

Supporting Information

Comparative Theoretical Study of 1,3-Dipolar Cycloadditions of Allyl-Anion Type Dipoles to Free and Pt-Bound Nitriles

Maxim L. Kuznetsov,* Vadim Yu. Kukushkin, and Armando J. L. Pombeiro*

*Centro de Química Estrutural, Complexo I, Instituto Superior Técnico, TU Lisbon, Av. Rovisco Pais,
1049-001 Lisbon, Portugal and Department of Chemistry, St. Petersburg State University, 198504 Stary
Petergof, Russian Federation*

max@mail.ist.utl.pt; pombeiro@ist.utl.pt

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Equilibrium structures of the products

1. Cycloadditions of azomethine (CH₂=N⁺(Me)–CH₂[–], D1) and carbonyl (CH₂=O⁺–CH₂[–], D2) ylides. While a lot of experimental structures of 4,5-dihydro-1*H*-imidazoles are known, there is only a limited number of those for nonfused 2,5-dihydro-1*H*-imidazoles (in particular, 4-alkyl-derivatives) and 2,5-dihydro-1,3-oxazoles. The computational results for **P(1-L)** and **P(2-L)** are in good agreement with the experimental X-ray structural parameters for 1-benzoyl-5-hydroxy-2,4-diphenyl-5-propionyloxy-2,5-dihydro-1*H*-imidazole^{1S} and 2,2-diphenyl-4,5,5-trimethyl-2,5-dihydro-1,3-oxazole,^{2S} respectively, with maximum deviation of 0.03 Å for the C(2)C(6) bond and not higher than 0.02 Å for the other bonds. There are no X-ray structures of transition metal complexes with 2,5-dihydro-1*H*-

imidazole or 2,5-dihydro-1,3-oxazole ligands which might be suitable for comparison with **P(1-Pt^{II})**, **P(2-Pt^{II})**, **P(1-Pt^{IV})** or **P(2-Pt^{IV})**. However, taking into account the good agreement between the experimental and theoretical geometries for products of CA of nitrones to nitriles,^{10c} we hope that the calculations performed in this work predict reasonably the main structural features of the CA products.

2. Cycloadditions of azomethine (CH₂=N⁺(Me)-NH⁻, D3) and carbonyl (CH₂=O⁺-NH⁻, D4) imines. The number of X-ray structures for 2,3(5)-dihydro-1*H*-1,2,4(3)-triazoles is very limited while for the 2,5-dihydro-1,2,4-oxadiazoles only two X-ray structures^{3S} are known and no structures are published for the 2,5-dihydro-1,2,3-oxadiazoles. The maximum deviation of the bond lengths calculated for **P(3-L)Mex** and **P(4-L)O** and experimentally determined for methyl 5-methoxycarbonylamino-2,4-dimethyl-5-phenylcarbamoyl-2,5-dihydro-1*H*-1,2,3-triazole-1-carboxylate^{4S} and 2-acetyl-5-ethyl-3-(*p*-tolyl)-2,5-dihydro-1,2,4-oxadiazole,^{3S} respectively, are 0.03 Å for the N(4)N(5) bond (in **P(3-L)Mex**) and not higher than 0.02 Å for other bonds. To the best of our knowledge, there are no experimental structural data for transition metal complexes with all these heterocycles and no X-ray data suitable for comparison with **P(3-L)O**.

3. Cycloadditions of nitrones (CH₂=N⁺(Me)-O⁻, D5) and carbonyl oxides (CH₂=O⁺-O⁻, D6). No X-ray structures are known for 5*H*-1,2,3-dioxazoles (the products of *meta*-CA of **D6**) and only one structure was obtained for each of 3*H*-1,2,4-dioxazoles (*ortho*-CA of **D6**)^{5S} and 2,3-dihydro-1,2,5-oxadiazoles (*meta*-CA of **D5**).^{6S} The maximum deviation of the bond lengths calculated for **P(6-L)O** and experimentally determined for methyl 3-benzyl-5-phenyl-3*H*-1,2,4-dioxazole-3-carboxylate^{5S} is 0.02 Å for the N(1)C(5) bond and not higher than 0.01 Å for other comparable bonds.

4. Cycloadditions of azoimines (NH=N⁺(Me)-NH⁻, D7) and nitrosimines (NH=O⁺-NH⁻, D8). Only four X-ray structures of 2,3-dihydro-1*H*-tetrazoles have been found.^{7S} In all of them, the heterocycle is bound with a metal (Tc or Cd) and, hence, the experimental structural parameters are not suitable for comparison with theoretically calculated species **P(7-L)**, **P(7-Pt^{II})** and **P(7-Pt^{IV})**. There are no X-ray structural data for the 2,5-dihydro-1,2,3,5-oxatriazoles.

Nature of Transition states and details of the reaction mechanisms

1. Cycloadditions of azomethine ($\text{CH}_2=\text{N}^+(\text{Me})-\text{CH}_2^-$, **D1) and carbonyl ($\text{CH}_2=\text{O}^+-\text{CH}_2^-$, **D2**) ylides. Reactions with free MeCN.** For these processes, the transition states **TS(1-L)** and **TS(2-L)** corresponding to a concerted mechanism were found [Scheme 1S(1)]. The topological analysis of the electron density distribution (AIM method) indicates that both TSs are cyclic. The $\text{N}(1)\cdots\text{C}(5)$ internuclear distance in **TS(1-L)** is significantly longer (by 0.28 Å) than the $\text{C}(2)\cdots\text{C}(3)$ distance whereas, in **TS(2-L)**, this difference is much smaller (0.03 Å). Despite this, both reactions are asynchronous. The calculated values of synchronicity S_y (see Computational details) are 0.69 and 0.64 for **TS(1-L)** and **TS(2-L)**, respectively (see Table 2S for additional characteristics of TSs). It was shown^{28a} that the average value of relative variations of Wiberg bond indices [δB_{av} , formula (9)] is a good quantitative measure of the “advancement” of TS along the reaction path. The low values of δB_{av} for **TS(1-L)** and **TS(2-L)** (0.238 and 0.174) indicate that both these TSs are “early” ones.

For each of the reactions, several triplet biradical or singlet dipolar acyclic intermediates of the stepwise mechanism were also found (Figure 2S). However, these intermediates (and/or TSs leading to them) have energies by 7.24–26.5 kcal/mol higher than the energy of **TS(1-L)** or **TS(2-L)**. Thus, the stepwise mechanism may be discarded.

Reactions with complex 1. In contrast, the mechanism of CAs to the Pt^{II} -nitrile complex **1** is stepwise. The reaction of the azomethine ylide **D1** includes the formation of the closed-shell zwitterionic intermediate **I(1-Pt^{II})** via the transition state **TS(1-Pt^{II})₁** followed by the transformation, via **TS(1-Pt^{II})₂**, to the final product [Scheme 1S(2)]. The first TS (**TS(1-Pt^{II})₁**) is very “early” with an extremely flat surrounding potential energy surface (PES). The $\text{C}(2)\text{C}(3)$ and $\text{N}(1)\text{C}(5)$ distances are very long (2.988 and 3.375 Å, respectively) and the latter is comparable with the $\text{PtC}(5)$ distance (3.485 Å). Despite the long distance between the reacting molecules in this TS, it has a cyclic nature as indicated by the AIM analysis. However, the corresponding cycle is six-membered rather than five-membered. The bond critical points were found for the $\text{C}(2)\text{C}(3)$ and $\text{PtC}(5)$ contacts but not for the $\text{N}(1)\text{C}(5)$ contact

(Figure 3S).

The intermediate **I(1-Pt^{II})** represents a six-membered cyclic structure bearing Pt–N and Pt–C bonds, the latter with the length of 2.118–2.230 Å. Organometallic compounds with Pt–C bonds are well known including those with four- or five-membered metallacycles. However, six-membered metallacycles of this type are rare.^{8S} The second TS (**TS(1-Pt^{II})₂**) is also cyclic, bearing both C(2)C(3) and N(1)C(5) bond critical points of the electron density field and a cyclic critical point corresponding to the imidazoline ring.

For the reaction of carbonyl ylide **D2**, the intermediate **I(2-Pt^{II})** and one TS (**TS(2-Pt^{II})₂**) were found. However, despite all attempts, we were unable to locate any TS for the formation of **I(2-Pt^{II})** from the starting reactants (**D2** and **1**). Such a situation may be caused by one of two reasons. First, the TS does not exist and, hence, this process is barrierless. Second, the PES near the TS is so flat that the optimization procedure failed to locate a saddle point. In any case, the character of PES indicates that even if such TS exists, the activation energy for the reaction should be very low. Note that no TS of the concerted mechanism was found for the CAs of **D1** or **D2** to **1**.

Reactions with complex 2. For these processes, transition states **TS(1-Pt^{IV})** and **TS(2-Pt^{IV})** of the concerted mechanism were found (Scheme 1S(1)). Both TSs are very “early” with long C(2)C(3) and particularly N(1)C(5) distances (2.956–3.043 and 3.708–4.332 Å, respectively). A bond critical point exists only for the first contact, thus indicating the acyclic nature of the TSs. The mechanism is highly asynchronous with the *S_y* parameter of 0.40 and 0.31 for **TS(1-Pt^{IV})** and **TS(2-Pt^{IV})**, respectively, that is also seen from the general view of the TSs (Figure 4S) and the great difference of the C(2)C(3) and N(1)C(5) distances.

Taking into account the extremely “early” character of **TS(1-Pt^{IV})** and **TS(2-Pt^{IV})**, an additional investigation of the nature of these TSs has been performed. First, the IRC calculations starting from **TS(1-Pt^{IV})** and **TS(2-Pt^{IV})** were attempted to be carried out. However, these calculations failed because of very flat PES near these TSs. Therefore, the following procedure was done: the atoms in these TSs were shifted from their equilibrium positions along the vectors corresponding to the imaginary

frequency and then the geometry optimization with small step size was carried out. Such an optimization resulted in the formation of the final products **P(1-Pt^{IV})** and **P(2-Pt^{IV})** instead of acyclic intermediates that allowed the assignment of the mechanism to the concerted type.

2. Cycloadditions of azomethine (CH₂=N⁺(Me)-NH⁻, D3) and carbonyl (CH₂=O⁺-NH⁻, D4) imines. Reactions with free MeCN. For all the reaction channels, cyclic transition states of the concerted mechanism **TS(3-L)O/Men/ex** and **TS(4-L)O/M** were found [Scheme 1S(1)]. The N(1)X(5) distances are noticeably longer than the C(2)Z(3) contacts (by 0.15–0.49 Å), particularly in *meta*-TSs, except **TS(4-L)O** where the N(1)C(5) distance is by 0.02 Å shorter than the C(2)N(3) contact. The synchronicity is rather high for *ortho*-CAs of **D3** (*S_y* = 0.79–0.81) while other processes are more asynchronous (*S_y* = 0.69–0.73). The reactions of azomethine and carbonyl imines CH₂YNH are generally more synchronous than those of the corresponding ylides CH₂YCH₂. The stepwise mechanism is not favorable. The energies of acyclic intermediates found (Figure 2S) are by 7.7–32.8 kcal/mol higher than those of **TS(3-L)Oen** or **TS(4-L)O**.

Reactions with complex 1. The mechanism of these processes depends on the followed regio- and stereoisomeric pathway. In the cases of *ortho-exo*- and *meta-endo*-additions of **D3** and *meta*-addition of **D4**, both concerted and stepwise mechanisms may be operating, and the former is slightly (by 0.7–2.1 kcal/mol) more favorable than the latter. For the *ortho-endo*- and *meta-exo*-additions of **D3** and the *ortho*-addition of **D4**, only the stepwise pathway was found [Scheme 1S(2)]. All TSs of the concerted pathways (**TS(3-Pt^{II})** and **TS(4-Pt^{II})**) have a cyclic nature and correspond to an asynchronous CAs with *S_y* values of 0.63–0.71, the reactions being more asynchronous than those involving free MeCN. The natures of TSs and intermediates of the stepwise mechanism are similar to those for the reaction of **D1**.

