In addition, the tetrahedral shape of the sp^3 carbon introduces a high degree of repulsive steric interactions in the transition state, as opposed to the planar sp^2 carbon. In Figure 9 the close unfavorable contacts between hydrogens from the two coupling partners are shown. In the homo-coupling transition state two hydrogens are only 2.26 Å apart, which is closer than the sum of their van der Waals radii (r_W = 1.20 Å for hydrogen). The absence of homo-coupling can therefore be

ascribed to unfavorable steric interactions in the transition state, coupled with the lower migratory power of sp^3 carbons.

Alkyne polymerization. The absence of alkyne polymerization was assumed to arise either from an endergonic, reversible polymerization reaction, or from a high reaction barrier of the alkyne homo-coupling step. An initial investigation of reactant and product stabilities proved the alkyne homo-coupling to be exergonic by 88 kJ/mol (Figure 10). However, the relative barriers clearly show that in the carbopalladation step, the alkyne cannot compete with the alkene; the difference is 22 kJ/mol. An energy difference this high will lead to complete selectivity for the cross-coupling reaction, in accordance with experimental observations. Reaction selectivities can frequently be rationalized in terms of Bell-Evans-Polanyi theory,[17] but in this case, the relationship obviously does not apply, since the alkyne homocoupling is more exergonic than the alkyne-alkene coupling. Instead, the source of the selectivity must be found in the polar nature of the transition state. The reaction can be viewed at least partially as a nucleophilic addition to an unsaturated system. Compared to the non-polar alkyne, the polarized Michael acceptor is of course better able to react with an incoming nucleophile.

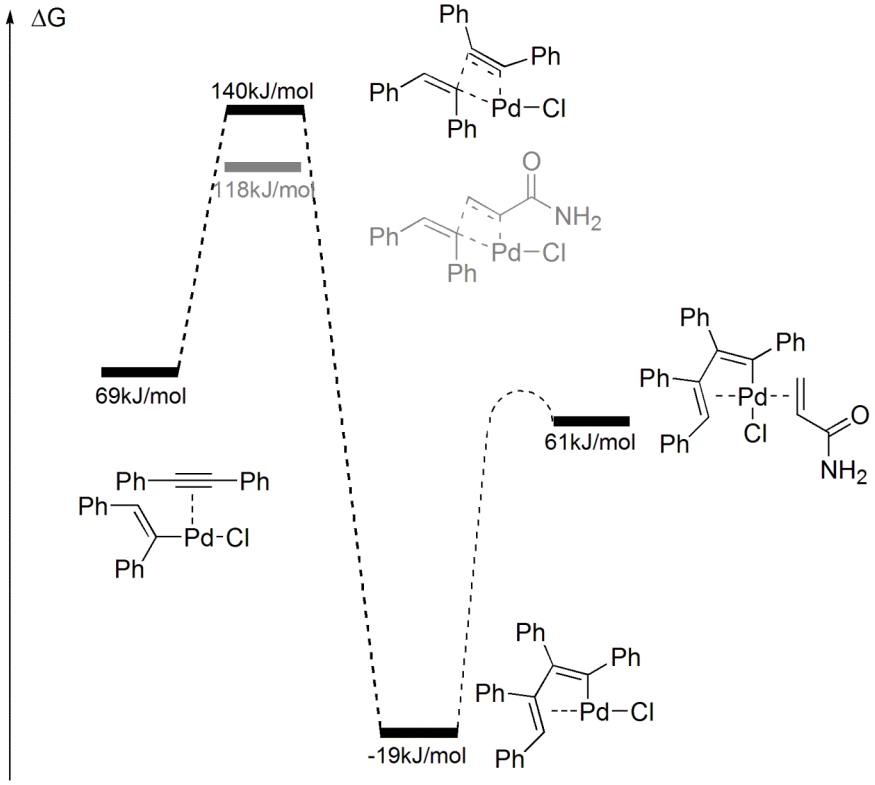


Figure 10 Energy profile for alkyne polymerization.

Conclusions

In a qualitative sense, the current DFT investigation has validated the proposed mechanism of the title reaction.[2] The hydropalladation step is found to be rate limiting. However, the alkene substrate undergoes facile and reversible hydropalladation, and would be expected to undergo fast hydrogen exchange under the reaction conditions. What stops the alkene insertion product from competing in the coupling is the subsequent carbopalladation step.

The role of the tris(*tert*-butyl)phosphine ligand yielded some surprises. The phosphine must dissociate to enable the carbopalladation step, but will then re-associate to enable the β-hydride elimination. The phosphine ligand is also essential for the stability of the active catalyst, Pd(II)-hydride **1a**. In the hydropalladation step, the phosphine seems optional; barriers with and without coordinated phosphine are similar, but when considering standard state corrections, a path without coordinating phosphine may be favored.

The absence of alkene homo-coupling can be explained by an extremely high barrier for the coupling step (step IVa, Figure 2). This arises from steric repulsions between the two coupling partners in the transition state and the sp^3 character of the migrating carbon. Likewise, the transition state for alkyne-alkyne coupling in a potential polymerization reaction is energetically unfavorable compared to the transition state for the ene-yne cross-coupling. This explains why these undesired side reactions are not observed.

Computational methods

All calculations have been performed in Jaguar[18] with the B3LYP hybrid functional[19] and the basis set LACVP**.[20] Previous studies on the Heck reaction show that it is important to include both entropy and solvation energy when evaluating a reaction path and not merely to use the potential energy surface.[21] Thus, this approach has been used in the present study of the closely related ene-yne coupling as well. The complexes have been optimized in the gas phase and the entropic contribution has been computed from a vibrational analysis at 373.15 K using the analytic Hessian. The number of negative eigenvalues from the vibrational analysis (zero or one for minima and transition states, respectively) was used to validate the nature of all stationary points. The solution phase potential energies were obtained by single point calculations on the gas phase structure. Solvent was modeled by Jaguar's Poisson-Boltzmann solver[22] with parameters describing DMF (dielectricity constant: epsout = 38; probe radius: radprb = 2.47982). Solution phase Gibbs free energies were estimated by adding the gas phase thermodynamic contribution to the single point solution phase energy. This procedure will lead to overestimated entropic contributions. The entropy in solvent should be substantially lower than what it is in gas phase,[23] and the harmonic approximation will overestimate the influence of low frequency vibrations.[24] In addition, the B3LYP method is known to be over-repulsive.[14] Since only relative energies are used to draw conclusions, most of these systematic errors will cancel. The most important exception is comparisons with different molecularity, where the current methodology would be expected to overestimate the energy penalty for association, possibly by more than 20 kJ/mol.

Prior to the DFT study of the reaction path a MCMM[25] conformational search of the acryl amide was performed in MacroModel.[26] The lowest energy conformation (s-*cis*) was used when building the different Pd(II)-π-alkene complexes used as starting points for the subsequent DFT calculations.

Acknowledgment

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Supporting information

1a

E_scf = -1402.50417576463 a.u.

E_sol = -1402.53356 a.u.

G(T)-E(0) = 0.315321 a.u.

Lowest frequency: -22.97 cm-1

C	2.13445	-3.45897	-1.11864
C	3.84987	-1.09641	0.15276
C	2.91479	-0.93293	-2.89481
C	4.38006	-1.22682	-3.28360
H	4.62590	-2.29018	-3.24274
H	4.53626	-0.89650	-4.31766
H	5.09567	-0.68288	-2.66454
C	1.99020	-1.58085	-3.94836
H	2.16212	-2.65121	-4.07437
H	0.93334	-1.41485	-3.72268
H	2.19512	-1.10585	-4.91501
C	2.66100	0.59207	-2.97789
H	2.87507	0.91904	-4.00295
H	1.61870	0.83378	-2.75318
H	3.29141	1.17476	-2.30821
C	5.09219	-2.00497	0.03156
H	5.52996	-2.00911	-0.96839
H	5.85803	-1.62701	0.71983
H	4.88678	-3.03720	0.32349
C	4.27387	0.37450	-0.05758
H	4.80556	0.53986	-0.99639
H	3.42013	1.05512	0.00240
H	4.96148	0.64423	0.75252
C	3.30601	-1.18026	1.60048
H	4.11357	-0.86574	2.27304
H	2.46151	-0.50579	1.76035
H	3.01216	-2.18528	1.89840
C	2.07309	-3.97517	0.33604
H	3.04360	-3.96658	0.83432
H	1.35949	-3.40765	0.93985
H	1.73157	-5.01690	0.31364
C	3.22402	-4.24505	-1.88154
H	4.23006	-4.05614	-1.50328
H	3.02676	-5.31703	-1.75994
H	3.21632	-4.03999	-2.95406
C	0.75578	-3.78193	-1.74087
H	0.62773	-4.87127	-1.73167

H	-0.05554	-3.34206	-1.15640
H	0.65048	-3.44919	-2.77269
Cl	0.39913	1.26436	1.31237
P	2.43520	-1.54048	-1.11454
Pd	0.64092	-0.35971	-0.41068
H	0.16196	-1.16345	-1.62195

1b

E_scf = -836.08465368175 a.u.

E_sol = -836.11685 a.u.

G(T)-E(0) = 0.061706 a.u.

Lowest frequency: -190.31 cm-1

Pd	-0.31193	-0.90730	0.00000
H	-1.80111	-0.83078	0.00000
Cl	-0.48635	-3.17999	0.00000
C	0.92881	1.88608	0.00000
O	-0.12349	1.22149	0.00000
N	0.93282	3.22347	0.00000
H	1.92395	1.41739	0.00000
C	-0.36057	3.91612	0.00000
H	-0.18815	4.99197	0.00000
H	-0.94038	3.63939	-0.88487
H	-0.94038	3.63939	0.88487
C	2.20423	3.95470	0.00000
H	1.99452	5.02399	0.00000
H	2.79624	3.72436	0.89145
H	2.79624	3.72436	-0.89145

1c

E_scf = -1402.50881623093 a.u.

E_sol = -1402.53331 a.u.

G(T)-E(0) = 0.310776 a.u.

Lowest frequency: 39.09 cm-1

C	2.10322	-3.47217	-1.17869
C	3.71887	-1.06681	0.12332
C	2.80415	-0.90564	-2.91157
C	4.26947	-1.17807	-3.31445
H	4.52182	-2.24048	-3.29983
H	4.42452	-0.82011	-4.33968
H	4.98442	-0.64852	-2.68160
C	1.87686	-1.54681	-3.96661
H	2.06719	-2.61091	-4.11508
H	0.81976	-1.40811	-3.72222
H	2.05765	-1.04946	-4.92688
C	2.52838	0.61601	-2.97033
H	2.68810	0.95486	-4.00111
H	1.49595	0.84533	-2.69324
H	3.18811	1.20110	-2.33125
C	4.97688	-1.95759	0.08549
H	5.45973	-1.95881	-0.89437
H	5.70629	-1.56953	0.80780
H	4.76995	-2.99277	0.36509
C	4.14643	0.40239	-0.09264
H	4.72121	0.55143	-1.00803
H	3.29010	1.08293	-0.09894
H	4.79230	0.69650	0.74346
C	3.09167	-1.11491	1.54008
H	3.84768	-0.79630	2.26836
H	2.24965	-0.41727	1.63661
H	2.74734	-2.10352	1.83709
C	2.03049	-4.00259	0.27095
H	2.98326	-3.94469	0.80083
H	1.26489	-3.48303	0.85483
H	1.74783	-5.06128	0.23363
C	3.21038	-4.23870	-1.93116
H	4.20795	-4.04496	-1.53021
H	3.02232	-5.31497	-1.83210
H	3.22176	-4.01539	-3.00016
C	0.72938	-3.79781	-1.81560
H	0.57488	-4.88224	-1.76092

H	-0.08475	-3.31161	-1.27230
H	0.65602	-3.51155	-2.86407
Cl	-1.44971	0.47779	0.66686
P	2.33046	-1.54648	-1.14769
Pd	0.41746	-0.54327	-0.29592
H	-0.19530	-0.75284	-1.64940

1d

E_scf = -2217.44417761744 a.u.

E_sol = -2217.46008 a.u.

G(T)-E(0) = 0.657440 a.u.