Reactions with complex 2. The mechanism of all these reactions is concerted asynchronous (via **TS(3-Pt^{IV})O/M** or **TS(4-Pt^{IV})O/M**), especially for the *ortho*-CA of **D4** with *S_y* values of only 0.33. The *ortho*-TSs **TS(3-Pt^{IV})Oen/ex** are acyclic (no critical point for the N(1)C(5) bond was found) whereas the *meta*-TSs **TS(3-Pt^{IV})Men/ex** and **TS(4-Pt^{IV})M** are cyclic ones. Surprisingly, **TS(4-Pt^{IV})O** also has

the cyclic nature despite the great asynchronicity of the reaction.

3. Cycloadditions of nitrones ($\text{CH}_2=\text{N}^+(\text{Me})-\text{O}^-$, **D5**) and carbonyl oxides ($\text{CH}_2=\text{O}^+-\text{O}^-$, **D6**).

Reactions with free MeCN occur via a concerted route through formation of the cyclic TSs **TS(5-L)O/M** and **TS(6-L)O/M** [Scheme 1S(1)]. **TS(6-L)O** along with **TS(4-L)O** (see above) are the only concerted TSs among all studied in this work, in which the C(2)Z(3) contact is longer than the N(1)X(5) contact. The *ortho*-CA of **D5** is highly synchronous ($S_y = 0.92^{10c}$) while the other processes are rather asynchronous ($S_y = 0.70\text{--}0.77$). The stepwise mechanism is less favorable than the concerted one, the energies of found acyclic intermediates^{10c} (Figure 2S) being by 17.4–49.3 kcal/mol higher compared to the energy of **TS(5-L)O** or **TS(6-L)O**.

The mechanism of the reactions of **D5** with **1** is also concerted while, for the reactions **D6** + **1**, both concerted and stepwise pathways were found. The former mechanism is more plausible (by 3.3 kcal/mol) than the latter one in the case of *ortho*-CA whereas both these routes have the same activation barriers for the *meta*-CA. The reactions with **2** proceed via cyclic TSs along the concerted route. Coordination of MeCN to Pt decreases noticeably the synchronicity for the *ortho*-channels but the change is insignificant for the *meta*-channels (Table 2S). The additional discussion of the reaction mechanism is given in Supporting Information.

4. Cycloadditions of azoimines ($\text{NH}=\text{N}^+(\text{Me})-\text{NH}^-$, **D7**) and nitrosimines ($\text{NH}=\text{O}^+-\text{NH}^-$, **D8**).

All reactions with free MeCN proceed via a concerted mechanism with formation of cyclic transition states **TS(7-L)** and **TS(8-L)** [Scheme 1S(1)]. The N(1)N(5) contacts in the TSs are noticeably (by 0.09–0.40 Å) longer than the C(2)N(3) contacts. Nevertheless, the mechanism is rather synchronous with the S_y parameter of 0.77–0.90. It is interesting that the synchronicity varies significantly (by 10 %) depending on the stereoisomeric path (Table 2S). The located acyclic triplet intermediates or transition states of the stepwise mechanism (Figure 2S) have energies higher, by 11.7–39.8 kcal/mol, than those of **TS(7-L)exex** or **TS(8-L)en**.

The reaction of **D8** with complex **1** may occur via both concerted and stepwise mechanisms, and the former is more favorable than the latter by 5.2 kcal/mol. For the reactions of **D7** with **1** and of both

dipoles *with complex 2*, only the concerted mechanism involving cyclic TSs was found. The synchronicity of the CAs decreases on going from free MeCN to complexes **1** and **2** up to $S_y = 0.59$ – 0.64 for **D7** and $S_y = 0.68$ – 0.76 for **D8**.

5. Cycloadditions of azoxy compounds ($\text{NH}=\text{N}^+(\text{Me})-\text{O}^-$, **D9) and nitroso oxides ($\text{NH}=\text{O}^+-\text{O}^-$, **D10**).** For all the reactions examined in this section, cyclic transition states of the concerted mechanism were found. The IRC calculations and following geometry optimizations starting from the last points on the reaction paths indicated that **TS(10-L)O/M** correspond to the formation of the acyclic products **P(10-L)O/M_{acyc}**, while all other TSs lead to the heterocycles. The synchronicity of the reaction $\text{NHN}(\text{Me})\text{O} + \text{MeCN}$ is rather high ($S_y = 0.77$ – 0.89) but it is significantly lower for the reactions with **1** and **2** ($S_y = 0.65$ – 0.74). For the CA $\text{NHN}(\text{Me})\text{O} + \text{MeCN}$, three triplet stepwise intermediates were found (Figure 2S), but their energy is by 21.8 – 41.6 kcal/mol higher than that of **TS(9-L)O_{ex}**. No stepwise intermediates were found for the reaction $\text{NHOO} + \text{MeCN}$.

6. Cycloadditions of nitro compounds ($\text{O}=\text{N}^+(\text{Me})-\text{O}^-$, **D11) and ozone ($\text{O}=\text{O}^+-\text{O}^-$, **D12**).** Reactions of $\text{ON}(\text{Me})\text{O}$ with MeCN, **1**, and **2** and of OOO with MeCN and **2** occur via concerted mechanism involving cyclic TSs while, for the CA of OOO to **1**, both concerted and stepwise mechanisms are possible (Scheme 1S). They have similar activation barriers and the former is only by 1.4 kcal/mol more favorable than the latter. The reactions with free MeCN are rather synchronous with the S_y parameter of 0.79 – 0.83 and the coordination of the nitrile decreases S_y to 0.67 – 0.73 . Triplet biradical acyclic intermediates were found for the reactions of $\text{ON}(\text{Me})\text{O}$ or OOO with MeCN, but their energy (and/or energy of TSs leading to them) is by 4.36 – 41.8 kcal/mol higher than that of **TS(11-L)** or **TS(12-L)**. No triplet acyclic intermediate for the reaction $\text{OOO} + \text{2}$ was obtained; instead, the elimination of oxygen molecule occurs during the geometry optimization.

Additional details of the reaction mechanism

There are several additional interesting features concerning the reaction mechanisms. First, all reactions of the dipoles studied with free MeCN and the Pt^{IV} complex **2** occur via the concerted

mechanism. This is in agreement with a large amount of literature data suggesting that, for the majority of the [2 + 3] cycloaddition reactions, the concerted pathway is preferable over the stepwise one.¹³ In contrast, reactions of many dipoles studied with the Pt^{II} complex **1** occur via the stepwise mechanism or this route is energetically comparable with the concerted one. This may be explained by the fact that the coordination sphere of platinum is not saturated in the square-planar Pt^{II} complex **1**, and there is a possibility for the formation of relatively stable metallacyclic intermediates of the **I(B-Pt^{II})** type (Scheme 1S).

Second, it was indicated that for some reactions with **1**, both concerted and stepwise mechanisms exist, in principle (*e.g.* in the case of **D3**, **D4**, **D6**, **D8**, **D12**). Meanwhile, for other dipoles (**D5**, **D7**, **D9–D11**) the stepwise mechanism was not found, and this is because no transition states **TS(B-Pt^{II})₂** – which connect intermediates **I(B-Pt^{II})** and final products **P(B-Pt^{II})** (Scheme 1S) – exist for these processes. Indeed, all attempts to optimize these structures resulted either in the collapse of the system to separated molecules of the initial reactants or in the formation of **TS(B-Pt^{II})** of the concerted mechanism. Thus, the CA adducts **P(B-Pt^{II})** and the acyclic intermediates **I(B-Pt^{II})** are formed along two different reaction channels which are not connected with each other. This allows to rule out the stepwise mechanism involving the formation of **I(B-Pt^{II})** for these reactions.

The absence of **TS(B-Pt^{II})₂** for these reactions, in turn, may be related to thermodynamic stabilities of intermediates **I(B-Pt^{II})** and products **P(B-Pt^{II})**. Indeed, CA products of the reactions of **D11**, **D9**, **D7**, and **D5** are the least thermodynamically stable (Figure 15A). Intermediates **I(7-Pt^{II})** and **I(5-Pt^{II})** are also less stable than intermediates of the other reactions (Table 11S) while **I(9-Pt^{II})** and **I(11-Pt^{II})** do not exist at all (all attempts to optimize them led to decomposition of the system to the starting reactants). Conceivably, the decrease of the stability of **I(B-Pt^{II})** and **P(B-Pt^{II})** relative to reactants changes the curvature of the surrounding PES so that the channel between **I(B-Pt^{II})** and **P(B-Pt^{II})** which connects them disappears in the case of the low stable systems.

Another possible reason is the degree of advancement of the concerted **TS(B-Pt^{II})** along the reaction path. When **TS(B-Pt^{II})** is early (reactions of **D1–D4**, **D6**, **D8**, **D12**), the structures of **TS(B-**

$\text{Pt}^{\text{II}})_2$ and $\text{TS}(\text{B-Pt}^{\text{II}})$ are significantly different (Scheme 2S(A)), and the corresponding saddle points are far from each other on the PES. When $\text{TS}(\text{B-Pt}^{\text{II}})$ is later (reactions of **D5**, **D7**, **D9**, **D11**), $\text{TS}(\text{B-Pt}^{\text{II}})$ and the expected $\text{TS}(\text{B-Pt}^{\text{II}})_2$ should be structurally closer to each other (Scheme 2S(B)). Such a spatial proximity of the saddle point of $\text{TS}(\text{B-Pt}^{\text{II}})$ on PES leads to the disappearance of the saddle point for $\text{TS}(\text{B-Pt}^{\text{II}})_2$ and the formation of a hill between $\text{I}(\text{B-Pt}^{\text{II}})$ and $\text{P}(\text{B-Pt}^{\text{II}})$ instead of a channel.

For the reaction **D10** + **1**, $\text{TS}(\text{10-Pt}^{\text{II}})_2$ was also not found although the stability of $\text{I}(\text{10-Pt}^{\text{II}})$ and $\text{P}(\text{10-Pt}^{\text{II}})$ is significant (Table 11S) and $\text{TS}(\text{10-Pt}^{\text{II}})$ is as early as, *e.g.*, $\text{TS}(\text{12-Pt}^{\text{II}})$ (Table 2S). The reason is due to the very low stability of the OO bond in the cyclic structures of this type (see section 5 of the article). Indeed, during the attempts to locate $\text{TS}(\text{10-Pt}^{\text{II}})_2$, the cleavage of the OO bond always occurred. Thus, in this case, the disappearance of the saddle point of $\text{TS}(\text{10-Pt}^{\text{II}})_2$ is due to overlapping with another reaction channel leading to the acyclic products $\text{P}(\text{10-Pt}^{\text{II}})_{\text{acyc}}$.

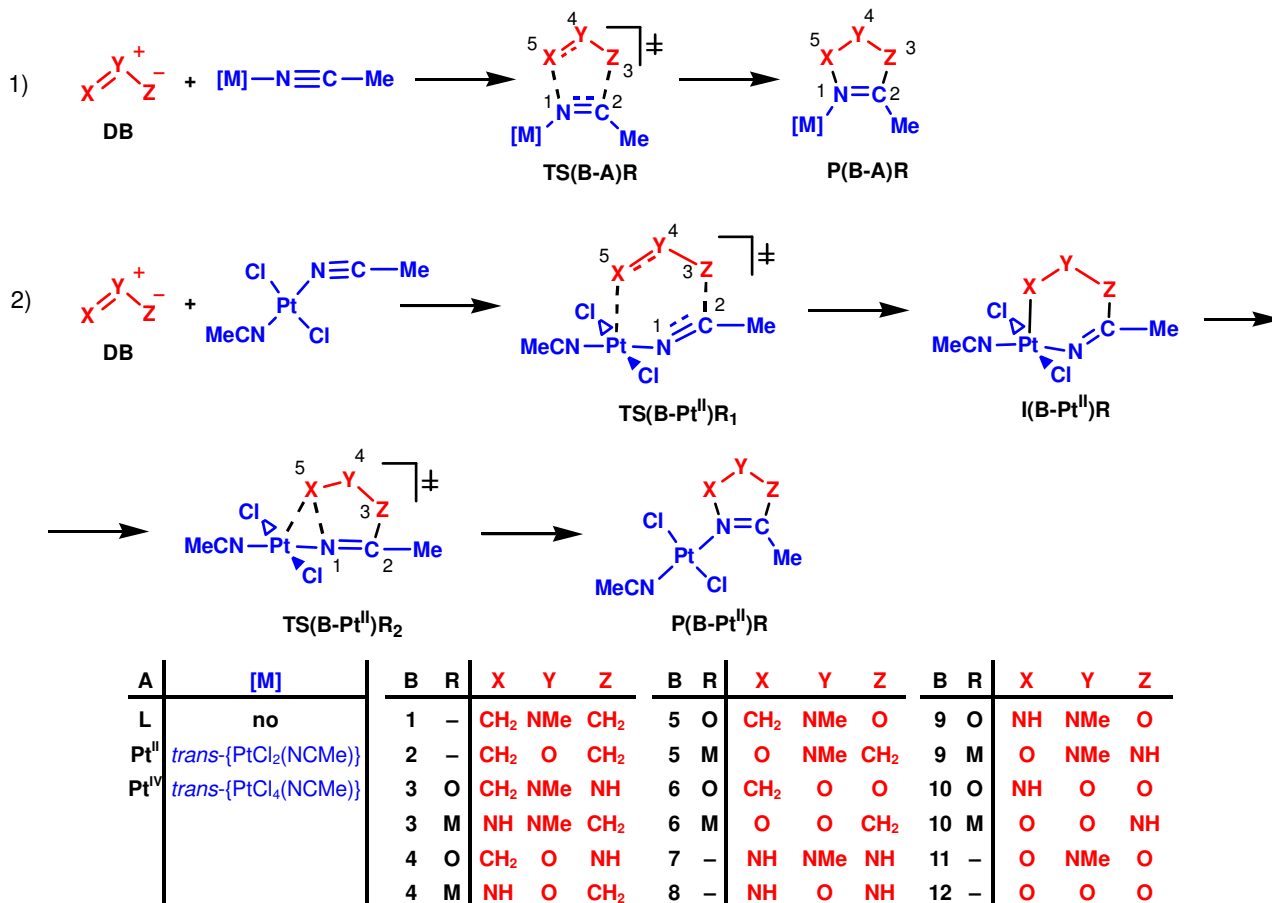
Finally, it should be mentioned that the ΔG value of formation of $\text{I}(\text{5-Pt}^{\text{II}})$ and $\text{I}(\text{7-Pt}^{\text{II}})$ is strongly positive (20–30 kcal/mol) and that of the formation of $\text{I}(\text{10-Pt}^{\text{II}})$ is slightly negative (–3.6 kcal/mol). Thus, the processes $\text{Dipole} + \mathbf{1} = \text{I}(\text{B-Pt}^{\text{II}})$ ($\text{B} = 5, 7$, and 10) are reversible and the relatively low stability of $\text{I}(\text{B-Pt}^{\text{II}})$ should prevent a competition of the formation of $\text{I}(\text{B-Pt}^{\text{II}})$ vs. the formation of $\text{P}(\text{B-Pt}^{\text{II}})$.

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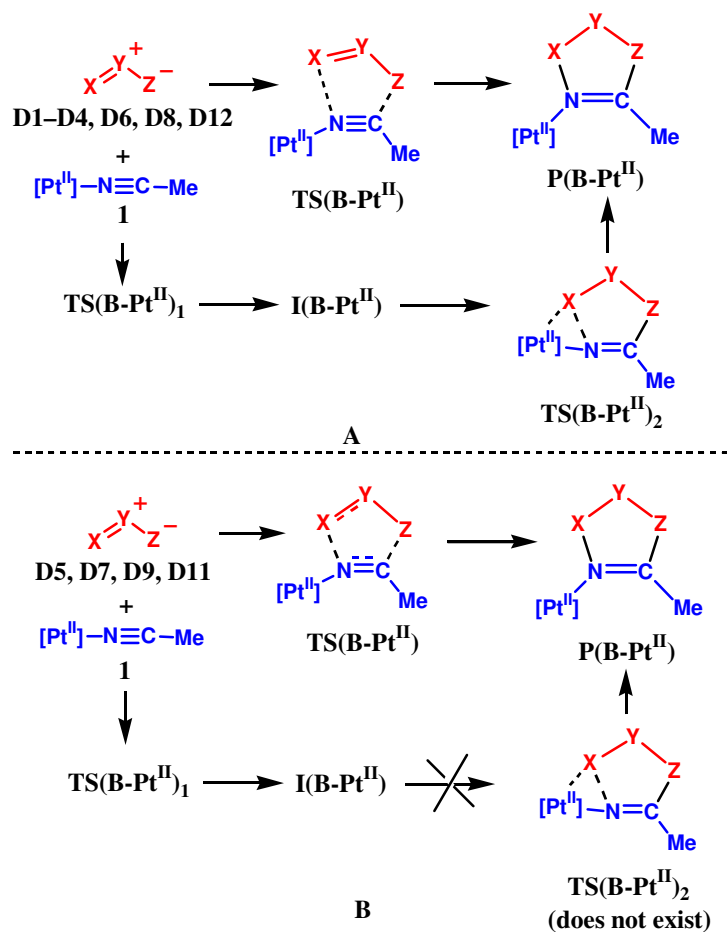
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SCHEME 1S. Concerted (1) and Stepwise (2) Mechanisms of CAs to Nitriles



SCHEME 2S. Transition States for the Early (A) and Late (B) Cycloadditions

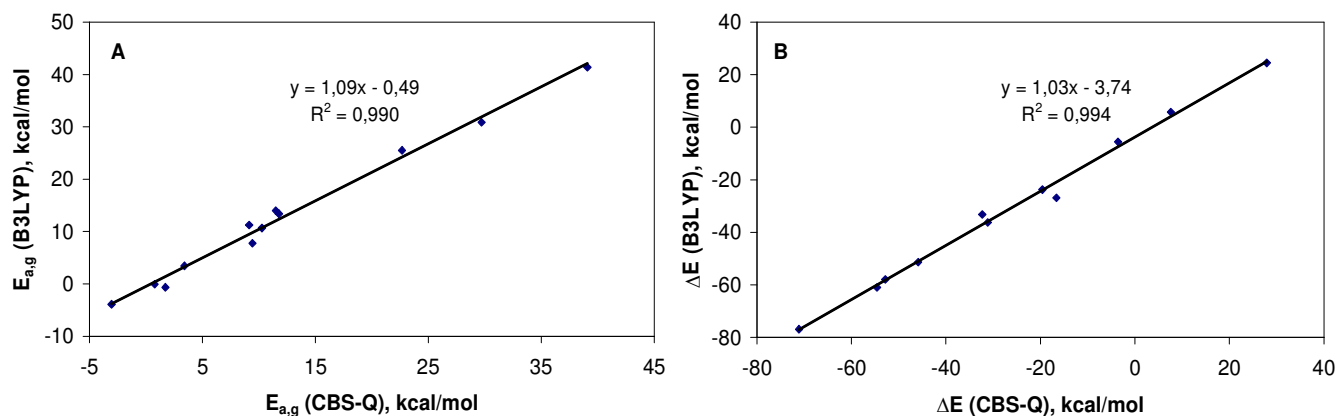
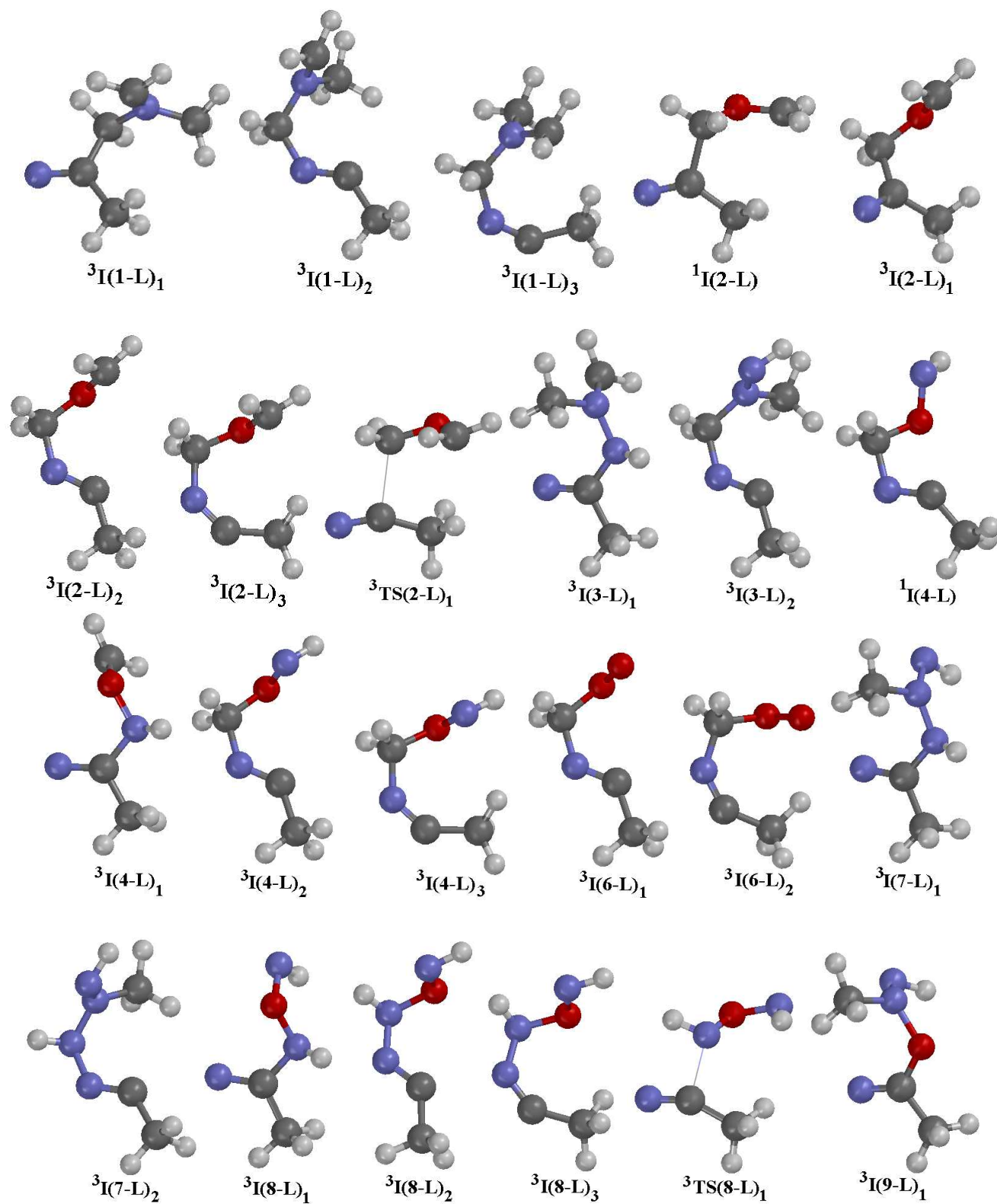


FIGURE 1S. Plots of the B3LYP vs. CBS-Q activation (A) and reaction (B) energies.