Lowest frequency: -15.69 cm-1

C	-2.42274	2.07197	-0.24762
C	-2.58654	-0.54036	1.54987
C	-3.16151	-0.69464	-1.56130
C	-4.66869	-0.74421	-1.22302
H	-5.09041	0.22760	-0.96982
H	-5.21274	-1.11842	-2.09966
H	-4.88035	-1.43304	-0.40157
C	-2.96367	0.05532	-2.89860
H	-3.41390	1.04832	-2.91076
H	-1.90315	0.15120	-3.15143
H	-3.44142	-0.52583	-3.69752
C	-2.70759	-2.14661	-1.84201
H	-3.40157	-2.58350	-2.57177
H	-1.70758	-2.17426	-2.27743
H	-2.71129	-2.78923	-0.96263
C	-3.93619	-0.01703	2.08617
H	-4.77513	-0.25423	1.42913
H	-4.13603	-0.49447	3.05436
H	-3.93165	1.06033	2.25796
C	-2.65400	-2.08300	1.50099
H	-3.51056	-2.45548	0.93470
H	-1.73914	-2.51728	1.08758
H	-2.76176	-2.45536	2.52753
C	-1.46773	-0.18854	2.56008
H	-1.72640	-0.62906	3.53195
H	-0.50454	-0.59668	2.24228
H	-1.33373	0.88222	2.70370
C	-1.97839	2.75666	1.06611
H	-2.61615	2.50413	1.91575
H	-0.93663	2.53947	1.30511
H	-2.06375	3.84087	0.91740
C	-3.90057	2.45128	-0.48576
H	-4.56903	2.05075	0.28049
H	-3.97966	3.54504	-0.44122
H	-4.27580	2.14817	-1.46471
C	-1.54995	2.68229	-1.37179

H	-1.72931	3.76514	-1.39541
H	-0.48902	2.52295	-1.16731
H	-1.78469	2.29385	-2.36335
C	2.23153	-3.47953	-1.04053
C	3.88413	-1.13244	0.25780
C	2.92253	-0.90945	-2.75950
C	4.37711	-1.20565	-3.18334
H	4.60817	-2.27260	-3.19087
H	4.52604	-0.83335	-4.20534
H	5.11073	-0.70246	-2.55172
C	1.97849	-1.52910	-3.81336
H	2.16470	-2.59219	-3.98117
H	0.92638	-1.39093	-3.54818
H	2.14795	-1.01896	-4.76993
C	2.68040	0.61884	-2.80725
H	2.89639	0.97247	-3.82402
H	1.64098	0.86295	-2.57135
H	3.30916	1.18002	-2.11781
C	5.09177	-2.09261	0.18890
H	5.55315	-2.12336	-0.80133
H	5.85461	-1.72569	0.88745
H	4.85359	-3.11390	0.49123
C	4.42039	0.29967	0.02597
H	4.98131	0.39926	-0.90566
H	3.62273	1.04275	0.06184
H	5.11890	0.52581	0.84192
C	3.29895	-1.15041	1.69159
H	4.10457	-0.89701	2.39306
H	2.51328	-0.39949	1.79876
H	2.90627	-2.12347	1.98835
C	2.14187	-4.01691	0.40621
H	3.08575	-3.96165	0.94935
H	1.37679	-3.48880	0.98375
H	1.85306	-5.07490	0.36702
C	3.36857	-4.21398	-1.78637
H	4.36290	-3.96299	-1.41934
H	3.23415	-5.29505	-1.65302
H	3.34275	-4.02216	-2.86181
C	0.90034	-3.89641	-1.70930
H	0.87838	-4.99246	-1.76655
H	0.04068	-3.57758	-1.11789
H	0.77504	-3.51380	-2.72140
Cl	1.28109	1.64969	0.62940
P	2.42580	-1.53026	-0.98537

Pd	0.32185	-0.40199	-0.43714
H	-0.26013	-1.64625	-1.08480
P	-2.05110	0.15119	-0.18627

2a

E_scf = -1941.98160408482 a.u.

E_sol = -1941.99979 a.u.

G(T)-E(0) = 0.476334 a.u.

Lowest frequency: 16.54 cm-1

C	7.72682	1.61557	-3.56210
C	9.33287	-1.11810	-3.43373
C	9.97761	1.29104	-1.31694
C	10.90604	2.18154	-2.16630
H	10.39923	3.06846	-2.55279
H	11.72794	2.53504	-1.53113
H	11.35491	1.64200	-3.00633
C	9.24597	2.15980	-0.26478
H	8.58810	2.91378	-0.69360
H	8.65644	1.54014	0.41673
H	10.00469	2.68476	0.32909
C	10.85495	0.30568	-0.50872
H	11.36274	0.88524	0.27222
H	10.27170	-0.47931	-0.02157
H	11.63207	-0.15832	-1.11478
C	9.83706	-0.70668	-4.83176
H	10.59009	0.08601	-4.79503
H	10.31297	-1.58312	-5.28886
H	9.03316	-0.39910	-5.50288
C	10.49967	-1.84239	-2.73022
H	11.42286	-1.25858	-2.76037
H	10.26332	-2.11887	-1.70229
H	10.69036	-2.76893	-3.28653
C	8.19200	-2.15270	-3.59089
H	8.54638	-2.95577	-4.25022
H	7.93324	-2.59475	-2.62642
H	7.28645	-1.73738	-4.03592
C	6.58081	0.85590	-4.26811
H	6.94642	0.10596	-4.97281
H	5.91480	0.36657	-3.55259
H	5.98736	1.57652	-4.84412
C	8.60210	2.28151	-4.65277
H	8.99201	1.58139	-5.38745
H	7.96911	2.99490	-5.19533
H	9.43870	2.84677	-4.24364
C	7.09307	2.76993	-2.75321

H	6.39351	3.30300	-3.40856
H	6.53325	2.42020	-1.88282
H	7.83827	3.49877	-2.42582
Cl	8.49817	-2.39645	0.20420
P	8.61608	0.35018	-2.35017
Pd	7.10805	-0.55667	-0.78192
H	6.18523	0.53845	-1.32059
C	5.15412	-1.55147	0.25430
C	5.59802	-0.78216	1.10412
C	6.70435	1.51091	4.48559
C	7.52828	0.47296	4.04270
C	7.17896	-0.27784	2.92376
C	5.98365	0.00965	2.23535
C	5.15804	1.05754	2.68333
C	5.52023	1.80033	3.80366
H	6.98369	2.09267	5.35980
H	8.44996	0.24656	4.57148
H	7.81352	-1.07911	2.55631
H	4.23771	1.27560	2.15085
H	4.87674	2.60610	4.14566
C	3.29557	-4.50921	-2.13473
C	2.63077	-3.30970	-1.86968
C	3.24081	-2.32707	-1.09446
C	4.53050	-2.54165	-0.57359
C	5.19972	-3.75111	-0.84618
C	4.57716	-4.72493	-1.62146
H	2.81589	-5.27379	-2.73970
H	1.63412	-3.13956	-2.26717
H	2.72845	-1.39345	-0.88268
H	6.20128	-3.89434	-0.45129
H	5.09610	-5.65702	-1.82694

2b

E_scf = -1375.58536167758 a.u.

E_sol = -1375.61175 a.u.

G(T)-E(0) = 0.225259 a.u.

Lowest frequency: 16.16 cm-1

Cl	8.17394	-2.44821	0.47136
H	5.92777	-0.95293	0.24640
C	6.23247	1.30686	-1.15852
C	5.80589	0.51079	-2.01256
C	3.97422	-1.33125	-5.36041
C	5.35852	-1.40926	-5.18943
C	5.96490	-0.81172	-4.08963
C	5.18435	-0.11956	-3.14439
C	3.79027	-0.04463	-3.32031
C	3.19408	-0.64790	-4.42482
H	3.50445	-1.80435	-6.21798
H	5.96693	-1.94238	-5.91430
H	7.03843	-0.86893	-3.94150
H	3.18749	0.48143	-2.58648
H	2.11705	-0.58824	-4.55286
C	7.18929	4.71958	1.16422
C	5.85434	4.35946	0.96717
C	5.53453	3.23696	0.20747
C	6.55754	2.46087	-0.36685
C	7.90084	2.82817	-0.16326
C	8.20890	3.95215	0.59590
H	7.43455	5.59316	1.76150
H	5.05908	4.95167	1.41074
H	4.49878	2.94891	0.05702
H	8.68278	2.22015	-0.60590
H	9.24811	4.22833	0.74977
Pd	7.10016	-0.67725	-0.65092
O	8.93464	-0.26111	-2.06237
C	9.94674	-0.97680	-1.96414
H	9.99200	-1.78715	-1.22307
N	11.04681	-0.83372	-2.72807
C	11.12538	0.19770	-3.75317
H	10.19635	0.76652	-3.74456
H	11.96832	0.86954	-3.55350
H	11.26927	-0.25601	-4.74084
C	12.19588	-1.71057	-2.56417

H	13.08853	-1.13204	-2.29833
H	11.99817	-2.43316	-1.76987
H	12.40063	-2.25628	-3.49289

3a

E_scf = -1941.96775080361 a.u.

E_sol = -1941.98705 a.u.

G(T)-E(0) = 0.481653 a.u.

Lowest frequency: -517.92 cm-1

C	-2.06686	1.94008	0.49558
C	-2.58131	-1.07841	1.27815
C	-2.53142	-0.20742	-1.77926
C	-3.88824	0.49311	-2.00604
H	-3.82373	1.58264	-1.99385
H	-4.25579	0.20824	-3.00002
H	-4.64727	0.18339	-1.28318
C	-1.51337	0.27938	-2.83933
H	-1.28680	1.34413	-2.76849
H	-0.57921	-0.28289	-2.76531
H	-1.93812	0.09990	-3.83538
C	-2.73961	-1.71668	-2.04243
H	-3.04117	-1.82946	-3.09165
H	-1.82003	-2.28576	-1.89731
H	-3.53883	-2.14831	-1.43654
C	-4.12087	-1.14169	1.17212
H	-4.45984	-1.57390	0.22927
H	-4.49689	-1.79040	1.97377
H	-4.59949	-0.16836	1.29288
C	-2.00848	-2.50625	1.12457
H	-2.22157	-2.95960	0.15874
H	-0.92466	-2.52466	1.25419
H	-2.46110	-3.13767	1.90014
C	-2.21259	-0.61988	2.70669
H	-2.52412	-1.40296	3.40869
H	-1.13399	-0.48236	2.82891
H	-2.72424	0.29731	3.00602
C	-1.19876	2.34967	1.70903
H	-1.43242	1.79912	2.61834
H	-0.13122	2.23512	1.51341
H	-1.38175	3.41204	1.91417
C	-3.53505	2.25058	0.86521
H	-3.83381	1.76486	1.79700
H	-3.63404	3.33175	1.02525
H	-4.24710	1.97068	0.08961
C	-1.63524	2.86343	-0.66654

H	-1.65437	3.90259	-0.31513
H	-0.61646	2.64461	-1.00017
H	-2.29695	2.80505	-1.53170
Cl	0.57282	-2.53737	-1.25571
P	-1.72472	0.08434	-0.02456
Pd	0.66877	-0.37458	-0.11180
H	0.94978	0.99127	0.58921
C	2.87504	-0.53534	0.12870
C	2.62217	0.66247	0.43297
C	4.19721	4.48115	1.46524
C	2.98895	4.40397	0.77125
C	2.44766	3.16440	0.43712
C	3.11362	1.98081	0.79005
C	4.33454	2.06620	1.48550
C	4.86753	3.30760	1.81878
H	4.61479	5.44850	1.72922
H	2.46454	5.31196	0.48710
H	1.51335	3.10482	-0.11120
H	4.85507	1.15385	1.75817
H	5.80869	3.35837	2.35904
C	5.45712	-3.86666	-0.32019
C	5.31303	-3.24461	0.92186
C	4.45216	-2.16057	1.06347
C	3.72080	-1.68618	-0.04352
C	3.85681	-2.32802	-1.28753
C	4.73076	-3.40359	-1.41906
H	6.12776	-4.71459	-0.42899
H	5.86965	-3.60548	1.78229
H	4.33057	-1.67711	2.02838
H	3.26313	-1.98889	-2.12709
H	4.83179	-3.89356	-2.38319

3b

E_scf = -1375.57287369412 a.u.

E_sol = -1375.60228 a.u.

G(T)-E(0) = 0.229432 a.u.

Lowest frequency: -494.01 cm-1

Cl	8.12416	-2.55974	0.44749
H	5.97817	-1.00591	-0.51497
C	5.60349	0.50264	-1.13171
C	6.47107	0.87016	-1.98529
C	7.74826	3.22460	-5.27923
C	8.64922	2.90821	-4.25977
C	8.24855	2.12356	-3.18172
C	6.92322	1.65621	-3.10351
C	6.02049	1.97701	-4.13759
C	6.43463	2.75412	-5.21546
H	8.06847	3.83220	-6.12092
H	9.67140	3.27389	-4.30680
H	8.94646	1.85566	-2.39748
H	5.00281	1.60138	-4.08951
H	5.73107	2.99162	-6.00836
C	1.96969	1.18791	0.96631
C	2.28713	1.92758	-0.17637
C	3.47805	1.69409	-0.85568
C	4.37311	0.70721	-0.39683
C	4.04862	-0.02961	0.75389
C	2.85443	0.21236	1.42794
H	1.03810	1.37276	1.49328
H	1.60343	2.68941	-0.53992
H	3.72746	2.27016	-1.74161
H	4.74115	-0.78305	1.11900
H	2.61689	-0.36389	2.31730
Pd	7.42660	-0.70800	-0.93152
O	9.49625	-0.41699	-1.74115
C	10.42529	-1.17943	-1.40999
H	10.26776	-1.95395	-0.64859
N	11.65654	-1.12399	-1.94549
C	11.99142	-0.16129	-2.98630
H	11.08309	0.35968	-3.28623
H	12.72693	0.56417	-2.61856
H	12.41727	-0.68080	-3.85197
C	12.70955	-2.02396	-1.49728

H	13.55111	-1.45667	-1.08232
H	12.32141	-2.69030	-0.72450
H	13.07831	-2.63034	-2.33278

4a

E_scf = -1942.00529754402 a.u.

E_sol = -1942.02672 a.u.

G(T)-E(0) = 0.487024 a.u.

Lowest frequency: 3.81 cm-1

C	-1.40081	0.93267	-1.78787
C	-2.57269	0.04657	1.00058
C	-1.71587	-2.14119	-1.11779
C	-3.21224	-2.38842	-1.40178
H	-3.63363	-1.66812	-2.10644
H	-3.32873	-3.38579	-1.84606
H	-3.81911	-2.37181	-0.49476
C	-0.93249	-2.36270	-2.43072
H	-1.30536	-1.75727	-3.25956
H	0.13750	-2.16886	-2.30716
H	-1.04251	-3.41377	-2.72590
C	-1.20052	-3.21634	-0.12995
H	-1.36194	-4.20571	-0.57699
H	-0.13115	-3.10048	0.06695
H	-1.71004	-3.20130	0.83187
C	-3.94445	0.52119	0.47613
H	-4.42939	-0.21687	-0.16734
H	-4.60627	0.68580	1.33624
H	-3.89152	1.46700	-0.06709
C	-2.81206	-1.16774	1.92770
H	-3.36891	-1.97199	1.44234
H	-1.87742	-1.56107	2.33154
H	-3.42071	-0.82698	2.77498
C	-1.95587	1.15075	1.89497
H	-2.66093	1.36858	2.70770
H	-1.01963	0.81378	2.34568
H	-1.77425	2.08674	1.36668
C	-1.37174	2.34557	-1.16145
H	-2.28696	2.59816	-0.62450
H	-0.52383	2.47165	-0.48102
H	-1.25743	3.08080	-1.96809
C	-2.63622	0.82114	-2.70498
H	-3.57831	0.87213	-2.15675
H	-2.62723	1.65576	-3.41837
H	-2.63475	-0.09938	-3.29335
C	-0.12814	0.84365	-2.66074

H	-0.15951	1.64711	-3.40806
H	0.77724	0.98608	-2.06494
H	-0.03289	-0.09752	-3.19980
Cl	0.71253	-1.31103	2.69389
P	-1.26952	-0.40137	-0.37562
Pd	1.12448	-0.50959	0.48507
C	3.88409	-0.77224	1.87403
C	3.10642	-0.50919	0.82203
H	3.37180	-1.05842	2.78982
C	8.15727	-0.70565	2.32444
C	7.60170	-0.49275	1.06033
C	6.22094	-0.50844	0.88229
C	5.35638	-0.73702	1.96880
C	5.93316	-0.95594	3.23368
C	7.31453	-0.93860	3.41170
H	9.23547	-0.69353	2.45828
H	8.24983	-0.31661	0.20565
H	5.81295	-0.34907	-0.10947
H	5.28067	-1.14039	4.08348
H	7.73256	-1.10943	4.40024
C	3.56023	0.77176	-3.22359
C	3.61460	1.71224	-2.18628
C	3.46999	1.30705	-0.86582
C	3.29631	-0.06596	-0.54780
C	3.21059	-0.99784	-1.61501
C	3.34924	-0.57737	-2.93767
H	3.67941	1.09579	-4.25372
H	3.77197	2.76256	-2.41468
H	3.52215	2.02558	-0.05349
H	3.09104	-2.05044	-1.37689
H	3.30281	-1.30507	-3.74271

4b

E_scf = -1375.59085409233 a.u.

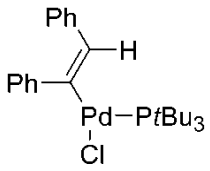
E_sol = -1375.62560 a.u.

G(T)-E(0) = 0.230475 a.u.

Lowest frequency: 17.77 cm-1

Cl	9.11170	-2.20793	0.97351
H	5.38730	-0.86337	-0.06219
C	5.31327	0.02992	-0.70803
C	6.42357	0.35026	-1.39039
C	7.19288	2.83588	-4.77129
C	7.90094	3.03898	-3.58349
C	7.65966	2.23040	-2.47555
C	6.68412	1.21554	-2.53039
C	5.98139	1.01776	-3.73735
C	6.23561	1.82067	-4.84534
H	7.38578	3.46592	-5.63527
H	8.64297	3.83029	-3.52179
H	8.21266	2.38087	-1.55354
H	5.23508	0.23117	-3.78842
H	5.68411	1.65737	-5.76717
C	1.44787	1.87697	-0.43059
C	2.48557	2.54256	-1.08804
C	3.74908	1.96631	-1.18095
C	4.00177	0.69869	-0.62270
C	2.95159	0.04662	0.04895
C	1.68844	0.62715	0.14139
H	0.46401	2.33231	-0.35949
H	2.31122	3.52149	-1.52675
H	4.54572	2.50262	-1.68345
H	3.13144	-0.92737	0.49772
H	0.89171	0.10294	0.66188
Pd	7.81151	-0.74089	-0.49508
O	9.26530	-0.47752	-2.06005
C	10.35591	-1.08402	-1.93556
H	10.53700	-1.73416	-1.07170
N	11.34957	-0.97546	-2.82507
C	11.22007	-0.13550	-4.01092
H	10.26380	0.38457	-3.97076
H	12.03589	0.59488	-4.04108
H	11.26574	-0.75025	-4.91698
C	12.59357	-1.71273	-2.64659

H	13.44206	-1.02158	-2.59209
H	12.55011	-2.29053	-1.72142
H	12.75529	-2.39948	-3.48517



E_scf = -1942.00432856358 a.u.

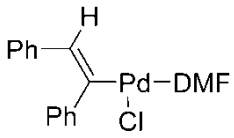
E_sol = -1942.02761 a.u.

G(T)-E(0) = 0.483476 a.u.

Lowest frequency: 10.25 cm-1

C	-2.51442	1.85459	0.52532
C	-2.23765	-1.25832	1.08219
C	-1.93648	-0.12888	-1.88257
C	-3.35771	-0.67017	-2.15220
H	-4.14359	0.00794	-1.81457
H	-3.47941	-0.79525	-3.23550
H	-3.52978	-1.64725	-1.69718
C	-1.74065	1.15657	-2.71528
H	-2.53887	1.88693	-2.56560
H	-0.77905	1.63778	-2.51725
H	-1.75377	0.87837	-3.77617
C	-0.90152	-1.15067	-2.40939
H	-1.11992	-1.33973	-3.46847
H	0.11821	-0.76370	-2.33607
H	-0.92444	-2.10667	-1.89032
C	-3.76275	-1.22691	1.32335
H	-4.33836	-1.23482	0.39477
H	-4.03657	-2.13159	1.88010
H	-4.08538	-0.37551	1.92526
C	-1.89662	-2.61870	0.43399
H	-2.46898	-2.81337	-0.47501
H	-0.83018	-2.72653	0.22563
H	-2.16806	-3.40139	1.15343
C	-1.50257	-1.23168	2.44526
H	-1.88261	-2.06242	3.05307
H	-0.42728	-1.37973	2.31587
H	-1.65895	-0.31311	3.01059
C	-2.44606	1.98704	2.06349
H	-3.05276	1.24653	2.58633
H	-1.41954	1.92334	2.43365
H	-2.83478	2.97477	2.34113
C	-3.99301	1.91299	0.07775
H	-4.58715	1.06278	0.41190

H	-4.44440	2.81563	0.50884
H	-4.09285	1.99846	-1.00642
C	-1.80373	3.10226	-0.04451
H	-2.30632	3.99042	0.35843
H	-0.75626	3.14335	0.24839
H	-1.85472	3.17140	-1.12985
Cl	1.71478	-2.17150	0.12560
P	-1.57142	0.23000	-0.00622
Pd	0.76664	0.05067	0.27147
C	1.67738	2.69470	-0.50997
C	1.38178	1.92301	0.55336
H	1.18512	2.45102	-1.45044
C	4.33774	6.03479	-0.99341
C	3.40802	5.69737	-1.97789
C	2.56063	4.60822	-1.79238
C	2.61127	3.83275	-0.61760
C	3.56196	4.18092	0.36085
C	4.41021	5.26848	0.17189
H	5.00492	6.88023	-1.13546
H	3.34497	6.27960	-2.89329
H	1.84231	4.34732	-2.56638
H	3.64680	3.59111	1.26524
H	5.14004	5.51454	0.93852
C	2.36692	2.27246	4.70784
C	2.94152	1.26287	3.93358
C	2.64032	1.15993	2.57647
C	1.74626	2.06787	1.96761
C	1.17711	3.08476	2.76360
C	1.48821	3.18524	4.11647
H	2.60661	2.35334	5.76440
H	3.63252	0.55579	4.38339
H	3.10283	0.38165	1.97566
H	0.50054	3.79959	2.30573
H	1.04648	3.97917	4.71261



E_scf = -1375.61644609303 a.u.

E_sol = -1375.64499 a.u.

G(T)-E(0) = 0.231687 a.u.

Lowest frequency: 22.94 cm-1

Cl	8.27570	1.18530	-1.32547
H	5.59077	1.59410	-0.17287
C	5.20029	0.76586	0.41421
C	5.92915	-0.35265	0.41681
C	6.72142	-4.10383	2.24403
C	6.46363	-4.02799	0.88455
C	6.09711	-2.80021	0.30261
C	6.01242	-1.62413	1.10416
C	6.30263	-1.72866	2.49440
C	6.62694	-2.95131	3.04972
H	6.99018	-5.05476	2.69502
H	6.51853	-4.91753	0.26414
H	5.76370	-2.76513	-0.73123
H	6.25739	-0.83079	3.10240
H	6.82631	-3.02309	4.11533
C	1.53649	1.68105	2.46333
C	1.99527	0.36108	2.43508
C	3.17468	0.03584	1.77048
C	3.93183	1.02690	1.11847
C	3.44968	2.34866	1.14498
C	2.27003	2.67337	1.81144
H	0.61532	1.93049	2.98226
H	1.42673	-0.42164	2.93052
H	3.50742	-0.99673	1.74938
H	4.01712	3.12624	0.63974
H	1.92359	3.70337	1.82052
Pd	7.62300	-0.91536	-0.43010
O	9.50323	-1.98113	-1.10073
C	10.46891	-1.33324	-1.54071
H	10.39040	-0.25190	-1.71461
N	11.66359	-1.87884	-1.83762
C	11.91226	-3.30144	-1.65073
H	11.00936	-3.76105	-1.25051

H	12.17102	-3.77235	-2.60627
H	12.74245	-3.45303	-0.95101
C	12.75496	-1.06475	-2.35008
H	13.06951	-1.41794	-3.33934
H	12.43118	-0.02549	-2.43653
H	13.61887	-1.10849	-1.67612

5a

E_scf = -2189.30009167708 a.u.

E_sol = -2189.32852 a.u.

G(T)-E(0) = 0.552836 a.u.

Lowest frequency: 12.03 cm-1

C	1.67568	-4.19557	-0.32047
C	-0.98009	-2.92705	-1.40823
C	-0.28849	-2.74315	1.66657
C	-1.33167	-3.85399	1.91514
H	-0.94007	-4.85688	1.73907
H	-1.64926	-3.80867	2.96534
H	-2.22952	-3.72757	1.30768
C	0.84397	-2.90083	2.70608
H	1.30333	-3.89141	2.69537
H	1.62692	-2.14650	2.57830
H	0.41841	-2.75495	3.70688
C	-0.94839	-1.37643	1.96424
H	-1.34733	-1.39754	2.98646
H	-0.22579	-0.55891	1.91337
H	-1.76971	-1.13173	1.29319
C	-1.48971	-4.37701	-1.55842
H	-1.86518	-4.79170	-0.62020
H	-2.32752	-4.37512	-2.26787
H	-0.74052	-5.06197	-1.95900
C	-2.19654	-2.04650	-1.03981
H	-2.72296	-2.40077	-0.15100
H	-1.92097	-0.99862	-0.91130
H	-2.91069	-2.09797	-1.87181
C	-0.47917	-2.41634	-2.78139
H	-1.29615	-2.51222	-3.50834
H	-0.20843	-1.35948	-2.72582
H	0.36720	-2.98163	-3.17301
C	2.01129	-4.42232	-1.81213
H	1.17927	-4.82963	-2.38686
H	2.34756	-3.50446	-2.30332
H	2.83426	-5.14533	-1.87782
C	1.16690	-5.52915	0.26876
H	0.19693	-5.83005	-0.12824
H	1.88358	-6.32228	0.01714
H	1.09630	-5.50179	1.35826
C	3.02818	-3.86238	0.35258

H	3.66522	-4.75564	0.32293
H	3.55703	-3.07864	-0.19181
H	2.94096	-3.55935	1.39544
Cl	-0.32688	0.99408	-1.29092
P	0.47241	-2.65989	-0.12775
C	2.49394	2.89902	-0.21431
C	2.03775	1.87125	0.50400
H	2.67591	2.72921	-1.27167
C	3.25254	7.00086	0.82201
C	3.29655	6.56146	-0.50114
C	3.05482	5.22329	-0.79946
C	2.75553	4.29002	0.21038
C	2.72318	4.74713	1.54133
C	2.96834	6.08570	1.83794
H	3.44171	8.04375	1.06066
H	3.52059	7.25992	-1.30292
H	3.09317	4.88679	-1.83256
H	2.51328	4.05721	2.34890
H	2.93917	6.41626	2.87298
C	0.62493	1.66159	4.53509
C	1.91392	1.21648	4.23136
C	2.38117	1.26926	2.91987
C	1.56407	1.77905	1.88799
C	0.25649	2.20641	2.20701
C	-0.20050	2.15512	3.52018
H	0.26410	1.62302	5.55930
H	2.55806	0.83516	5.01888
H	3.39025	0.94336	2.68667
H	-0.37969	2.57081	1.40741
H	-1.20457	2.49817	3.75386
Pd	1.60877	-0.00105	-0.14335
C	3.89169	-0.39731	0.00832
C	3.47638	-0.45525	-1.30550
H	4.37599	0.50206	0.37051
H	3.17538	-1.40659	-1.73964
H	3.97034	-1.28665	0.62030
C	3.77671	0.63487	-2.31253
N	2.76150	0.90290	-3.18898
O	4.88004	1.16221	-2.36549
H	1.79803	0.75495	-2.89906
H	2.92999	1.67035	-3.82549

5b

E_scf = -1622.93762247964 a.u.