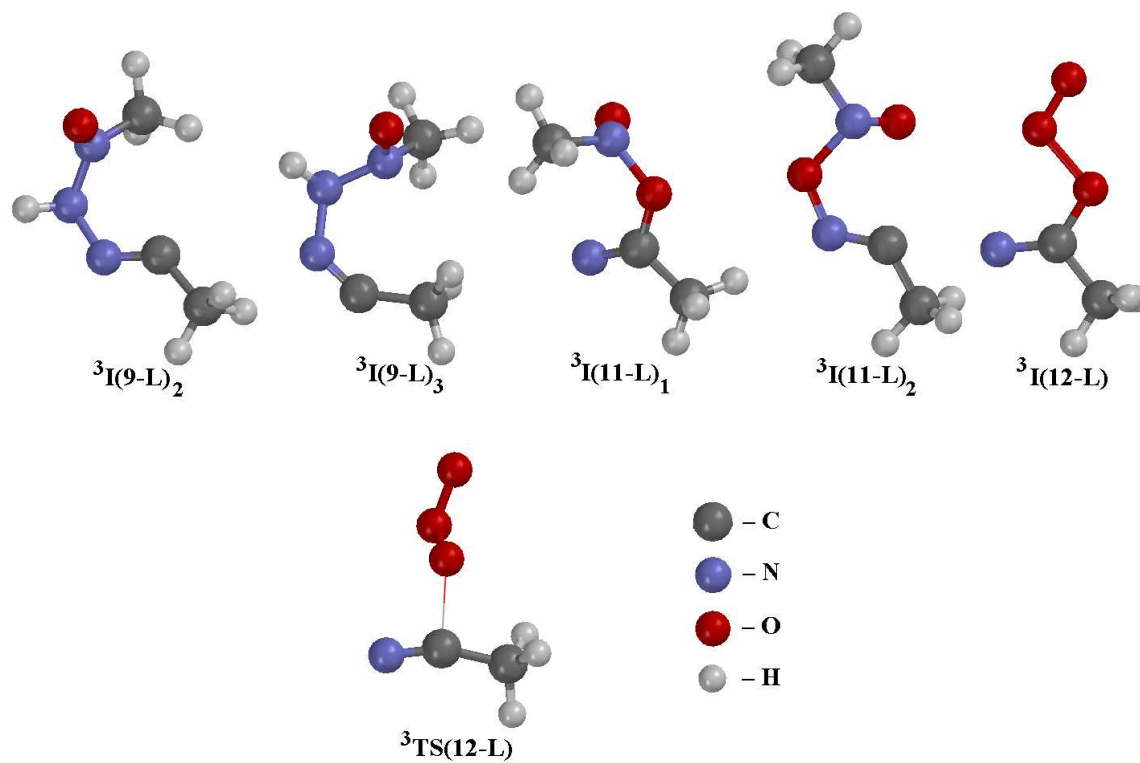


FIGURE 2S. Equilibrium structures of stepwise intermediates and some transition states for the reactions of **D1–D12** with MeCN.

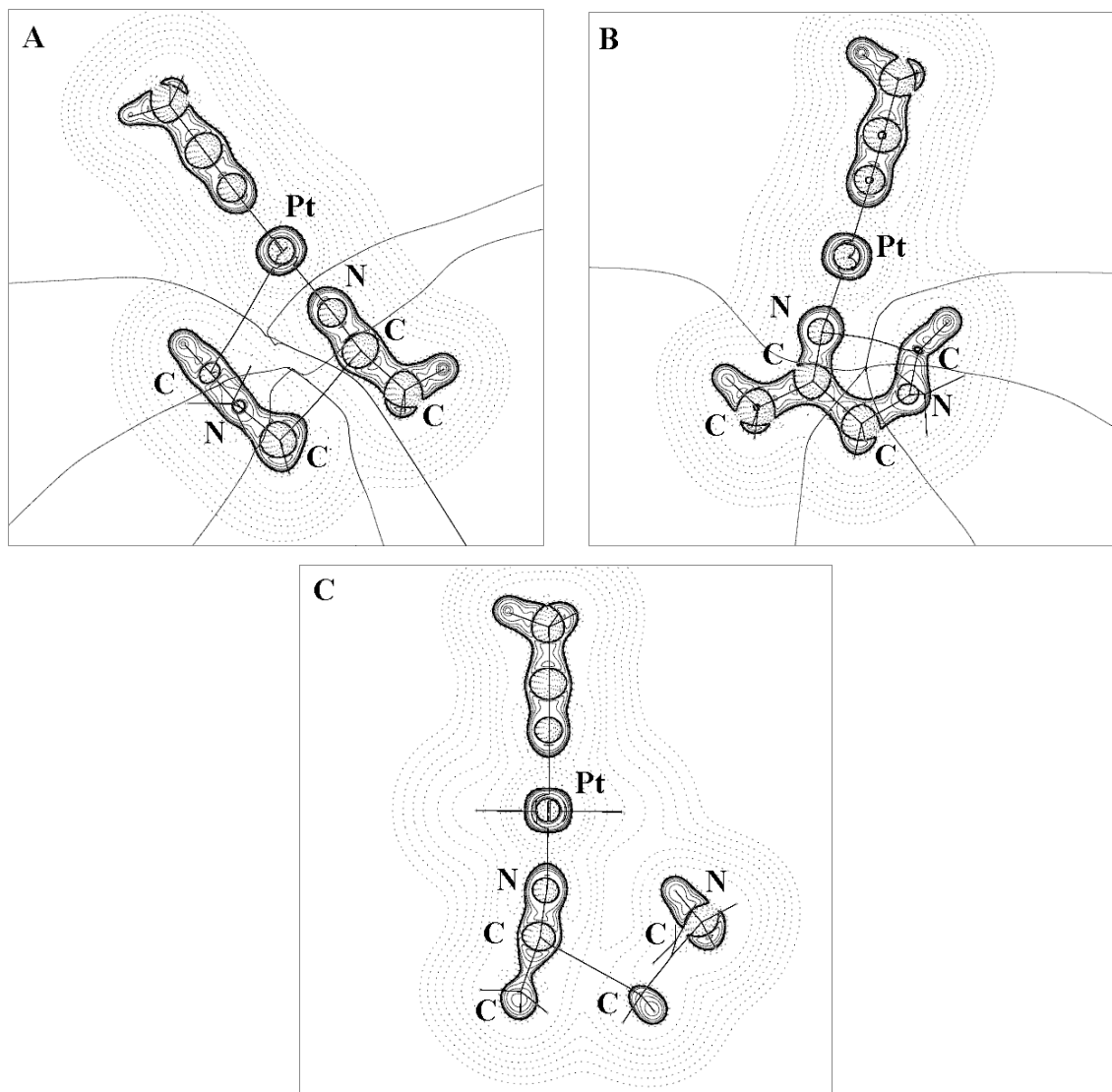


FIGURE 3S. Contour line diagrams of the Laplacian distribution $\nabla^2\rho(\mathbf{r})$ bond paths and selected zero-flux surfaces for **TS(1-Pt^{II})₁** (A), **TS(1-Pt^{II})₂** (B), and **TS(1-Pt^{IV})** (C). Dashed lines indicate charge depletion ($\nabla^2\rho(\mathbf{r}) > 0$), solid lines indicate charge concentration ($\nabla^2\rho(\mathbf{r}) < 0$).

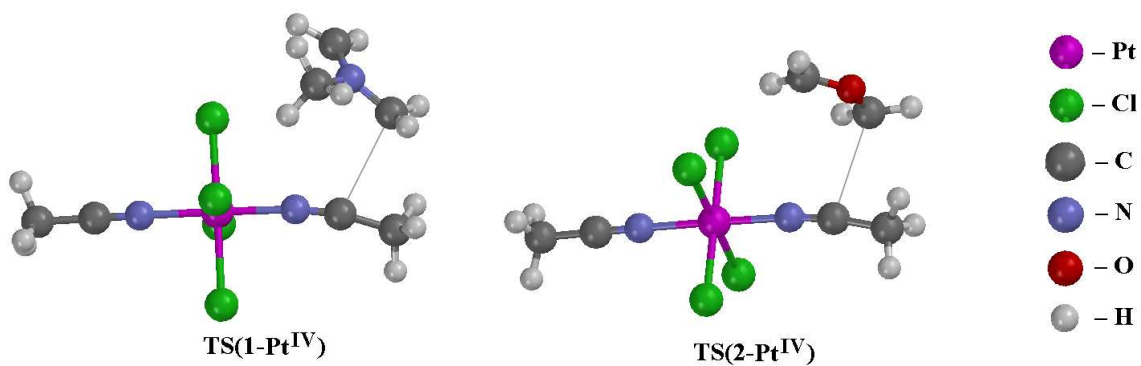


FIGURE 4S. Equilibrium structures of transition states **TS(1-Pt^{IV})** and **TS(2-Pt^{IV})**.

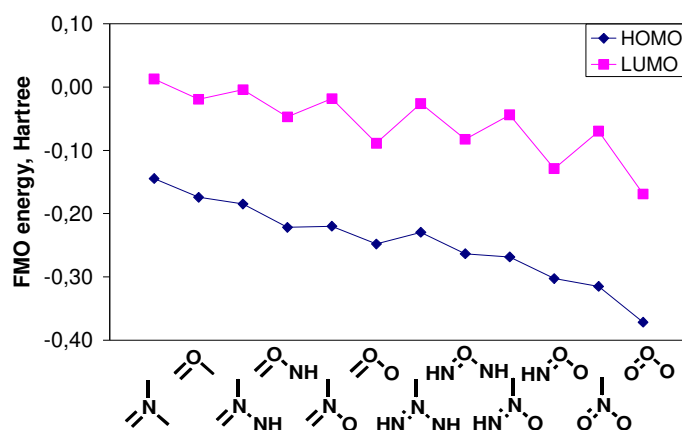


FIGURE 5S. Plots of FMO energies in the series of 1,3-dipoles of allyl anion type.

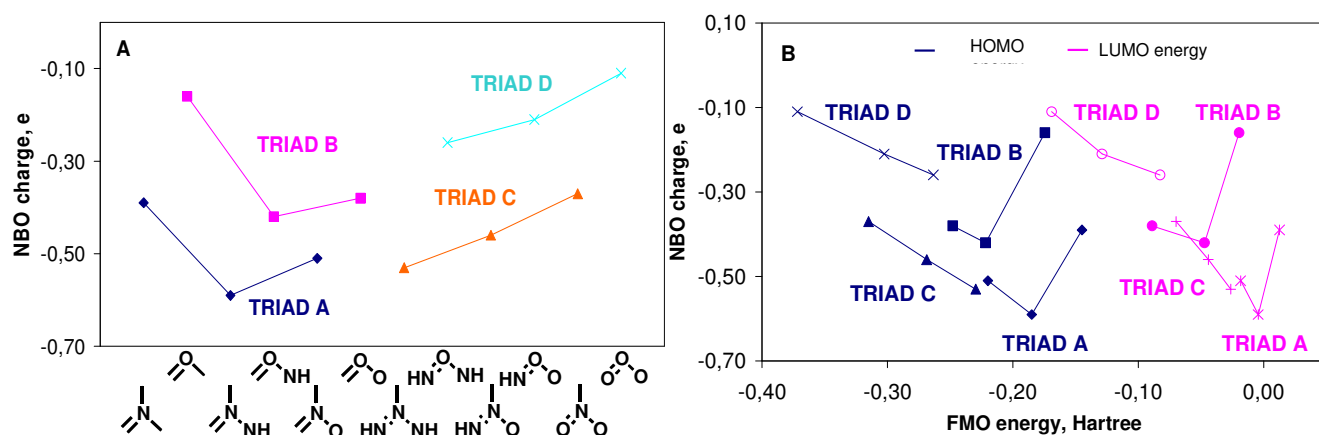


FIGURE 6S. Plots of NBO atomic charge on the Z atom of dipole $X=Y^+-Z^-$ vs. dipoles nature (A) and dipole FMO energy (B).

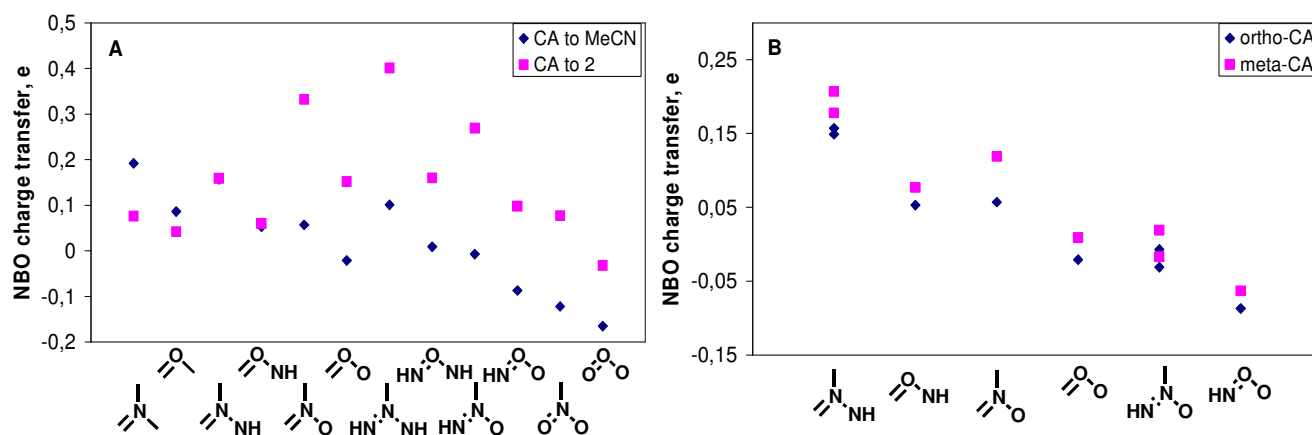


FIGURE 7S. Dipole-to-nitrile NBO charge transfer for CAs to MeCN and **2** along the most favorable regio- and stereoisomeric pathways (A) and for CAs to MeCN along all regio- and stereoisomeric pathways (B).