E_sol = -1622.96934 a.u.

G(T)-E(0) = 0.303116 a.u.

Lowest frequency: 16.51 cm-1

Cl	-0.79234	0.71926	-0.52741
C	2.32169	2.71778	-0.54706
C	2.02153	1.73715	0.32020
H	2.29779	2.47209	-1.60839
C	3.32968	6.85108	0.08530
C	3.75259	6.17120	-1.05747
C	3.41412	4.83190	-1.23871
C	2.65860	4.13335	-0.27911
C	2.22400	4.83845	0.85799
C	2.55902	6.17860	1.03635
H	3.58608	7.89730	0.22784
H	4.34171	6.68562	-1.81214
H	3.73928	4.31115	-2.13664
H	1.60529	4.33922	1.59455
H	2.20596	6.70452	1.91961
C	2.27771	1.72692	4.61079
C	3.39242	2.05379	3.83438
C	3.30111	2.06582	2.44350
C	2.08741	1.75610	1.79459
C	0.97305	1.42066	2.58888
C	1.07031	1.41415	3.98084
H	2.34939	1.71715	5.69479
H	4.33637	2.30139	4.31273
H	4.16622	2.33438	1.84379
H	0.03557	1.18100	2.09704
H	0.19512	1.16664	4.57592
C	3.53829	-0.62218	-1.09631
C	3.42751	-0.94195	0.23885
H	3.37032	-1.39003	-1.84496
H	3.78052	-0.24945	0.99749
H	3.99769	0.30907	-1.40753
C	3.13103	-2.34617	0.70248
N	2.72963	-2.41547	2.00939
O	3.28605	-3.33425	-0.00323
H	2.40350	-1.59027	2.49217
H	2.41670	-3.31450	2.34511

Pd	1.46758	-0.04465	-0.44111
C	-0.28800	-2.42134	-1.52301
O	0.87428	-2.04903	-1.28857
H	-1.13144	-1.72099	-1.45990
N	-0.59898	-3.68552	-1.85363
C	0.43726	-4.71131	-1.93796
H	1.35491	-4.32836	-1.48996
H	0.10885	-5.60589	-1.39832
H	0.62457	-4.98451	-2.98357
C	-1.96168	-4.06149	-2.19644
H	-2.01853	-4.40850	-3.23522
H	-2.31398	-4.86770	-1.54289
H		-2.62338	-3.20049	-2.07953

5e

E_scf = -1374.38991873981 a.u.

E_sol = -1374.42413 a.u.

G(T)-E(0) = 0.211973 a.u.

Lowest frequency: 15.86 cm-1

Cl	-1.30124	0.53786	0.59013
C	1.73400	2.20046	-0.59846
C	1.68187	1.56302	0.57304
H	1.34999	1.67572	-1.47064
C	3.22675	6.08357	-1.66455
C	2.88246	5.14448	-2.63698
C	2.39775	3.89528	-2.25773
C	2.25235	3.55011	-0.90178
C	2.59420	4.51021	0.06711
C	3.07519	5.75986	-0.31419
H	3.60298	7.06047	-1.95465
H	2.98584	5.38537	-3.69151
H	2.12320	3.17000	-3.02037
H	2.47309	4.28491	1.11950
H	3.32966	6.48882	0.45033
C	2.88053	2.51447	4.54927
C	3.83958	2.17497	3.59048
C	3.45217	1.85516	2.29181
C	2.08637	1.88520	1.93727
C	1.12449	2.21710	2.91266
C	1.52540	2.53454	4.20734
H	3.18817	2.75772	5.56259
H	4.89271	2.15669	3.85692
H	4.18421	1.57765	1.53961
H	0.07454	2.21062	2.63786
H	0.77901	2.79407	4.95263
Pd	0.88056	-0.28988	0.54016
C	2.65052	-1.51818	1.18311
C	2.67926	-1.46481	-0.19383
H	3.32994	-0.89804	1.75722
H	2.17990	-2.23382	-0.78263
H	2.15342	-2.33211	1.70401
C	3.68271	-0.59366	-0.90284
N	3.56997	-0.59314	-2.26306
O	4.55067	0.03287	-0.30899
H	2.78878	-1.01682	-2.73807
H	4.18242	0.01668	-2.78383

6e

E_scf = -1374.37465656918 a.u.

E_sol = -1374.40606 a.u.

G(T)-E(0) = 0.214668 a.u.

Lowest frequency: -239.19 cm-1

Cl	-0.51890	-1.78997	0.02684
C	2.67530	2.08904	-0.32015
C	2.44851	1.40367	0.82853
H	2.85554	1.48909	-1.21283
C	2.81296	6.27880	-1.20519
C	3.23926	5.32654	-2.13254
C	3.17823	3.97192	-1.81756
C	2.70348	3.53763	-0.56425
C	2.26583	4.50945	0.35671
C	2.32272	5.86232	0.03608
H	2.85252	7.33632	-1.44979
H	3.61406	5.63771	-3.10344
H	3.50416	3.23219	-2.54457
H	1.86923	4.20373	1.31757
H	1.97535	6.59738	0.75665
C	2.60957	2.60779	4.93638
C	3.72960	2.75087	4.11351
C	3.66783	2.37334	2.77465
C	2.47833	1.84972	2.23008
C	1.35762	1.71148	3.07193
C	1.42447	2.08858	4.41182
H	2.66005	2.90103	5.98106
H	4.65357	3.15531	4.51701
H	4.53898	2.48305	2.13518
H	0.42748	1.31866	2.66875
H	0.54867	1.97925	5.04478
Pd	1.21799	-0.21605	0.42594
C	3.56815	-0.48303	0.71186
C	2.81449	-1.52731	0.12169
H	4.27909	0.02110	0.06913
H	2.51411	-2.38774	0.71749
H	3.79154	-0.52011	1.77143
C	2.94546	-1.72080	-1.37759
N	2.15048	-2.69945	-1.89083
O	3.74090	-1.05537	-2.03632
H	1.28105	-2.90258	-1.40309

H	2.12235	-2.74900	-2.90039

7e

E_scf = -1374.42574640514 a.u.

E_sol = -1374.45345 a.u.

G(T)-E(0) = 0.220132 a.u.

Lowest frequency: 31.02 cm-1

Cl	-0.85202	-0.61209	-0.49244
C	3.15793	1.52690	-0.04316
C	3.06764	0.84859	1.17848
H	3.64623	0.97775	-0.84797
C	2.47723	5.62796	-1.10580
C	3.38120	4.83770	-1.81778
C	3.58912	3.51125	-1.44897
C	2.91579	2.95131	-0.34720
C	2.00166	3.75975	0.35830
C	1.78462	5.08119	-0.02301
H	2.30645	6.66026	-1.39756
H	3.91794	5.25178	-2.66649
H	4.28244	2.89461	-2.01532
H	1.45801	3.35404	1.20517
H	1.07037	5.68663	0.52746
C	2.68108	2.61399	5.08061
C	3.59870	3.12450	4.16137
C	3.70244	2.56626	2.88820
C	2.89129	1.48177	2.51598
C	1.98583	0.96292	3.45631
C	1.87533	1.53104	4.72395
H	2.59598	3.05520	6.06955
H	4.23677	3.96027	4.43434
H	4.41841	2.96793	2.17805
H	1.34753	0.12719	3.18232
H	1.15748	1.12777	5.43234
Pd	1.18640	0.43947	0.03440
C	3.40898	-0.65865	1.12899
C	2.32182	-1.25023	0.24433
H	4.39965	-0.82361	0.69291
H	1.63971	-1.95493	0.72043
H	3.38220	-1.08143	2.13484
C	2.75660	-1.66678	-1.14910
N	1.80351	-2.31179	-1.87607
O	3.90016	-1.46038	-1.55327
H	0.82724	-2.17818	-1.62965
H	2.02249	-2.48305	-2.84738

8a

E_scf = -2189.34062333017 a.u.

E_sol = -2189.36660 a.u.

G(T)-E(0) = 0.556513 a.u.

Lowest frequency: 14.41 cm-1

C	-0.58642	1.99922	-1.90584
C	-2.35991	-0.31245	-0.70334
C	-0.87378	-0.73703	-3.47264
C	-2.23151	-0.56096	-4.18356
H	-2.50156	0.48674	-4.33025
H	-2.17180	-1.02465	-5.17673
H	-3.04851	-1.05277	-3.65204
C	0.23693	-0.17182	-4.38613
H	0.07249	0.86903	-4.67197
H	1.22749	-0.26199	-3.92922
H	0.25544	-0.76081	-5.31131
C	-0.57113	-2.24904	-3.32901
H	-0.57973	-2.69994	-4.32939
H	0.41659	-2.41922	-2.89142
H	-1.29710	-2.78308	-2.71859
C	-3.58743	0.53668	-1.09724
H	-3.85967	0.42169	-2.14907
H	-4.44604	0.19994	-0.50222
H	-3.45803	1.60097	-0.89145
C	-2.74491	-1.80233	-0.85480
H	-3.11546	-2.04647	-1.85259
H	-1.91748	-2.46659	-0.59879
H	-3.56240	-2.00928	-0.15264
C	-2.04706	-0.10022	0.79891
H	-2.93964	-0.37019	1.37786
H	-1.23008	-0.74791	1.12546
H	-1.80077	0.93159	1.04952
C	-0.83340	2.69355	-0.54691
H	-1.87367	2.65069	-0.22231
H	-0.20235	2.28230	0.24632
H	-0.57138	3.75399	-0.64987
C	-1.53794	2.61494	-2.95442
H	-2.58675	2.38034	-2.76614
H	-1.43684	3.70744	-2.92584
H	-1.29515	2.30000	-3.97174
C	0.86755	2.36617	-2.28953

H	0.91651	3.44853	-2.46345
H	1.56035	2.14226	-1.47428
H	1.22504	1.87414	-3.19328
Cl	0.46166	-2.85307	0.45054
P	-0.73798	0.06506	-1.70807
C	2.91588	1.38063	1.19310
C	3.88308	0.99924	0.33081
H	1.97204	0.83589	1.10660
C	2.66453	4.37682	4.25594
C	1.89064	3.21712	4.31372
C	1.99884	2.25558	3.31134
C	2.89508	2.41856	2.23797
C	3.65887	3.59964	2.18811
C	3.54279	4.56411	3.18583
H	2.57755	5.13298	5.03133
H	1.19677	3.06339	5.13577
H	1.38644	1.35787	3.35677
H	4.33420	3.76806	1.35723
H	4.13672	5.47215	3.12349
C	7.96188	2.36995	0.32496
C	7.21102	2.40450	-0.85041
C	5.88821	1.96269	-0.85032
C	5.28701	1.49258	0.32900
C	6.05783	1.45525	1.50300
C	7.38091	1.89022	1.50051
H	8.99428	2.70821	0.32405
H	7.65512	2.77344	-1.77088
H	5.31281	1.99800	-1.77202
H	5.61104	1.07988	2.41801
H	7.96108	1.84939	2.41828
Pd	1.31001	-0.93152	-0.72146
C	3.56163	-0.07090	-0.69847
C	3.27359	-1.43645	-0.20496
H	2.59048	0.29772	-1.27993
H	3.30723	-1.61581	0.86691
H	4.26065	-0.12246	-1.53836
C	3.70597	-2.56666	-1.09952
N	3.46837	-3.81605	-0.59459
O	4.25279	-2.36464	-2.18433
H	2.68038	-3.90914	0.04134
H	3.59667	-4.56924	-1.25725

8e

E_scf = -1374.39522986097 a.u.

E_sol = -1374.43126 a.u.

G(T)-E(0) = 0.215555 a.u.

Lowest frequency: 18.70 cm-1

Cl	-0.60343	-0.05523	-1.28789
C	2.04396	-1.29874	3.32611
C	3.15105	-1.41385	2.55869
H	1.25019	-0.66431	2.92283
C	0.86773	-3.04476	7.06417
C	0.40665	-1.78428	6.68323
C	0.80757	-1.23358	5.46793
C	1.69286	-1.91866	4.61578
C	2.13535	-3.19614	5.00686
C	1.72695	-3.74935	6.21706
H	0.55106	-3.48100	8.00736
H	-0.27163	-1.23265	7.32814
H	0.43540	-0.25582	5.17068
H	2.79122	-3.75983	4.35302
H	2.07464	-4.73984	6.49751
C	6.88890	-3.22694	3.67335
C	6.18373	-2.44409	4.59100
C	4.97210	-1.86256	4.23017
C	4.43406	-2.05629	2.94420
C	5.16719	-2.82258	2.01940
C	6.37845	-3.40879	2.38824
H	7.83475	-3.68073	3.95620
H	6.58245	-2.27975	5.58837
H	4.43515	-1.24793	4.94482
H	4.79924	-2.95568	1.00569
H	6.92593	-4.00441	1.66325
Pd	1.18825	0.23704	0.14802
C	3.11748	-0.81939	1.15256
C	2.21633	-1.48929	0.15311
H	2.73977	0.27079	1.29362
H	1.55098	-2.25556	0.55766
H	4.11112	-0.67351	0.72363
C	2.83615	-1.89918	-1.17609
N	1.98699	-2.01882	-2.21953
O	4.03348	-2.17786	-1.22160

H	1.06260	-1.59918	-2.18981
H	2.38475	-2.27860	-3.11064

9a

E_scf = -2189.33366686557 a.u.

E_sol = -2189.36193 a.u.

G(T)-E(0) = 0.554720 a.u.

Lowest frequency: -640.03 cm-1

C	-0.42269	2.03554	-1.79970
C	-2.30864	-0.29629	-0.81677
C	-0.64460	-0.63061	-3.50228
C	-1.95968	-0.41301	-4.27994
H	-2.21603	0.64221	-4.39397
H	-1.84334	-0.83070	-5.28817
H	-2.80790	-0.92337	-3.82005
C	0.51667	-0.03146	-4.32686
H	0.36682	1.02022	-4.57950
H	1.47837	-0.14155	-3.81725
H	0.58606	-0.58286	-5.27247
C	-0.35886	-2.14938	-3.40385
H	-0.31963	-2.56051	-4.42041
H	0.60604	-2.34236	-2.92579
H	-1.11817	-2.70006	-2.85109
C	-3.49514	0.58446	-1.26468
H	-3.69033	0.52170	-2.33771
H	-4.39731	0.22915	-0.75083
H	-3.37345	1.63604	-0.99756
C	-2.69490	-1.77491	-1.05180
H	-2.99535	-1.97801	-2.08182
H	-1.89414	-2.45666	-0.75912
H	-3.56213	-1.99748	-0.41751
C	-2.10635	-0.13839	0.71078
H	-3.04310	-0.42091	1.20815
H	-1.32268	-0.80521	1.07619
H	-1.87574	0.88237	1.01487
C	-0.73682	2.66599	-0.42363
H	-1.79483	2.62545	-0.16218
H	-0.15863	2.20377	0.38146
H	-0.45383	3.72538	-0.45812
C	-1.31782	2.70421	-2.86685
H	-2.37582	2.46850	-2.74668
H	-1.21448	3.79322	-2.77926
H	-1.02141	2.43806	-3.88389
C	1.04715	2.41527	-2.09763

H	1.10212	3.50596	-2.20565
H	1.70486	2.13685	-1.27103
H	1.43903	1.97612	-3.01439
Cl	0.29357	-2.85844	0.60596
P	-0.61855	0.09507	-1.70055
C	2.91794	1.20074	1.34626
C	3.81867	0.83988	0.40329
H	2.02628	0.57476	1.40635
C	2.69594	4.43657	4.15531
C	2.03151	3.23136	4.38402
C	2.12876	2.19541	3.45829
C	2.90811	2.32811	2.29286
C	3.56121	3.55596	2.07029
C	3.45329	4.59425	2.99199
H	2.61641	5.25044	4.87075
H	1.43043	3.09971	5.27952
H	1.59927	1.26228	3.63596
H	4.14031	3.70303	1.16571
H	3.95858	5.53654	2.79715
C	7.68178	2.64860	-0.17025
C	6.78774	2.56203	-1.23760
C	5.53522	1.97572	-1.05736
C	5.15097	1.47974	0.19832
C	6.06461	1.56145	1.26218
C	7.31752	2.14265	1.07925
H	8.65880	3.10205	-0.31168
H	7.06438	2.95106	-2.21344
H	4.84390	1.91954	-1.89453
H	5.78313	1.16717	2.23407
H	8.01182	2.19721	1.91337
Pd	1.27461	-0.97463	-0.64512
C	3.55947	-0.33056	-0.49455
C	3.26709	-1.62762	-0.01482
H	2.22710	0.11028	-1.30846
H	3.15651	-1.80456	1.05080
H	4.09261	-0.33559	-1.44503
C	3.60250	-2.79636	-0.90624
N	3.23035	-4.00985	-0.40084
O	4.19706	-2.64982	-1.97274
H	2.40920	-4.02103	0.20210
H	3.31875	-4.78112	-1.04901

9e

E_scf = -1374.37467713294 a.u.

E_sol = -1374.41044 a.u.

G(T)-E(0) = 0.215112 a.u.

Lowest frequency: -142.99 cm-1

Cl	0.25193	1.44429	-0.34561
C	1.51480	-2.17051	2.93818
C	2.68175	-2.17770	2.24012
H	0.62945	-1.84005	2.39805
C	0.49386	-3.16146	6.97515
C	-0.30443	-2.30561	6.21486
C	0.05179	-2.00724	4.90300
C	1.22715	-2.53275	4.32828
C	2.01459	-3.40627	5.10558
C	1.64637	-3.71570	6.41116
H	0.21525	-3.40443	7.99669
H	-1.20749	-1.87746	6.64024
H	-0.57843	-1.34851	4.31038
H	2.90391	-3.85557	4.68043
H	2.26023	-4.39794	6.99239
C	6.57504	-2.85032	3.94674
C	5.76857	-1.81223	4.41768
C	4.50406	-1.60385	3.87028
C	4.02509	-2.43084	2.84161
C	4.85007	-3.46127	2.36538
C	6.11311	-3.67343	2.91910
H	7.55948	-3.01398	4.37589
H	6.12498	-1.16200	5.21166
H	3.87765	-0.79762	4.23993
H	4.49515	-4.11312	1.57128
H	6.73454	-4.48297	2.54707
Pd	2.25393	0.31957	0.27646
C	2.69618	-1.90108	0.79158
C	1.59004	-1.62606	-0.05699
H	3.67968	-0.24841	0.56355
H	0.57394	-1.63533	0.33044
H	3.58172	-2.24002	0.25959
C	1.73380	-1.91559	-1.54192
N	0.74956	-1.37154	-2.30903
O	2.63690	-2.62520	-1.96776
H	0.25133	-0.55645	-1.96133

H	0.87313	-1.45116	-3.30876

$9a_z$

E_scf = -2189.32133798743 a.u.

E_sol = -2189.35018 a.u.

G(T)-E(0) = 0.552938 a.u.

Lowest frequency: -597.63 cm-1

C	-0.62718	2.13512	-1.53912
C	-2.08804	-0.58293	-0.82732
C	-1.08774	-0.03724	-3.78803
C	-2.56686	0.19855	-4.16396
H	-2.90911	1.20721	-3.92320
H	-2.67599	0.06839	-5.24846
H	-3.24318	-0.51319	-3.68895
C	-0.22763	0.90325	-4.66138
H	-0.53961	1.94782	-4.59969
H	0.83713	0.84159	-4.42194
H	-0.34247	0.59662	-5.70833
C	-0.68340	-1.47900	-4.17567
H	-0.86837	-1.61302	-5.24947
H	0.37599	-1.66490	-3.98376
H	-1.24330	-2.24573	-3.64325
C	-3.37904	0.25449	-0.71066
H	-3.82889	0.47483	-1.68174
H	-4.11389	-0.32686	-0.13950
H	-3.23506	1.19490	-0.17478
C	-2.47279	-1.97264	-1.38637
H	-3.01216	-1.91866	-2.33376
H	-1.60486	-2.62456	-1.49742
H	-3.14979	-2.44479	-0.66320
C	-1.51449	-0.83656	0.58888
H	-2.29407	-1.31371	1.19648
H	-0.65972	-1.51644	0.54889
H	-1.21166	0.07493	1.10537
C	-0.57148	2.34614	-0.00911
H	-1.50430	2.08816	0.49429
H	0.23996	1.77199	0.44921
H	-0.37863	3.40736	0.19154
C	-1.82085	2.93146	-2.11183
H	-2.78866	2.55004	-1.78718
H	-1.74708	3.97112	-1.76849
H	-1.81265	2.95783	-3.20388
C	0.66641	2.77315	-2.10011

H	0.67537	3.83259	-1.81498
H	1.56929	2.31931	-1.68526
H	0.74081	2.73092	-3.18531
Cl	0.84941	-3.21804	-1.34394
P	-0.66978	0.21521	-1.90524
C	4.73698	2.17112	-1.16078
C	4.35099	0.91743	-1.51312
H	4.45494	2.49051	-0.15668
C	6.86955	5.33331	-3.13406
C	6.77322	5.27577	-1.74299
C	6.08027	4.23158	-1.13612
C	5.48053	3.20696	-1.89510
C	5.57862	3.28588	-3.29924
C	6.26185	4.33812	-3.90420
H	7.40316	6.14888	-3.61396
H	7.23198	6.04677	-1.12997
H	6.00195	4.19888	-0.05176
H	5.10548	2.53465	-3.91795
H	6.31662	4.38328	-4.98861
C	5.46202	-0.83197	-5.28531
C	4.11607	-0.63200	-4.98239
C	3.75014	-0.08568	-3.75041
C	4.72324	0.27592	-2.80927
C	6.07384	0.05315	-3.11867
C	6.43921	-0.49285	-4.34565
H	5.74940	-1.25608	-6.24368
H	3.34730	-0.89991	-5.70215
H	2.69965	0.06124	-3.51607
H	6.83134	0.29797	-2.38273
H	7.48966	-0.66037	-4.56703
Pd	1.44609	-0.83210	-1.24446
C	3.51052	0.18652	-0.52052
C	3.43010	-1.22470	-0.35115
H	3.28894	0.77730	0.36784
H	3.06422	-1.55455	0.62208
H	2.07480	0.60498	-1.05236
C	4.47380	-2.17498	-0.92043
N	4.02279	-3.32913	-1.44766
O	5.66335	-1.89554	-0.78253
H	3.02501	-3.52195	-1.53358
H	4.71088	-4.00398	-1.74653

10a

E_scf = -2189.34246350534 a.u.

E_sol = -2189.37132 a.u.

G(T)-E(0) = 0.554433 a.u.

Lowest frequency: 12.15 cm-1

C	-0.21831	2.00532	-2.40660
C	-2.10518	0.07373	-0.76228
C	-0.80347	-0.92534	-3.48885
C	-2.19649	-0.75922	-4.13407
H	-2.40706	0.26996	-4.43175
H	-2.23374	-1.37420	-5.04198
H	-3.00443	-1.10097	-3.48499
C	0.26769	-0.59511	-4.55167
H	0.14104	0.39470	-4.99507
H	1.28128	-0.67980	-4.15060
H	0.17614	-1.32517	-5.36505
C	-0.59432	-2.41194	-3.11118
H	-0.71069	-3.01694	-4.01908
H	0.41133	-2.58309	-2.71698
H	-1.30787	-2.77678	-2.37403
C	-3.28147	0.93898	-1.26659
H	-3.60106	0.68229	-2.27891
H	-4.13746	0.76213	-0.60344
H	-3.07136	2.00968	-1.23075
C	-2.60074	-1.38548	-0.63952
H	-3.03075	-1.76946	-1.56686
H	-1.81281	-2.05441	-0.28838
H	-3.39990	-1.40122	0.11205
C	-1.72553	0.52942	0.66805
H	-2.61717	0.42561	1.29951
H	-0.94467	-0.10364	1.09261
H	-1.41154	1.57098	0.72391
C	-0.31400	2.90754	-1.15537
H	-1.33130	3.01274	-0.77655
H	0.32750	2.54963	-0.34477
H	0.03280	3.91174	-1.42895
C	-1.21182	2.51777	-3.47385
H	-2.25590	2.38975	-3.18778
H	-1.04323	3.59213	-3.61890
H	-1.06111	2.03891	-4.44398
C	1.21416	2.20872	-2.95263

H	1.30676	3.25283	-3.27761
H	1.96038	2.03413	-2.17499
H	1.45676	1.57613	-3.80568
Cl	0.43205	-2.29607	0.96354
P	-0.51575	0.14315	-1.89326
C	3.12225	0.67781	1.72157
C	3.95348	0.59922	0.64694
H	2.42553	-0.15054	1.84237
C	2.35415	3.63035	4.73563
C	1.95878	2.30191	4.89810
C	2.23197	1.36736	3.90319
C	2.92765	1.72680	2.73019
C	3.30738	3.07605	2.57773
C	3.02060	4.01140	3.56791
H	2.13555	4.36544	5.50556
H	1.42780	1.99515	5.79509
H	1.90359	0.33819	4.02524
H	3.81263	3.39657	1.67533
H	3.31484	5.04786	3.42473
C	7.13441	3.36336	-0.24126
C	6.14807	3.10638	-1.19406
C	5.11484	2.21289	-0.91056
C	5.04185	1.57347	0.33689
C	6.04900	1.82949	1.28138
C	7.08362	2.71763	0.99594
H	7.94112	4.05649	-0.46323
H	6.18207	3.60083	-2.16112
H	4.35080	2.02000	-1.65905
H	6.01259	1.32694	2.24341
H	7.85394	2.90289	1.73961
Pd	1.37952	-0.79598	-0.83687
C	3.84433	-0.52469	-0.30578
C	3.38015	-1.78881	-0.04853
H	2.01126	-0.05479	-2.01405
H	3.06644	-2.07667	0.94824
H	4.31712	-0.38613	-1.27574
C	3.53319	-2.88553	-1.06762
N	2.85749	-4.02597	-0.73049
O	4.22493	-2.77251	-2.07516
H	2.07255	-3.94784	-0.08862
H	2.82415	-4.74828	-1.43560

10e

E_scf = -1374.39197645814 a.u.