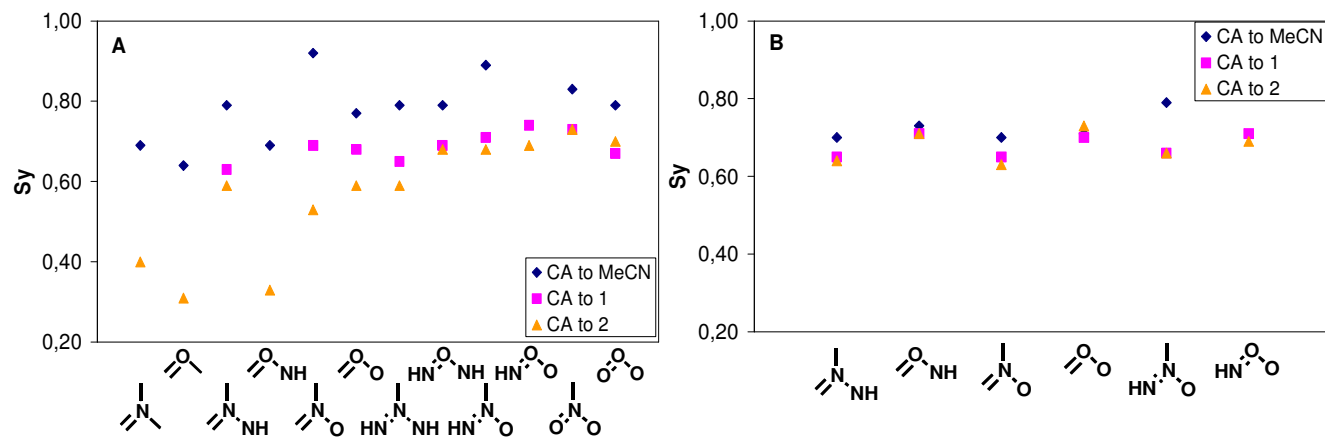


FIGURE 8S. Synchronicity (S_y) of the CAs to MeCN, **1**, and **2**. For reactions of **D3**, **D4**, **D5**, **D6**, **D9**, and **D10**, *ortho*-additions are considered in part (A) and *meta*-additions are considered in part (B). Only the most favorable stereoisomeric pathways are considered in both parts of the Figure.

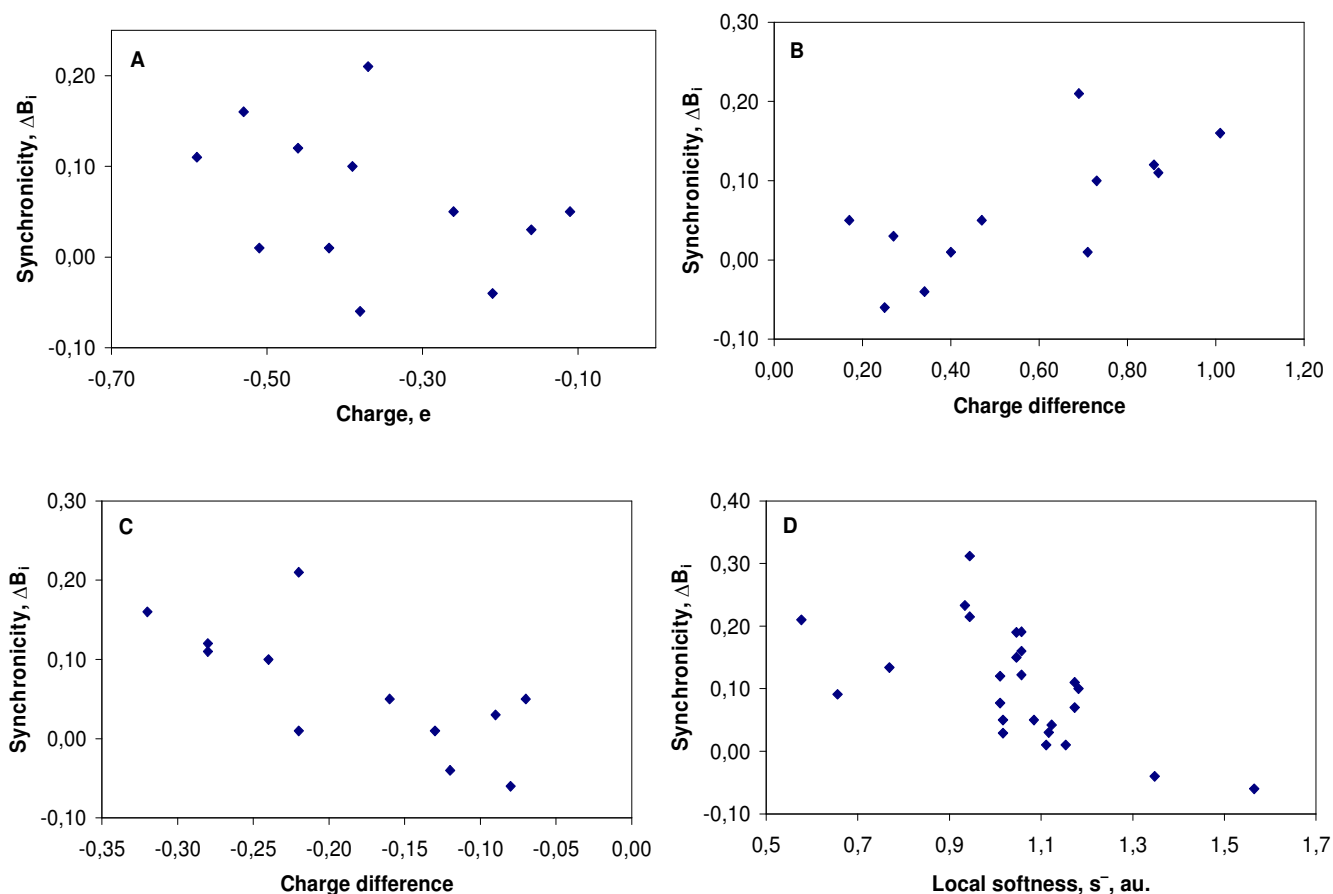


FIGURE 9S. Plots of synchronicity in terms of $\Delta B_i = B_{C(2)Z(3)} - B_{N(1)X(5)}$ in TS vs. NBO charge (A) and local softness s^- (D) on the atom Z(3) of dipole XYZ and charge differences $[qC(2) - qZ(3)] - [qX(5) - qN(1)]$ (B) and $[qC(2) \times qZ(3)] - [qX(5) \times qN(1)]$ (C) for CAs to MeCN.

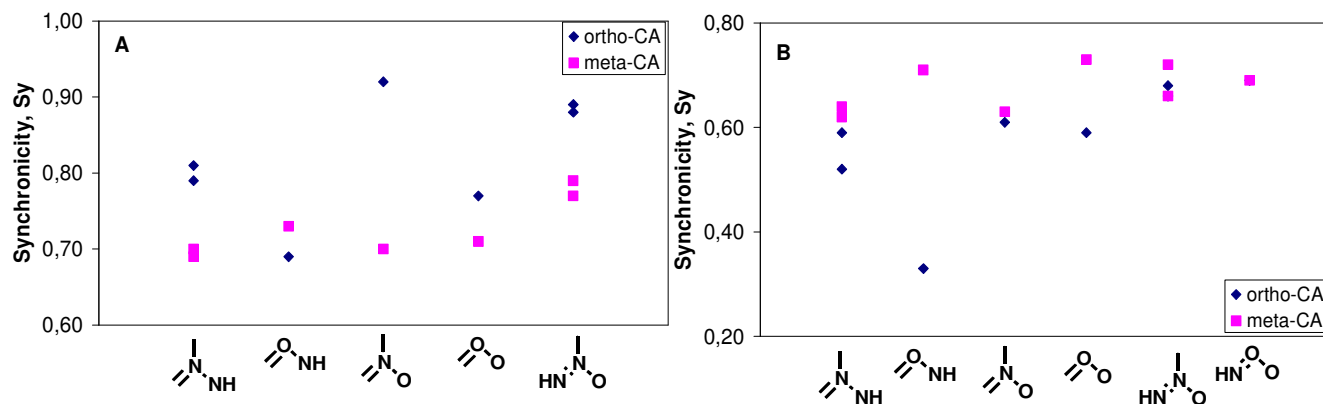


FIGURE 10S. Synchronicity S_y of the *ortho*- and *meta*-CAs to MeCN (A) and **2** (B).

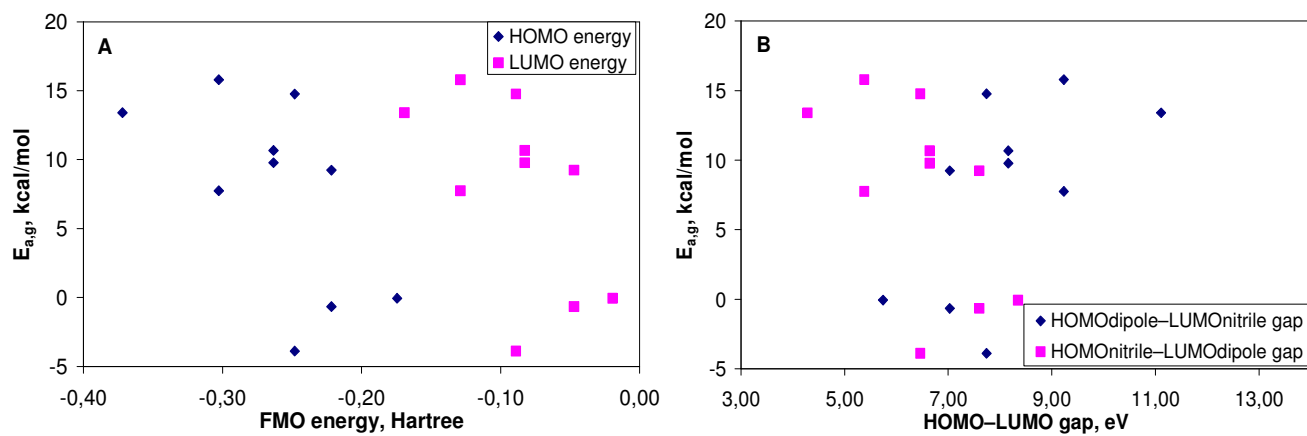


FIGURE 11S. Plots of activation energy $E_{a,g}$ vs. FMO energies (A) and HOMO-LUMO gaps (B) for dipoles with the central O atom and CAs to MeCN.

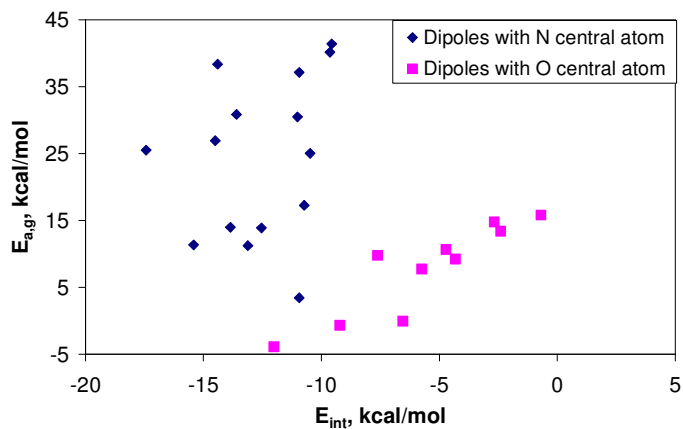


FIGURE 12S. Plot of activation energy $E_{a,g}$ vs. interaction energy E_{int} for CAs to MeCN.