E_sol = -1374.42827 a.u.

G(T)-E(0) = 0.217603 a.u.

Lowest frequency: -18.24 cm-1

Cl	0.55621	1.64648	-1.06885
C	1.55648	-2.13473	3.04898
C	2.72873	-2.09374	2.38353
H	0.67233	-1.78391	2.52032
C	0.51483	-3.38356	7.02103
C	-0.24102	-2.42851	6.34033
C	0.12077	-2.04449	5.05141
C	1.25624	-2.58586	4.42004
C	1.99847	-3.55988	5.11373
C	1.62867	-3.95128	6.39806
H	0.23259	-3.69181	8.02386
H	-1.11614	-1.98740	6.80929
H	-0.47817	-1.30679	4.52231
H	2.85660	-4.02317	4.64096
H	2.21082	-4.70995	6.91397
C	6.57438	-2.92122	4.13699
C	5.77392	-1.89626	4.64441
C	4.52656	-1.63629	4.07926
C	4.05719	-2.39669	2.99601
C	4.87803	-3.41467	2.48393
C	6.12301	-3.67922	3.05559
H	7.54469	-3.12660	4.58041
H	6.12005	-1.29821	5.48288
H	3.90225	-0.84419	4.48135
H	4.53175	-4.02011	1.64994
H	6.73907	-4.48019	2.65655
Pd	2.24629	0.50400	0.02330
C	2.81876	-1.68351	0.92264
C	1.61145	-1.39992	0.09003
H	3.47323	-0.71459	0.91529
H	0.63184	-1.40380	0.56730
H	3.47382	-2.35525	0.35533
C	1.60527	-2.03871	-1.29421
N	0.62060	-1.60236	-2.12314
O	2.40473	-2.92423	-1.58133
H	0.21683	-0.68337	-1.96983

H	0.66357	-1.93948	-3.07481

J

E_scf = -786.81575364321 a.u.

E_sol = -786.83944 a.u.

G(T)-E(0) = 0.211452 a.u.

Lowest frequency: 33.22 cm-1

C	3.05234	0.69578	1.63810
C	3.96521	0.59070	0.63435
H	2.28478	-0.07641	1.65982
C	2.49480	3.52512	4.81595
C	1.42507	2.78560	4.30936
C	1.63408	1.87589	3.27596
C	2.90976	1.69352	2.70675
C	3.98095	2.43513	3.24281
C	3.77259	3.33768	4.28198
H	2.33777	4.23211	5.62546
H	0.42844	2.91329	4.72256
H	0.79776	1.29740	2.89082
H	4.98067	2.29219	2.85070
H	4.61512	3.89455	4.68261
C	6.84603	3.58271	-0.49835
C	5.50851	3.93636	-0.30744
C	4.57642	2.97474	0.07539
C	4.96389	1.63992	0.27624
C	6.30736	1.29344	0.06219
C	7.24236	2.25801	-0.31369
H	7.57199	4.33361	-0.79720
H	5.18899	4.96304	-0.46321
H	3.53677	3.25214	0.21563
H	6.61973	0.26174	0.19945
H	8.27939	1.97246	-0.46626
C	3.96514	-0.59174	-0.23993
C	3.60832	-1.84381	0.09943
H	3.31974	-2.08981	1.11937
H	4.31251	-0.45174	-1.26247
C	3.62999	-2.93021	-0.91905
N	3.23942	-4.16052	-0.45127
O	3.98591	-2.76401	-2.08131
H	2.82285	-4.28189	0.45752
H	3.15568	-4.90725	-1.12392

K

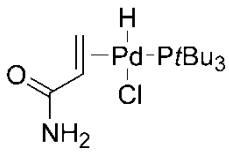
E_scf = -786.80693962291 a.u.

E_sol = -786.82760 a.u.

G(T)-E(0) = 0.213429 a.u.

Lowest frequency: 26.55 cm-1

C	3.92525	-3.16281	-1.00612
C	3.06430	-2.13600	-1.24809
H	3.48880	-4.04377	-0.53518
C	8.13183	-3.70936	-1.64320
C	7.45504	-4.39928	-0.63671
C	6.08894	-4.20196	-0.45565
C	5.36632	-3.29571	-1.25691
C	6.06250	-2.62081	-2.27908
C	7.42623	-2.82875	-2.46643
H	9.19662	-3.86411	-1.79267
H	7.98987	-5.09552	0.00325
H	5.56575	-4.74932	0.32483
H	5.53097	-1.94561	-2.93845
H	7.94133	-2.30293	-3.26551
C	4.33931	1.67089	-2.79794
C	4.83674	1.20647	-1.57873
C	4.42604	-0.02963	-1.08195
C	3.50706	-0.81862	-1.79247
C	3.01165	-0.34088	-3.01450
C	3.42822	0.89313	-3.51415
H	4.65976	2.63318	-3.18691
H	5.54760	1.80490	-1.01561
H	4.82375	-0.39611	-0.14039
H	2.29175	-0.93479	-3.56928
H	3.03501	1.24848	-4.46209
C	1.64697	-2.37501	-0.94381
C	0.57270	-1.55865	-0.92512
H	1.43293	-3.41945	-0.71817
H	-0.39356	-2.02818	-0.75438
C	0.41780	-0.09207	-1.20949
N	1.11665	0.76820	-0.40499
O	-0.38976	0.29443	-2.04536
H	1.93646	0.44061	0.08227
H	1.11802	1.73677	-0.69523



E_scf = -1649.82880891677 a.u.

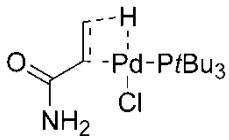
E_sol = -1649.85474 a.u.

G(T)-E(0) = 0.383247 a.u.

Lowest frequency: 16.05 cm-1

C	7.61001	1.65386	-3.56851
C	9.05114	-1.17841	-3.47679
C	9.99401	1.16904	-1.54611
C	10.87745	2.00465	-2.49833
H	10.37095	2.89622	-2.87380
H	11.74890	2.35218	-1.92968
H	11.25482	1.43587	-3.35022
C	9.50475	2.08327	-0.39639
H	8.94493	2.95120	-0.74189
H	8.90454	1.53126	0.32821
H	10.39210	2.45990	0.12784
C	10.87390	0.07717	-0.89524
H	11.64841	0.58242	-0.30531
H	10.30064	-0.54879	-0.20850
H	11.38979	-0.54769	-1.62689
C	10.34209	-0.92729	-4.28580
H	11.21092	-0.75285	-3.64916
H	10.55707	-1.82299	-4.88164
H	10.25113	-0.09030	-4.98126
C	9.27493	-2.37736	-2.52322
H	10.04563	-2.19935	-1.77488
H	8.35255	-2.64511	-1.99973
H	9.58396	-3.24212	-3.12339
C	7.94295	-1.61304	-4.46120
H	8.25445	-2.55547	-4.92738
H	6.99384	-1.80156	-3.95271
H	7.77830	-0.89605	-5.26786
C	6.18122	1.21107	-3.96112
H	6.14258	0.24938	-4.47145
H	5.52625	1.16049	-3.08855
H	5.77016	1.96378	-4.64547
C	8.40073	1.93117	-4.86695
H	8.40861	1.07168	-5.54069

H	7.91101	2.75301	-5.40390
H	9.43262	2.23253	-4.68533
C	7.43603	2.98127	-2.79708
H	6.79558	3.64330	-3.39256
H	6.94514	2.83122	-1.83096
H	8.37679	3.50807	-2.63337
Cl	8.16763	-0.67074	1.31512
P	8.45591	0.33190	-2.40691
H	6.16321	-0.66617	-2.19542
Pd	6.90867	-0.60888	-0.86152
C	4.59052	-1.20705	-0.53469
C	5.33247	-1.78035	0.45664
H	4.14130	-0.22731	-0.41040
H	5.50590	-1.26455	1.39518
H	4.29242	-1.80473	-1.38958
C	5.75900	-3.22614	0.34630
O	5.29622	-3.97611	-0.50709
H	7.24942	-2.88459	1.70383
N	6.65637	-3.60733	1.29951
H	7.05814	-4.52669	1.17844



E_scf = -1649.82468891724 a.u.

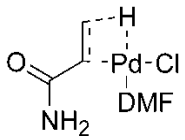
E_sol = -1649.84933 a.u.

G(T)-E(0) = 0.385502 a.u.

Lowest frequency: -579.35 cm-1

C	7.52919	1.56324	-3.57659
C	9.17954	-1.13799	-3.47883
C	9.94065	1.27505	-1.54948
C	10.68810	2.27296	-2.45939
H	10.06730	3.10702	-2.79140
H	11.51746	2.70344	-1.88435
H	11.12311	1.79374	-3.34005
C	9.35718	2.02455	-0.32643
H	8.60808	2.77180	-0.59033
H	8.91603	1.32291	0.38588
H	10.17737	2.54739	0.18167
C	10.98453	0.28276	-0.98724
H	11.70200	0.86115	-0.39174
H	10.53157	-0.45877	-0.32748
H	11.55664	-0.22239	-1.76781
C	10.41123	-0.76875	-4.33347
H	11.27680	-0.49533	-3.72787
H	10.69965	-1.64721	-4.92464
H	10.21533	0.04362	-5.03561
C	9.54812	-2.30869	-2.53725
H	10.32660	-2.06359	-1.81752
H	8.68132	-2.65643	-1.97069
H	9.91034	-3.14063	-3.15450
C	8.07753	-1.67563	-4.41838
H	8.43424	-2.61280	-4.86250
H	7.15243	-1.90303	-3.88027
H	7.85190	-0.99748	-5.24402
C	6.16046	0.99197	-4.01626
H	6.22870	0.06234	-4.57768
H	5.49763	0.82375	-3.16468
H	5.67717	1.73316	-4.66467
C	8.30502	1.93829	-4.85939
H	8.39270	1.09364	-5.54656

H	7.74930	2.72241	-5.38863
H	9.30480	2.32475	-4.66300
C	7.20544	2.85029	-2.78425
H	6.54105	3.47572	-3.39312
H	6.68107	2.62792	-1.84968
H	8.08686	3.44918	-2.55258
Cl	8.61434	-1.57324	0.89052
P	8.47288	0.31685	-2.40302
H	5.77463	-0.02948	-1.50451
Pd	7.00659	-0.61132	-0.72070
C	4.70259	-0.54210	-0.30977
C	5.37660	-1.40466	0.55887
H	4.44505	0.46413	0.00501
H	5.69749	-1.06822	1.54006
H	4.09136	-0.99729	-1.08495
C	5.29749	-2.88757	0.29209
O	4.55779	-3.34483	-0.57511
H	6.92626	-3.22167	1.46940
N	6.07087	-3.65003	1.11906
H	6.13337	-4.62505	0.85764



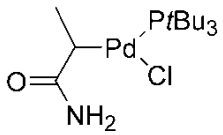
E_scf = -1083.41766662870 a.u.

E_sol = -1083.45424 a.u.

G(T)-E(0) = 0.131341 a.u.

Lowest frequency: -614.33 cm-1

Cl	7.54591	-3.09883	-0.23279
H	5.20440	-1.43431	-0.61451
O	8.70358	-0.12221	-1.35537
C	9.72201	-0.81356	-1.13297
H	9.61667	-1.83974	-0.75909
N	10.97556	-0.37782	-1.31812
C	11.26009	0.97053	-1.79341
H	10.34482	1.55972	-1.76214
H	12.01264	1.43722	-1.14960
H	11.64453	0.94722	-2.81986
C	12.11403	-1.25776	-1.08153
H	12.77843	-0.82620	-0.32475
H	11.76256	-2.22938	-0.73008
H	12.68503	-1.40262	-2.00570
Pd	6.66438	-0.97403	-0.89928
C	4.64877	0.06884	-0.94327
C	5.70276	0.86057	-1.43909
H	3.94182	-0.32941	-1.66677
H	6.17798	1.60021	-0.79735
H	4.27734	0.22675	0.06432
O	4.91892	0.81335	-3.70362
C	5.83794	1.04416	-2.92934
H	7.85912	1.29280	-2.74340
N	7.06124	1.52761	-3.32379
H	7.21365	1.51178	-4.32346



E_scf = -1649.83520525851 a.u.