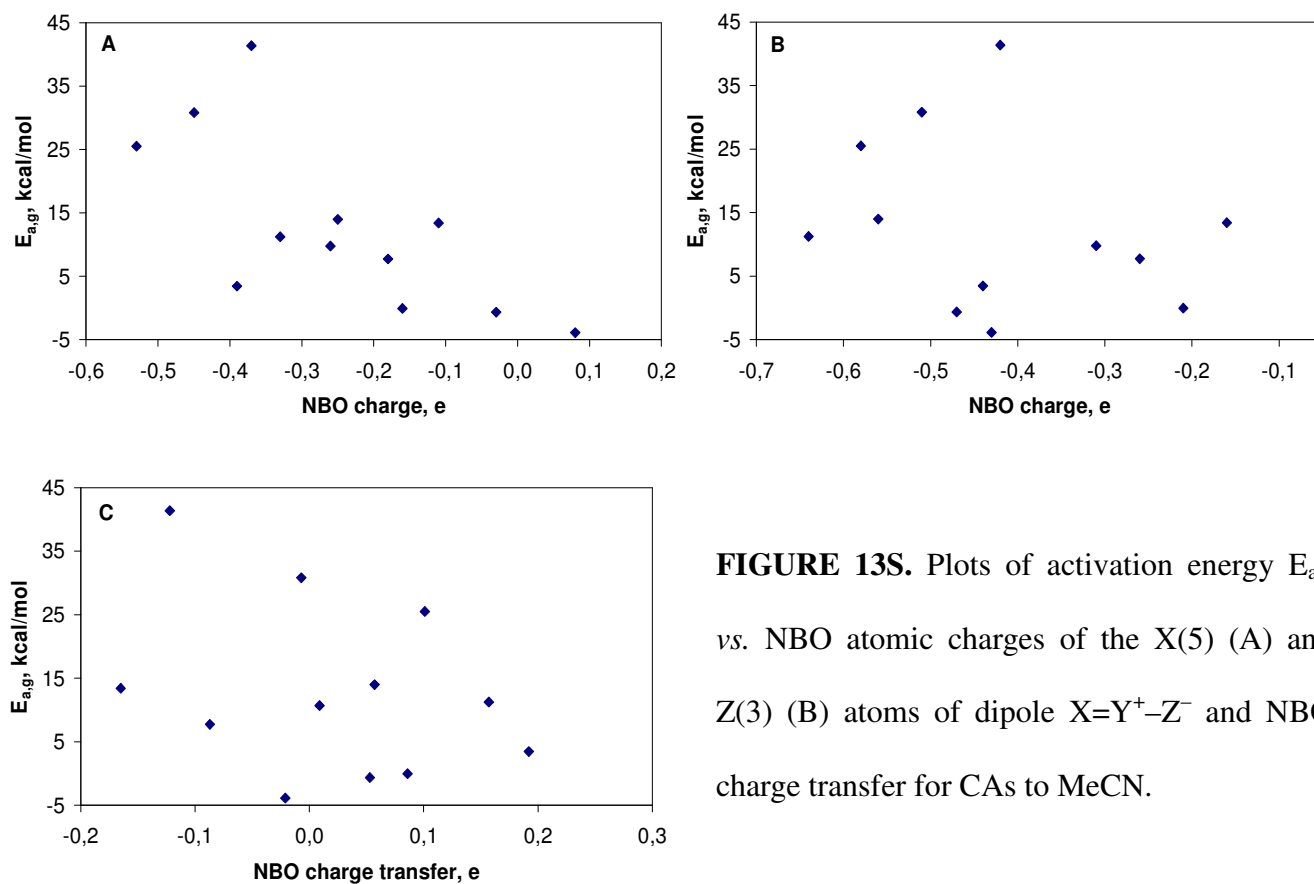


FIGURE 13S. Plots of activation energy $E_{a,g}$ vs. NBO atomic charges of the X(5) (A) and Z(3) (B) atoms of dipole $X=Y^+-Z^-$ and NBO charge transfer for CAs to MeCN.

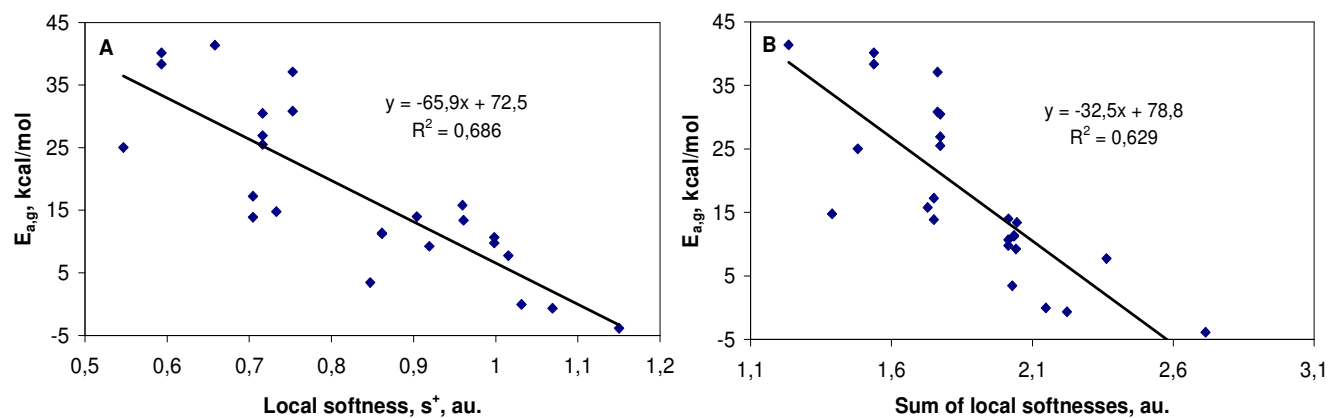


FIGURE 14S. Plots of activation energies $E_{a,g}$ vs. local softness s^+ of the X(5) atom of dipole XYZ (A) and sum of the softnesses $s^+(X(5)) + s^-(Z(3))$ (B).

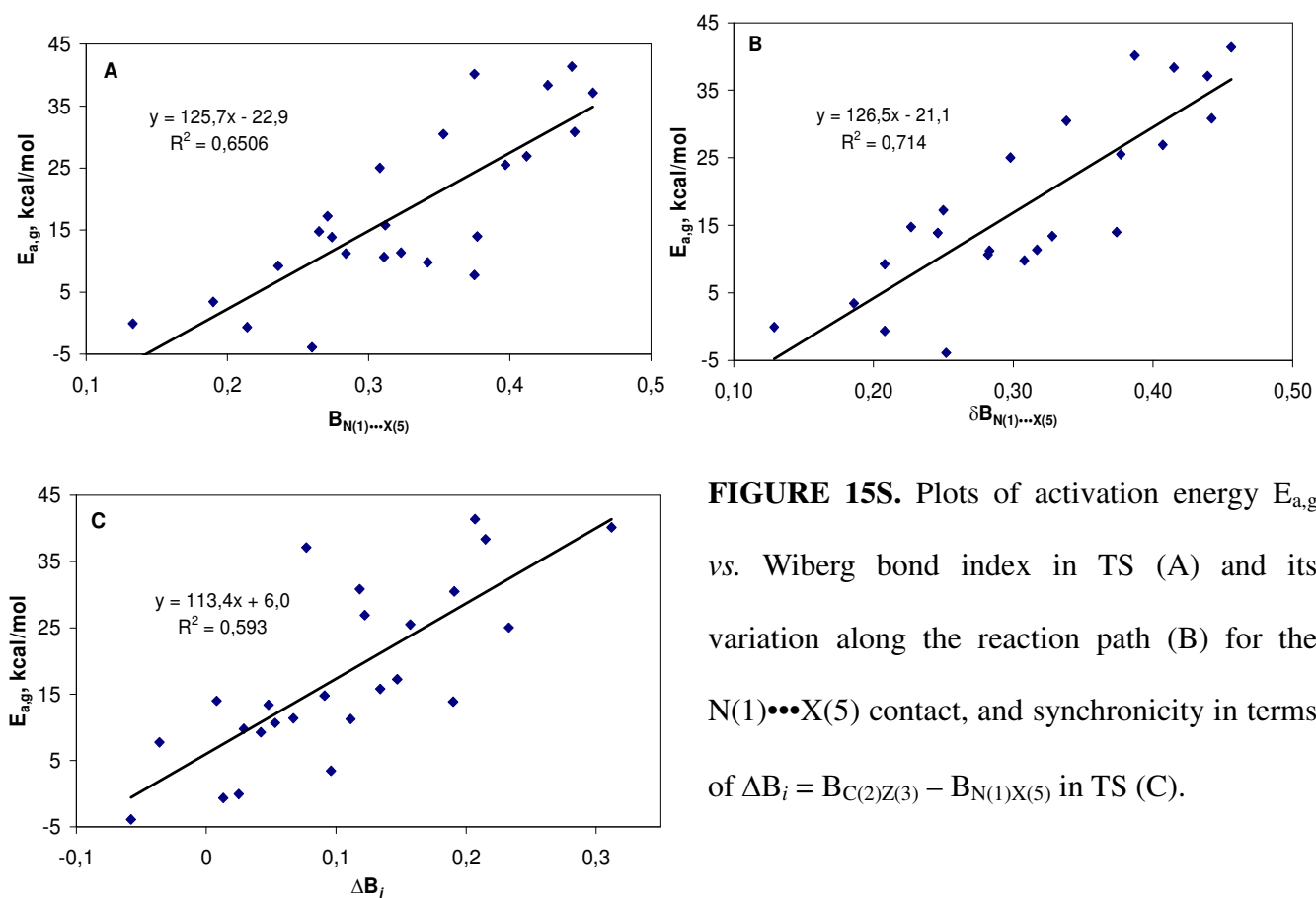


FIGURE 15S. Plots of activation energy $E_{a,g}$ vs. Wiberg bond index in TS (A) and its variation along the reaction path (B) for the $N(1)\cdots X(5)$ contact, and synchronicity in terms of $\Delta B_i = B_{C(2)Z(3)} - B_{N(1)X(5)}$ in TS (C).

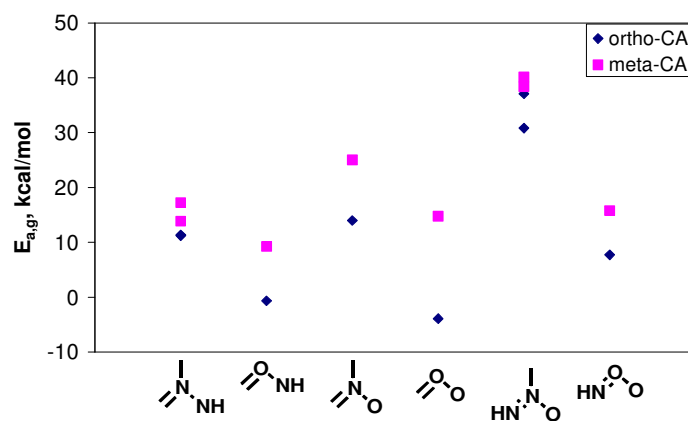


FIGURE 16S. Activation energies $E_{a,g}$ of the *ortho*- and *meta*-CAs to MeCN.