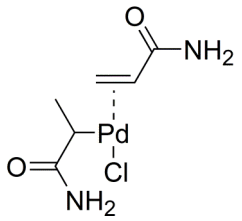
E_sol = -1649.85772 a.u.

G(T)-E(0) = 0.384200 a.u.

Lowest frequency: 13.96 cm-1

C	7.43799	1.45677	-3.47069
C	9.25213	-1.12811	-3.42757
C	9.87365	1.27956	-1.45775
C	10.59009	2.30950	-2.35507
H	9.93365	3.11607	-2.68864
H	11.39747	2.77533	-1.77577
H	11.04683	1.85267	-3.23624
C	9.24973	2.00368	-0.23902
H	8.48927	2.73686	-0.50937
H	8.80748	1.28613	0.45791
H	10.04620	2.53952	0.29274
C	10.93870	0.32058	-0.87801
H	11.62290	0.91367	-0.25820
H	10.49487	-0.44649	-0.23971
H	11.54462	-0.15847	-1.64942
C	10.45676	-0.67602	-4.27944
H	11.30974	-0.37267	-3.66942
H	10.78886	-1.52289	-4.89380
H	10.21555	0.14331	-4.95953
C	9.69204	-2.29615	-2.51418
H	10.47747	-2.02848	-1.80996
H	8.85662	-2.69089	-1.93266
H	10.07796	-3.10110	-3.15272
C	8.17668	-1.71360	-4.37003
H	8.58385	-2.61984	-4.83446
H	7.27111	-2.00563	-3.82932
H	7.90248	-1.03633	-5.18116
C	6.09992	0.78121	-3.85852
H	6.22060	-0.08676	-4.50382
H	5.52854	0.46675	-2.98167
H	5.48848	1.51118	-4.40330
C	8.14755	1.89298	-4.77010
H	8.31094	1.05646	-5.45308

H	7.51056	2.61487	-5.29725
H	9.10795	2.37776	-4.58859
C	7.05369	2.72085	-2.66892
H	6.34387	3.30916	-3.26331
H	6.56025	2.47248	-1.72394
H	7.90516	3.36751	-2.45304
Cl	8.51275	-1.88536	0.83358
P	8.46049	0.25855	-2.31994
H	5.29317	0.22443	-0.89711
Pd	6.97252	-0.69117	-0.56776
C	4.63760	-0.21590	-0.03894
C	5.40102	-1.26154	0.67843
H	4.38217	0.65775	0.56246
H	5.69915	-1.07431	1.70746
H	3.78761	-0.63257	-0.58492
C	5.05174	-2.68257	0.32913
O	4.23176	-2.94912	-0.54916
H	6.60467	-3.38526	1.44681
N	5.69162	-3.63408	1.07621
H	5.59687	-4.57794	0.72555



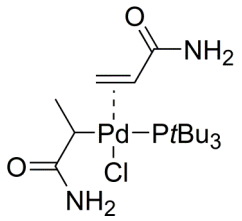
E_scf = -1082.22817332955 a.u.

E_sol = -1082.26078 a.u.

G(T)-E(0) = 0.117985 a.u.

Lowest frequency: 50.38 cm-1

Cl	8.72695	-1.00745	-0.39154
H	3.67893	-0.24528	-0.56977
C	4.51817	0.31549	-0.15638
C	5.82554	0.03799	-0.85926
H	4.28147	1.38231	-0.28368
H	6.64006	0.63411	-0.45014
H	4.59785	0.12844	0.91743
O	4.76299	-0.15051	-3.02490
C	5.78780	0.09384	-2.37767
H	7.82168	0.39051	-2.42943
N	6.95993	0.45897	-2.95997
H	7.01504	0.39826	-3.96686
Pd	6.55801	-1.88400	-0.54366
C	4.74383	-3.12337	-0.06635
C	4.68029	-2.79016	-1.39916
H	5.20750	-4.06400	0.22551
H	4.06524	-1.96537	-1.74174
H	4.15367	-2.59794	0.67618
C	5.27165	-3.68147	-2.46161
O	5.84690	-4.73037	-2.19222
H	4.80550	-2.23776	-3.86711
N	5.09067	-3.20044	-3.72354
H	5.54579	-3.69451	-4.47719



E_scf = -1897.13535258738 a.u.

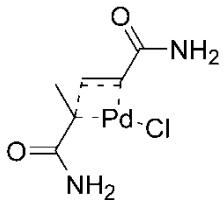
E_sol = -1897.16229 a.u.

G(T)-E(0) = 0.458871 a.u.

Lowest frequency: 18.12 cm-1

C	9.88519	1.66277	-1.34829
C	8.67500	0.51050	-4.01275
C	10.34903	-1.37753	-2.13293
C	11.78464	-0.98333	-2.54445
H	12.24186	-0.28092	-1.84571
H	12.40805	-1.88713	-2.53967
H	11.84433	-0.55533	-3.54571
C	10.39910	-1.99821	-0.71936
H	10.73636	-1.30476	0.04829
H	9.42361	-2.37474	-0.40641
H	11.10114	-2.84197	-0.74096
C	9.87302	-2.50910	-3.07141
H	10.51233	-3.38478	-2.90504
H	8.84497	-2.81899	-2.85747
H	9.95139	-2.25501	-4.12995
C	9.91504	0.56623	-4.93373
H	10.36677	-0.41685	-5.08090
H	9.59739	0.91945	-5.92368
H	10.68742	1.24804	-4.57903
C	7.70662	-0.53401	-4.62209
H	8.08449	-1.55431	-4.58430
H	6.72371	-0.51795	-4.15341
H	7.55527	-0.28601	-5.68048
C	7.94975	1.87334	-4.11474
H	7.58370	1.99608	-5.14173
H	7.08261	1.94872	-3.45351
H	8.60149	2.72166	-3.90448
C	8.74154	2.61579	-0.92322
H	8.14642	2.97882	-1.76226
H	8.06644	2.14218	-0.20482
H	9.17974	3.49400	-0.43212

C	10.86904	2.42489	-2.26310
H	10.39997	2.85841	-3.14729
H	11.29311	3.25900	-1.68932
H	11.70582	1.80247	-2.58847
C	10.65676	1.30178	-0.05912
H	10.96709	2.24046	0.41739
H	10.04024	0.75450	0.65389
H	11.56735	0.73261	-0.25671
Cl	8.20415	-0.65323	1.53607
P	9.04082	0.07523	-2.12360
H	6.01169	-1.99307	2.34808
C	5.09428	-1.76711	1.80119
C	5.18493	-0.47675	1.00470
H	4.89241	-2.61017	1.13359
H	4.29749	-0.36328	0.38566
H	4.25937	-1.70897	2.51415
C	5.39194	0.83393	1.73050
O	5.27226	1.92322	1.14953
H	6.13442	-0.04580	3.41119
N	5.66138	0.77837	3.06711
H	5.97870	1.65400	3.46307
Pd	6.76779	-0.43650	-0.39005
C	5.25216	-0.07410	-2.05678
C	5.52466	-1.42260	-1.94266
H	4.77512	-2.07276	-1.50181
H	6.31461	-1.90263	-2.50852
H	5.85707	0.57189	-2.68143
C	3.87729	0.46095	-1.72030
O	2.88458	-0.24340	-1.87401
H	4.55295	2.06588	-0.67257
N	3.83690	1.77673	-1.34512
H	2.90423	2.07071	-1.07754



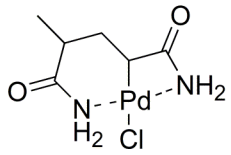
E_scf = -1082.17993720605 a.u.

E_sol = -1082.21977 a.u.

G(T)-E(0) = 0.115060 a.u.

Lowest frequency: -281.20 cm-1

Cl	8.27997	-3.36770	-1.22296
H	3.46345	0.90695	-0.24874
C	4.50270	1.04271	0.05688
C	5.45112	0.21516	-0.80126
H	4.75005	2.10337	-0.07983
H	6.47786	0.43565	-0.46103
H	4.61128	0.80852	1.11844
O	4.12860	0.42707	-2.79452
C	5.24399	0.45540	-2.28922
H	7.29801	0.67725	-2.62888
N	6.36844	0.73207	-3.01402
H	6.26934	0.81019	-4.01642
Pd	6.65699	-1.72907	-0.85636
C	4.35852	-1.58156	-0.47016
C	4.99104	-2.86823	-0.52653
H	4.04168	-1.29679	0.52680
H	4.89049	-3.47493	-1.42646
H	3.73318	-1.26505	-1.29919
C	5.13045	-3.62607	0.78652
O	4.55345	-3.24114	1.79736
H	6.60165	-4.81721	0.01072
N	5.86898	-4.76742	0.71239
H	6.06254	-5.21295	1.59916



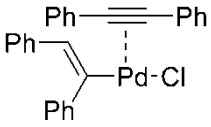
E_scf = -1082.24008033306 a.u.

E_sol = -1082.28743 a.u.

G(T)-E(0) = 0.123490 a.u.

Lowest frequency: 56.69 cm-1

Cl	8.78339	-2.36156	-2.82657
H	3.44099	-1.84357	1.84717
C	4.31429	-1.30387	2.22480
C	5.30601	-0.98256	1.10058
H	3.96824	-0.38034	2.69745
H	4.81024	-0.37283	0.33141
H	4.78929	-1.92975	2.98436
C	5.79738	-2.27784	0.45053
O	5.92457	-3.32750	1.03240
H	5.54253	-1.68356	-1.53248
N	6.20719	-2.16897	-0.93202
H	6.46139	-3.07483	-1.33100
Pd	7.98553	-1.00008	-1.00615
C	6.52981	-0.18340	1.63118
C	7.42420	0.32187	0.51494
H	6.15461	0.65183	2.23844
H	7.00189	1.14957	-0.06675
H	7.10874	-0.82217	2.30726
C	8.87034	0.46048	0.79015
O	9.50006	0.34627	1.81505
H	9.40390	1.20239	-1.14324
N	9.52665	0.39259	-0.53749
H	10.50590	0.11892	-0.47928



E_scf = -1666.54832292715 a.u.

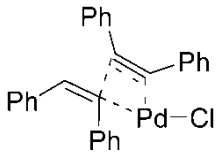
E_sol = -1666.57765 a.u.

G(T)-E(0) = 0.308575 a.u.

Lowest frequency: 18.26 cm-1

Cl	0.16357	-0.20334	-1.85883
C	1.76030	0.19748	3.43820
C	1.75694	0.63555	2.17797
H	1.27185	-0.75653	3.63319
C	3.46511	1.93413	6.97698
C	2.91379	0.65278	6.99438
C	2.35945	0.11625	5.83447
C	2.34688	0.84122	4.62896
C	2.89846	2.13600	4.62969
C	3.45112	2.67142	5.78986
H	3.89751	2.35715	7.87942
H	2.91442	0.06987	7.91159
H	1.93151	-0.88343	5.85412
H	2.88864	2.72833	3.72158
H	3.87116	3.67356	5.76989
C	3.34813	3.47972	-0.53978
C	1.98024	3.40736	-0.32703
C	1.46525	2.52559	0.63730
C	2.34390	1.68997	1.38760
C	3.74214	1.75927	1.12274
C	4.22806	2.65851	0.19333
H	3.74756	4.17288	-1.27433
H	1.30101	4.03928	-0.89008
H	0.40901	2.55410	0.89242
H	4.41008	1.10670	1.67580
H	5.29797	2.72569	0.01664
Pd	0.96107	0.00412	0.43849
C	-0.26260	-1.76082	1.22180
C	0.84391	-2.22495	0.90916
C	4.20927	-4.57675	-0.11683
C	3.58278	-3.78936	-1.08658
C	2.47918	-3.00943	-0.75600
C	1.99062	-3.01864	0.56571

C	2.62408	-3.81119	1.54032
C	3.72715	-4.58699	1.19385
H	5.07306	-5.18011	-0.38169
H	3.95750	-3.77936	-2.10603
H	1.98487	-2.38279	-1.49347
H	2.24666	-3.81244	2.55832
H	4.21298	-5.19814	1.94904
C	-4.26367	-0.97314	2.35433
C	-3.38927	-1.57855	3.25913
C	-2.07101	-1.83540	2.89277
C	-1.61857	-1.48811	1.60662
C	-2.50326	-0.87811	0.69513
C	-3.81764	-0.62733	1.07577
H	-5.29024	-0.76930	2.64571
H	-3.73309	-1.84846	4.25348
H	-1.38679	-2.30481	3.59242
H	-2.13557	-0.60715	-0.29101
H	-4.49661	-0.15569	0.37127



E_scf = -1666.52843442489 a.u.

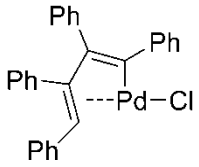
E_sol = -1666.55637 a.u.

G(T)-E(0) = 0.314453 a.u.