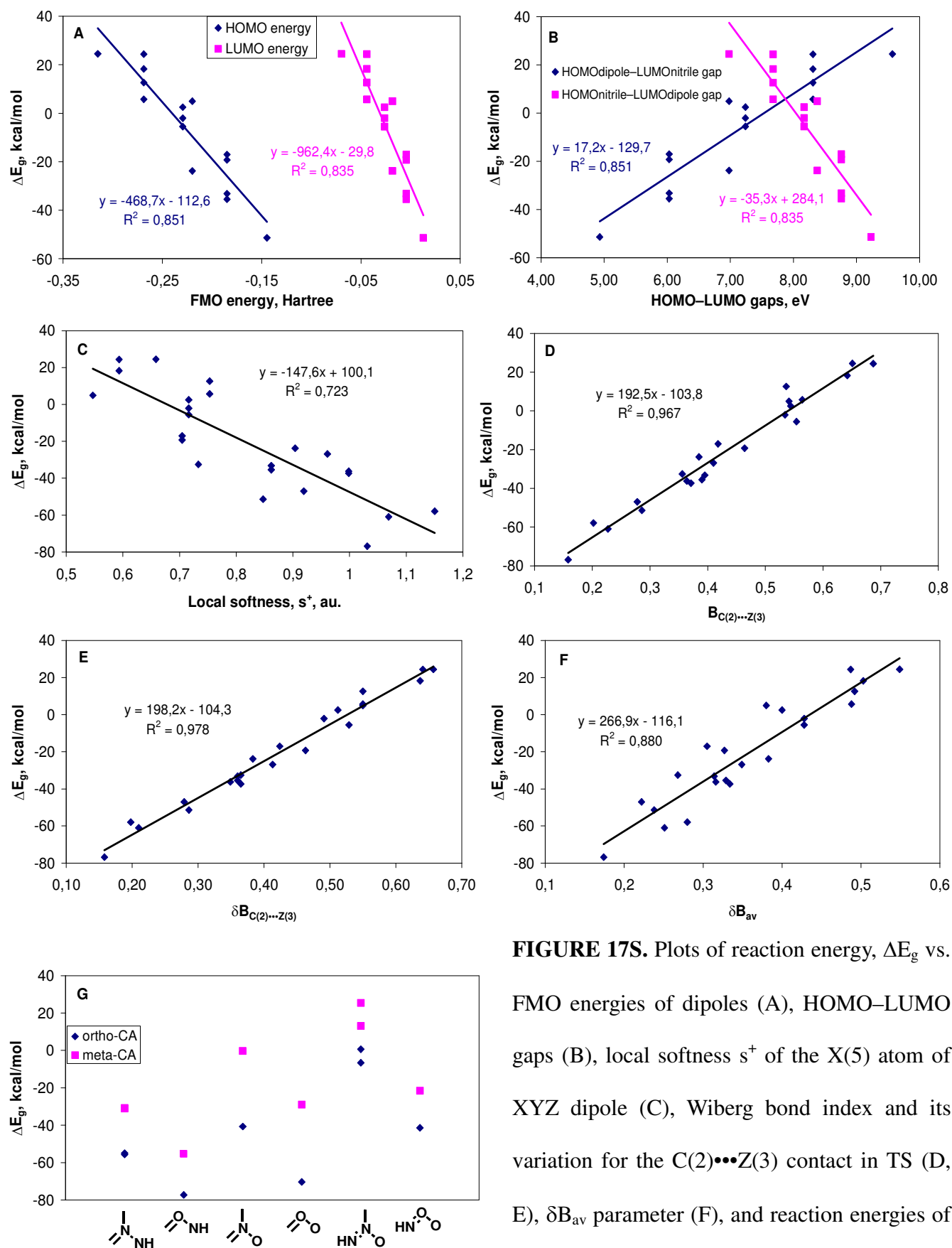


FIGURE 17S. Plots of reaction energy, ΔE_g vs. FMO energies of dipoles (A), HOMO–LUMO gaps (B), local softness s^+ of the X(5) atom of XYZ dipole (C), Wiberg bond index and its variation for the C(2)•••Z(3) contact in TS (D, E), δB_{av} parameter (F), and reaction energies of the *ortho*- and *meta*-CAs to MeCN (G).

TABLE 1S. Activation (E_a) and Reaction (ΔE) Energies (kcal/mol) of CAs of Dipoles **D1–D12** to MeCN Calculated at the CBS-Q and B3LYP Levels of Theory

Dipole	E_a		ΔE	
	CBS-Q	B3LYP	CBS-Q	B3LYP
D1	3.41	3.45	−45.89	−51.35
D2	0.77	−0.06	−71.10	−76.85
D3	9.14	11.24	−32.31	−33.18
D4	1.74	−0.65	−54.59	−60.96
D5	11.50	13.99	−19.59	−23.78
D6	−3.05	−3.88	−52.86	−57.89
D7	22.67	25.51	−3.56	−5.54
D8	10.28	10.67	−31.14	−36.22
D9	29.72	30.83	7.60	5.72
D10	9.43	7.75		
D11	39.08	41.37	27.90	24.47
D12	11.78	13.41	−16.63	−26.88

TABLE 2S. Some Characteristics of Concerted Transition States and Reaction Synchronicity^a

TS	CT	vi	ΔB_i	$\delta B_{C(2)\cdots Z(3)}$	$\delta B_{N(1)\cdots X(5)}$	δB_{av}	S_y
TS(1-L)	0.192	272i	0.10	0.286	0.186	0.24	0.69
TS(1-Pt ^{IV})	0.076	28i	0.03	0.047	0.019	0.07	0.40
TS(2-L)	0.086	190i	0.03	0.158	0.129	0.17	0.64
TS(2-Pt ^{IV})	0.042	9i	0.02	0.041	0.020	0.09	0.31
TS(3-L)Oex	0.149	416i	0.07	0.364	0.317	0.33	0.81
TS(3-L)Oen	0.157	373i	0.11	0.362	0.283	0.31	0.79
TS(3-L)Mex	0.207	361i	0.19	0.463	0.246	0.33	0.69
TS(3-L)Men	0.178	376i	0.15	0.424	0.250	0.31	0.70
TS(4-L)O	0.053	265i	0.01	0.210	0.208	0.25	0.69
TS(4-L)M	0.077	336i	0.04	0.279	0.208	0.22	0.73
TS(3-Pt ^{II})Oex	0.312	186i	0.27	0.339	0.135	0.25	0.63
TS(3-Pt ^{II})Men	0.269	212i	0.19	0.328	0.137	0.23	0.65
TS(4-Pt ^{II})M	0.149	229i	0.07	0.226	0.150	0.18	0.71
TS(3-Pt ^{IV})Oex	0.159	41i	0.11	0.118	0.040	0.11	0.59
TS(3-Pt ^{IV})Oen	0.096	41i	0.07	0.076	0.025	0.08	0.52
TS(3-Pt ^{IV})Mex	0.174	80i	0.09	0.151	0.060	0.12	0.62
TS(3-Pt ^{IV})Men	0.173	64i	0.07	0.129	0.059	0.11	0.64
TS(4-Pt ^{IV})O	0.060	35i	0.05	0.060	0.024	0.11	0.33
TS(4-Pt ^{IV})M	0.141	110i	0.04	0.131	0.093	0.11	0.71
TS(5-L)O	0.057	450i	0.01	0.383	0.374	0.38	0.92
TS(5-L)M	0.119	387i	0.23	0.550	0.298	0.38	0.70
TS(5-Pt ^{II})O	0.267	268i	0.35	0.506	0.216	0.36	0.69
TS(5-Pt ^{II})M	0.253	288i	0.33	0.533	0.207	0.35	0.65
TS(5-Pt ^{IV})O	0.332	143i	0.37	0.432	0.122	0.29	0.53
TS(5-Pt ^{IV})M	0.316	259i	0.27	0.419	0.148	0.28	0.63
TS(6-L)O	-0.021	277i	-0.06	0.198	0.252	0.28	0.77
TS(6-L)M	0.009	400i	0.09	0.365	0.227	0.27	0.71
TS(6-Pt ^{II})O	0.140	167i	0.19	0.276	0.121	0.24	0.68
TS(6-Pt ^{II})M	0.063	349i	0.15	0.348	0.194	0.25	0.70
TS(6-Pt ^{IV})O	0.152	102i	0.18	0.227	0.079	0.20	0.59
TS(6-Pt ^{IV})M	0.140	280i	0.09	0.281	0.191	0.21	0.73
TS(7-L)exex	0.101	485i	0.16	0.529	0.377	0.43	0.79
TS(7-L)exen	0.077	467i	0.12	0.491	0.407	0.43	0.87
TS(7-L)enen	0.102	425i	0.19	0.512	0.338	0.40	0.77
TS(8-L)ex	0.004	403i	0.03	0.365	0.308	0.33	0.90
TS(8-L)en	0.009	366i	0.05	0.349	0.282	0.32	0.79
TS(7-Pt ^{II})exex	0.317	271i	0.40	0.558	0.232	0.39	0.65
TS(7-Pt ^{II})exen	0.271	325i	0.33	0.502	0.266	0.36	0.69
TS(7-Pt ^{II})enen	0.294	248i	0.38	0.500	0.194	0.34	0.64
TS(8-Pt ^{II})ex	0.116	307i	0.14	0.346	0.225	0.26	0.80
TS(8-Pt ^{II})en	0.122	264i	0.16	0.314	0.186	0.24	0.69
TS(7-Pt ^{IV})exex	0.401	172i	0.43	0.462	0.115	0.32	0.59
TS(7-Pt ^{IV})exen	0.376	231i	0.41	0.477	0.182	0.33	0.64
TS(7-Pt ^{IV})enen	0.336	189i	0.36	0.401	0.118	0.27	0.61
TS(8-Pt ^{IV})ex	0.167	257i	0.13	0.309	0.201	0.23	0.76

TS	CT	vi	ΔB_i	$\delta B_{C(2)\cdots Z(3)}$	$\delta B_{N(1)\cdots X(5)}$	δB_{av}	S_y
TS(8-Pt^{IV})en	0.160	219i	0.15	0.276	0.159	0.21	0.68
TS(9-L)Oex	-0.007	527i	0.12	0.550	0.442	0.49	0.89
TS(9-L)Oen	-0.031	505i	0.08	0.550	0.439	0.49	0.88
TS(9-L)Mex	-0.017	463i	0.22	0.637	0.415	0.50	0.79
TS(9-L)Men	0.019	384i	0.31	0.641	0.387	0.49	0.77
TS(10-L)O	-0.087	384i	-0.04	0.184	0.238		
TS(10-L)M	-0.063	413i	0.13	0.324	0.176		
TS(9-Pt^{II})Oex	0.196	330i	0.38	0.619	0.316	0.44	0.71
TS(9-Pt^{II})Oen	0.152	349i	0.33	0.630	0.333	0.46	0.73
TS(9-Pt^{II})Mex	0.148	276i	0.43	0.677	0.308	0.47	0.66
TS(9-Pt^{II})Men	0.210	82i	0.54	0.709	0.291	0.47	0.65
TS(10-Pt^{II})O	0.044	321i	0.15	0.371	0.236	0.31	0.74
TS(10-Pt^{II})M	0.006	349i	0.27	0.430	0.211	0.31	0.71
TS(9-Pt^{IV})Oex	0.269	275i	0.45	0.666	0.321	0.46	0.68
TS(9-Pt^{IV})Oen	0.245	266i	0.40	0.688	0.297	0.46	0.66
TS(9-Pt^{IV})Mex	0.256	230i	0.47	0.687	0.307	0.48	0.66
TS(9-Pt^{IV})Men	0.212	155i	0.53	0.803	0.453	0.58	0.72
TS(10-Pt^{IV})O	0.098	288i	0.16	0.350	0.213	0.28	0.69
TS(10-Pt^{IV})M	0.088	315i	0.23	0.381	0.210	0.27	0.69
TS(11-L)	-0.122	496i	0.21	0.657	0.456	0.55	0.83
TS(11-Pt^{II})	0.013	234i	0.44	0.741	0.368	0.54	0.73
TS(11-Pt^{IV})	0.077	235i	0.44	0.773	0.425	0.57	0.73
TS(12-L)	-0.165	442i	0.05	0.413	0.328	0.35	0.79
TS(12-Pt^{II})	-0.127	364i	0.26	0.447	0.217	0.32	0.67
TS(12-Pt^{IV})	-0.032	377i	0.22	0.428	0.250	0.31	0.70

^a Dipole-to-nitrile charge transfer (CT, e), imaginary frequency (vi), difference of the Wiberg bond indices for the C(2)•••Z(3) and N(1)•••X(5) contacts ($\Delta B_i = B_{C(2)\cdots Z(3)} - B_{N(1)\cdots X(5)}$), relative variations of the Wiberg bond indices ($\delta B_{C(2)\cdots Z(3)}$ and $\delta B_{N(1)\cdots X(5)}$), average value of the relative variations of the Wiberg bond indices (δB_{av}), and synchronicity (S_y).