Lowest frequency: -238.84 cm-1

C	0.63045	0.20682	0.12048
C	0.06678	0.02042	2.13766
Cl	3.98662	-1.98467	1.75636
C	-0.25084	-0.58590	-0.53393
H	-0.59946	-1.46095	0.00848
C	-2.01013	-0.45267	-4.43946
C	-2.38260	-1.41792	-3.50336
C	-1.79067	-1.42816	-2.24454
C	-0.81630	-0.47501	-1.88496
C	-0.44682	0.48846	-2.84441
C	-1.04058	0.49522	-4.10314
H	-2.46631	-0.44201	-5.42534
H	-3.13059	-2.16477	-3.75452
H	-2.07858	-2.18675	-1.52063
H	0.30996	1.22654	-2.60933
H	-0.73987	1.24392	-4.83081
C	2.48526	3.90264	-1.02168
C	3.18033	2.69684	-1.12987
C	2.56433	1.50002	-0.76909
C	1.23845	1.48784	-0.28493
C	0.54834	2.71129	-0.18428
C	1.16888	3.90304	-0.55353
H	2.96299	4.83524	-1.30785
H	4.20004	2.68334	-1.50346
H	3.10038	0.56071	-0.88630
H	-0.47556	2.72006	0.17201
H	0.61972	4.83740	-0.47668
C	0.45775	-1.12904	2.56904
C	-2.15465	3.44670	3.33687
C	-0.80875	3.32744	3.68847
C	-0.07183	2.21753	3.27960
C	-0.68087	1.21250	2.51063

C	-2.03174	1.34442	2.14772
C	-2.76459	2.45225	2.56819
H	-2.72695	4.31193	3.65947
H	-0.33033	4.09890	4.28505
H	0.97357	2.11567	3.55407
H	-2.49718	0.57607	1.53771
H	-3.81169	2.54102	2.29261
C	-0.38968	-4.33878	5.20780
C	-1.39807	-3.45160	4.82050
C	-1.11471	-2.41428	3.93917
C	0.19630	-2.24495	3.44375
C	1.20474	-3.14647	3.82918
C	0.90538	-4.18307	4.70923
H	-0.61568	-5.15215	5.89185
H	-2.40759	-3.57166	5.20361
H	-1.89461	-1.72340	3.63485
H	2.20649	-3.02423	3.42760
H	1.68913	-4.87511	5.00338
Pd	2.02003	-0.74226	1.34032



E_scf = -1666.59393817859 a.u.

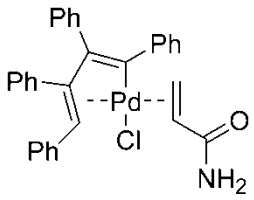
E_sol = -1666.61978 a.u.

G(T)-E(0) = 0.317170 a.u.

Lowest frequency: 16.10 cm-1

C	-0.01320	0.64556	0.53842
C	-0.06528	0.35409	2.02209
Cl	2.74095	-2.94067	0.42178
C	-0.78242	-0.21460	-0.27355
H	-1.55894	-0.77439	0.24264
C	-1.13933	-0.60308	-4.53823
C	-2.20798	-0.90590	-3.69285
C	-2.07314	-0.75734	-2.31452
C	-0.87488	-0.28452	-1.74839
C	0.19670	0.01260	-2.61479
C	0.06342	-0.14949	-3.99101
H	-1.23783	-0.73015	-5.61240
H	-3.14453	-1.26970	-4.10593
H	-2.90358	-1.01420	-1.66139
H	1.14002	0.36303	-2.20961
H	0.90638	0.07361	-4.63870
C	2.09448	4.17072	-0.73392
C	2.66367	3.31164	0.20746
C	1.98104	2.16799	0.61469
C	0.72480	1.85303	0.07179
C	0.15633	2.73077	-0.86558
C	0.83586	3.88033	-1.26284
H	2.62682	5.06312	-1.05089
H	3.64154	3.53118	0.62626
H	2.42753	1.50061	1.34507
H	-0.82134	2.51189	-1.28234
H	0.38117	4.54957	-1.98786
C	0.39472	-0.90170	2.19929
C	-1.37538	3.28089	4.87839
C	-0.48397	2.27701	5.26596
C	-0.04988	1.32433	4.34797

C	-0.50588	1.35363	3.01766
C	-1.39715	2.37147	2.63860
C	-1.82812	3.32470	3.55951
H	-1.70846	4.02466	5.59657
H	-0.11771	2.24052	6.28825
H	0.65307	0.55869	4.65657
H	-1.75968	2.41327	1.61583
H	-2.51902	4.10201	3.24458
C	0.43012	-3.56925	5.52536
C	-0.74247	-2.90930	5.15119
C	-0.74106	-2.05096	4.05627
C	0.44277	-1.83139	3.32113
C	1.61330	-2.51520	3.69457
C	1.60299	-3.36934	4.79361
H	0.42635	-4.24539	6.37586
H	-1.66163	-3.06820	5.70832
H	-1.65154	-1.53792	3.76323
H	2.51060	-2.39579	3.09774
H	2.51344	-3.89253	5.07150
Pd	1.03872	-1.33985	0.36048



E_scf = -1913.90290206564 a.u.

E_sol = -1913.93447 a.u.

G(T)-E(0) = 0.387623 a.u.

Lowest frequency: 13.52 cm-1

C	0.23836	0.57410	0.63820
C	0.14127	0.32775	2.12643
Cl	1.40934	-2.70631	-1.65460
C	-0.60274	-0.19195	-0.16555
H	-1.35381	-0.76071	0.38201
C	-1.58249	0.01861	-4.33076
C	-2.52636	-0.37189	-3.38139
C	-2.16755	-0.44541	-2.03751
C	-0.86832	-0.11590	-1.61371
C	0.07752	0.25596	-2.58463
C	-0.28068	0.32529	-3.92649
H	-1.85378	0.06987	-5.38175
H	-3.53759	-0.62681	-3.68589
H	-2.90406	-0.75824	-1.30085
H	1.09799	0.46495	-2.29133
H	0.46550	0.60464	-4.66487
C	2.69524	3.89185	-0.56199
C	3.22958	2.87369	0.22817
C	2.43669	1.79289	0.61010
C	1.10267	1.70049	0.18285
C	0.57488	2.73099	-0.61231
C	1.36375	3.81995	-0.97525
H	3.31174	4.73752	-0.85396
H	4.26556	2.91500	0.55147
H	2.86687	1.00623	1.22131
H	-0.45593	2.67852	-0.94664
H	0.93725	4.61185	-1.58473
C	0.56621	-0.91774	2.39738
C	-1.71764	3.31973	4.59340
C	-0.80256	2.42974	5.15779
C	-0.18083	1.46220	4.37206
C	-0.46668	1.35830	3.00001

C	-1.39068	2.26261	2.44628
C	-2.00841	3.23226	3.23197
H	-2.19841	4.07516	5.20864
H	-0.56533	2.49210	6.21637
H	0.53284	0.78624	4.82600
H	-1.64048	2.19625	1.39218
H	-2.72106	3.91668	2.77988
C	0.72516	-3.28923	5.95820
C	-0.28820	-3.48321	5.01690
C	-0.32704	-2.70993	3.85920
C	0.63751	-1.70957	3.62896
C	1.65662	-1.52888	4.58390
C	1.69718	-2.31222	5.73663
H	0.75723	-3.89665	6.85818
H	-1.04951	-4.24029	5.18358
H	-1.11289	-2.86402	3.12512
H	2.40969	-0.76179	4.42331
H	2.48846	-2.15577	6.46436
Pd	1.12187	-1.70194	0.59863
C	2.48942	-3.39009	1.29846
C	3.19781	-2.22489	1.49940
H	1.93191	-3.82924	2.12035
H	3.18777	-1.76284	2.47924
H	2.62134	-3.99635	0.40944
C	4.30193	-1.64676	0.64469
O	5.08536	-0.86201	1.17742
H	3.57808	-2.43300	-1.12621
N	4.40166	-2.07259	-0.63932
H	5.09830	-1.59689	-1.19585

***tert*-Butyl phosphine**

E_scf = -814.90239135606 a.u.

E_sol = -814.90717 a.u.

G(T)-E(0) = 0.312253 a.u.

Lowest frequency: 96.63 cm-1

C	7.60652	1.57022	-3.40238
C	9.36674	-1.03656	-3.47834
C	10.08893	1.29165	-1.48956
C	11.28309	1.65176	-2.39507
H	10.98826	2.27081	-3.24541
H	12.02343	2.22153	-1.81641
H	11.79545	0.76873	-2.78327
C	9.55494	2.59421	-0.85274
H	9.27277	3.34736	-1.59056
H	8.69668	2.40753	-0.19985
H	10.34729	3.03336	-0.23289
C	10.58939	0.43334	-0.30038
H	11.33371	1.00615	0.26853
H	9.76821	0.18386	0.37866
H	11.06433	-0.49784	-0.60748
C	9.95783	-0.55961	-4.81939
H	10.76952	0.15875	-4.68387
H	10.36950	-1.41975	-5.36555
H	9.20787	-0.10140	-5.46788
C	10.45997	-1.82184	-2.72012
H	11.37278	-1.24396	-2.56500
H	10.10534	-2.18013	-1.74870
H	10.73516	-2.70375	-3.31296
C	8.24283	-2.06763	-3.75213
H	8.66237	-2.91844	-4.30518
H	7.82283	-2.45049	-2.81685
H	7.42320	-1.66759	-4.34801
C	6.66873	0.78441	-4.34590
H	7.19975	0.27950	-5.15482
H	6.07292	0.04319	-3.80429
H	5.96806	1.48885	-4.81255
C	8.41274	2.57343	-4.25006
H	9.08617	2.07730	-4.95268
H	7.72286	3.19304	-4.83974
H	9.00749	3.25525	-3.63830
C	6.66521	2.34746	-2.44787
H	5.98536	2.97152	-3.04294

H	6.05512	1.66187	-1.85168		
H	7.19322	3.00868	-1.76155		
P			8.60543	0.31362	-2.29427

Diphenylacetylene

E_scf = -539.46525843564 a.u.

E_sol = -539.47424 a.u.

G(T)-E(0) = 0.140360 a.u.

Lowest frequency: 21.35 cm-1

C	0.00000	0.00000	0.60788
C	0.00000	0.00000	-0.60788
C	0.00000	0.00000	4.84339
C	0.00000	1.20793	4.14217
C	0.00000	1.21261	2.75058
C	0.00000	0.00000	2.03301
C	0.00000	-1.21261	2.75058
C	0.00000	-1.20793	4.14217
H	0.00000	0.00000	5.92958
H	0.00000	2.15052	4.68221
H	0.00000	2.14998	2.20391
H	0.00000	-2.14998	2.20391
H	0.00000	-2.15052	4.68221
C	0.00000	0.00000	-4.84339
C	0.00000	-1.20793	-4.14217
C	0.00000	-1.21261	-2.75058
C	0.00000	0.00000	-2.03301
C	0.00000	1.21261	-2.75058
C	0.00000	1.20793	-4.14217
H	0.00000	0.00000	-5.92958
H	0.00000	-2.15052	-4.68221
H	0.00000	-2.14998	-2.20391
H	0.00000	2.14998	-2.20391
H	0.00000	2.15052	-4.68221

scis-acrylamide

E_scf = -247.29812877893 a.u.
E_sol = -247.31672 a.u.
G(T)-E(0) = 0.041934 a.u.
Lowest frequency: -33.96 cm-1

C	0.99576	0.41173	0.00000
C	0.97991	1.74486	0.00000
H	1.93573	-0.13794	0.00000
H	1.89358	2.33049	0.00000
H	0.02984	2.27106	0.00000
C	-0.28481	-0.36382	0.00000
N	-0.12657	-1.72427	0.00000
O	-1.38956	0.16476	0.00000
H	0.77616	-2.16934	0.00000
H	-0.95605	-2.29768	0.00000

Ammonia

E_scf = -56.55640453274 a.u.
E_sol = -56.56851 a.u.
G(T)-E(0) = 0.009493 a.u.
Lowest frequency: 1081.07 cm-1

N	-1.29950	1.20334	-0.05486
H	-1.35643	2.21930	-0.04281
H	-1.98289	0.89234	-0.74170
H	-1.64863	0.89220	0.84890

Ammonium ion

E_scf = -56.90478402614 a.u.
E_sol = -57.04797 a.u.
G(T)-E(0) = 0.026890 a.u.
Lowest frequency: 1494.21 cm-1

N	0.00000	0.00000	0.00000
H	0.59319	0.59319	-0.59319
H	-0.59319	-0.59319	-0.59319
H	-0.59319	0.59319	0.59319
H	0.59319	-0.59319	0.59319

DMF

E_scf = -248.51676530937 a.u.

E_sol = -248.52908 a.u.

G(T)-E(0) = 0.064229 a.u.

Lowest frequency: 125.26 cm-1

C	0.93141	-0.37108	-0.00302
N	-0.19747	0.39909	0.00329
O	0.95800	-1.59078	-0.00901
H	1.85137	0.24672	-0.00163
C	-0.13400	1.84637	0.00936
H	-0.62077	2.26152	0.90161
H	0.91110	2.16695	0.00648
H	-0.62744	2.26853	-0.87579
C	-1.50604	-0.23173	0.00187
H	-2.08091	0.06168	0.88911
H	-2.07647	0.05514	-0.89049
H	-1.35697	-1.31203	0.00592