TABLE 3S. Activation and Reaction Total Energies, Enthalpies and Gibbs Free Energies (kcal/mol) for the Gas Phase and CH₂Cl₂ Solution (in Parentheses)

Reaction	E _a	ΔH [‡]	ΔG [‡]	ΔE	ΔH	ΔG
(D1 + L)	3.5 (8.5)	4.7 (9.8)	17.8 (19.0)	-51.4 (-43.1)	-47.7 (-39.4)	-32.9 (-28.8)
(D1 + 1)	-6.5 (3.0)	-6.2 (3.4)	9.0 (14.2)	-64.0 (-53.2)	-60.3 (-49.5)	-41.8 (-36.1)
(D1 + 2)	-5.7 (4.0)	-5.4 (4.3)	8.9 (14.4)	-68.7 (-57.6)	-64.9 (-53.8)	-45.4 (-39.6)
(D2 + L)	-0.1 (4.0)	1.5 (5.6)	13.9 (14.2)	-76.9 (-71.8)	-71.8 (-66.8)	-57.7 (-56.8)
(D2 + 1)	—	—	—	-87.5 (-80.2)	-82.1 (-74.8)	-66.4 (-63.6)
(D2 + 2)	-4.2 (3.6)	-2.8 (5.0)	8.8 (13.1)	-91.0 (-83.7)	-86.1 (-78.9)	-67.1 (-65.0)
(D3 + L)Oex	11.4 (17.5)	12.4 (18.6)	25.6 (27.9)	-35.5 (-28.3)	-32.4 (-25.3)	-18.3 (-15.3)
(D3 + L)Oen	11.2 (15.8)	12.2 (16.8)	25.5 (26.1)	-33.2 (-27.1)	-30.1 (-24.0)	-15.5 (-13.6)
(D3 + L)Mex	13.9 (16.8)	14.8 (17.8)	27.9 (26.9)	-19.3 (-11.4)	-16.5 (-8.6)	-2.4 (+1.4)
(D3 + L)Men	17.3 (20.7)	18.1 (21.5)	31.2 (30.8)	-17.0 (-10.0)	-14.3 (-7.2)	+0.5 (+3.3)
(D3 + 1)Oex	-0.8 (7.9)	0.2 (8.9)	13.8 (18.5)	-49.5 (-39.4)	-46.7 (-36.6)	-28.6 (-23.5)
(D3 + 1)Oen	-4.2 (4.7)	-2.8 (6.0)	13.3 (17.6)	-48.3 (-39.0)	-45.3 (-36.1)	-26.8 (-22.6)
(D3 + 1)Mex	0.6 (11.1)	1.4 (11.9)	16.1 (22.4)	-29.5 (-18.3)	-27.1 (-15.9)	-8.7 (-2.5)
(D3 + 1)Men	3.4 (12.3)	4.4 (13.2)	18.6 (23.3)	-27.9 (-16.3)	-24.9 (-13.2)	-7.9 (-1.0)
(D3 + 2)Oex	-7.3 (3.0)	-7.0 (3.2)	7.9 (13.9)	-55.6 (-45.6)	-52.6 (-42.7)	-33.9 (-29.0)
(D3 + 2)Oen	-6.3 (2.1)	-6.1 (2.3)	9.0 (13.1)	-54.9 (-45.4)	-51.9 (-42.4)	-33.0 (-28.6)
(D3 + 2)Mex	1.3 (9.5)	1.5 (10.3)	16.4 (19.0)	-31.1 (-19.9)	-28.7 (-17.5)	-10.1 (-4.0)
(D3 + 2)Men	0.9 (9.5)	1.6 (10.2)	14.6 (19.4)	-30.8 (-18.9)	-28.4 (-16.4)	-9.4 (-2.6)
(D4 + L)O	-0.7 (3.6)	0.7 (5.0)	12.9 (13.4)	-61.0 (-56.6)	-56.8 (-52.5)	-43.5 (-43.1)
(D4 + L)M	9.2 (12.5)	10.5 (13.8)	22.6 (22.1)	-47.0 (-41.8)	-43.3 (-38.0)	-29.8 (-28.6)
(D4 + 1)O	-6.8 (0.7)	-5.6 (2.0)	8.2 (11.7)	-72.0 (-64.5)	-68.1 (-60.6)	-50.6 (-48.0)
(D4 + 1)M	3.3 (10.6)	4.6 (11.9)	18.1 (21.4)	-54.1 (-44.7)	-50.0 (-40.6)	-34.3 (-29.4)
(D4 + 2)O	-7.9 (-0.7)	-6.7 (0.4)	5.4 (8.7)	-77.2 (-69.8)	-72.6 (-65.2)	-56.8 (-53.9)
(D4 + 2)M	2.5 (9.3)	3.7 (10.4)	16.6 (19.4)	-55.3 (-46.0)	-51.8 (-42.4)	-33.8 (-29.5)
(D5 + L)O	14.0 (21.7)	14.9 (22.6)	27.6 (31.5)	-23.8 (-14.0)	-21.1 (-11.3)	-7.6 (-1.8)
(D5 + L)M	25.0 (29.0)	25.7 (29.6)	38.3 (38.4)	+4.9 (+14.6)	+6.9 (16.5)	+20.5 (+26.1)
(D5 + 1)O	3.0 (12.9)	3.3 (13.1)	19.7 (25.0)	-35.2 (-21.4)	-32.8 (-19.0)	-15.2 (-6.2)
(D5 + 1)M	14.9 (22.6)	15.6 (23.3)	29.4 (33.1)	+0.4 (+12.4)	+2.5 (14.4)	+17.6 (+25.2)
(D5 + 2)O	-5.4 (5.6)	-3.9 (7.1)	8.0 (15.4)	-40.7 (-26.2)	-37.1 (-22.6)	-22.2 (-12.0)
(D5 + 2)M	12.1 (20.4)	12.8 (21.1)	25.8 (30.3)	-0.3 (+11.5)	+1.2 (13.0)	+18.9 (+25.8)
(D6 + L)O	-3.9 (2.0)	-2.8 (3.1)	9.4 (11.6)	-57.9 (-47.9)	-54.5 (-44.6)	-41.9 (-35.8)
(D6 + L)M	14.8 (18.9)	15.6 (19.8)	27.8 (28.2)	-32.6 (-22.5)	-30.0 (-20.0)	-17.1 (-11.0)
(D6 + 1)O	-7.5 (2.6)	-6.7 (3.5)	7.7 (13.7)	-65.6 (-52.2)	-62.6 (-49.2)	-45.1 (-36.6)
(D6 + 1)M	12.9 (20.7)	13.7 (21.5)	27.3 (31.1)	-29.7 (-18.2)	-27.6 (-16.0)	-11.0 (-4.1)
(D6 + 2)O	-11.3 (-0.6)	-10.4 (0.3)	3.0 (9.7)	-70.3 (-56.2)	-67.2 (-53.1)	-49.2 (-40.0)
(D6 + 2)M	13.8 (20.5)	14.0 (20.7)	28.6 (31.1)	-29.0 (-18.2)	-26.8 (-15.9)	-9.7 (-3.6)
(D7 + L)exex	25.5 (31.1)	26.2 (31.8)	39.6 (41.2)	-5.5 (+1.5)	-3.5 (+3.5)	+10.8 (+13.7)
(D7 + L)exen	26.9 (33.3)	27.4 (33.8)	40.8 (43.3)	-2.1 (+3.8)	0.0 (+5.9)	+14.3 (+16.1)
(D7 + L)enen	30.5 (32.8)	30.8 (33.2)	44.25(42.6)	+2.5 (+7.2)	+4.5 (+9.2)	+19.0 (+19.5)
(D7 + 1)exex	13.6 (22.3)	13.5 (22.3)	30.2 (34.3)	-16.4 (-4.6)	-14.7 (-2.9)	+3.4 (+10.3)
(D7 + 1)exen	13.1 (23.6)	13.7 (24.1)	28.7 (34.9)	-13.9 (-4.0)	-12.2 (-2.3)	+5.6 (+10.6)
(D7 + 1)enen	14.3 (21.2)	14.8 (21.8)	29.3 (32.1)	-9.2 (+1.1)	-7.5 (+2.7)	+11.2 (+16.3)
(D7 + 2)exex	6.5 (14.4)	6.5 (14.3)	21.6 (25.2)	-19.2 (-9.0)	-17.5 (-7.3)	+1.1 (+6.2)
(D7 + 2)exen	7.0 (17.0)	7.6 (17.6)	21.7 (27.5)	-17.4 (-7.4)	-15.1 (-5.1)	+0.9 (+6.4)
(D7 + 2)enen	8.6 (16.3)	9.2 (16.9)	22.5 (26.3)	-13.2 (-3.0)	-11.6 (-1.3)	+7.0 (+12.3)

Reaction	E _a	$\Delta H^\ddagger$	$\Delta G^\ddagger$	ΔE	ΔH	ΔG
(D8 + L)ex	9.8 (17.6)	10.8 (18.6)	23.2 (27.3)	-37.4 (-30.7)	-34.4 (-27.7)	-21.0 (-18.3)
(D8 + L)en	10.7 (16.1)	11.7 (17.1)	24.1 (25.7)	-36.2 (-31.0)	-33.7 (-28.5)	-20.4 (-19.1)
(D8 + 1)ex	4.2 (15.7)	5.1 (16.7)	18.7 (26.2)	-43.4 (-32.2)	-40.3 (-29.1)	-25.2 (-18.3)
(D8 + 1)en	3.6 (12.9)	4.6 (13.9)	18.5 (23.8)	-42.2 (-33.4)	-39.4 (-30.6)	-24.4 (-19.9)
(D8 + 2)ex	2.4 (14.2)	3.4 (15.1)	15.6 (23.6)	-44.9 (-33.7)	-42.4 (-31.2)	-24.7 (-18.3)
(D8 + 2)en	1.8 (11.2)	2.8 (12.3)	16.4 (21.8)	-43.1 (-35.4)	-40.9 (-33.2)	-23.1 (-20.3)
(D9 + L)Oex	30.8 (38.0)	31.3 (38.5)	44.5 (47.8)	+5.7 (+14.2)	+7.4 (+15.9)	+21.2 (+25.7)
(D9 + L)Oen	37.1 (42.7)	37.2 (42.7)	50.3 (52.0)	+12.6 (+19.9)	+14.1 (+21.4)	+27.9 (+31.2)
(D9 + L)Mex	38.4 (44.9)	38.6 (45.1)	51.7 (54.3)	+18.3 (+26.6)	+19.5 (+27.9)	+33.3 (+37.6)
(D9 + L)Men	40.2 (43.4)	40.2 (43.4)	53.3 (52.6)	+24.4 (+30.5)	+25.4 (+31.5)	+39.2 (+41.3)
(D9 + 1)Oex	21.3 (31.6)	21.5 (31.9)	35.7 (41.9)	-3.7 (+9.7)	-2.4 (+10.9)	+15.1 (+23.6)
(D9 + 1)Oen	24.4 (35.3)	23.9 (34.8)	41.2 (47.3)	+3.7 (+17.2)	+4.8 (+18.3)	+23.0 (+31.6)
(D9 + 1)Mex	29.7 (39.1)	29.9 (39.2)	45.1 (50.1)	+14.5 (+25.5)	+15.2 (+26.2)	+32.7 (+38.9)
(D9 + 1)Men	28.2 (34.7)	28.4 (34.9)	43.3 (45.5)	+19.1 (+28.0)	+19.7 (+28.6)	+36.7 (+40.9)
(D9 + 2)Oex	14.9 (25.0)	15.3 (25.4)	30.7 (36.4)	-6.6 (+6.6)	-5.3 (+7.8)	+12.6 (+20.8)
(D9 + 2)Oen	19.1 (30.0)	19.1 (30.0)	33.2 (40.0)	+0.6 (+15.2)	+1.7 (+16.2)	+19.8 (+29.4)
(D9 + 2)Mex	26.5 (35.2)	26.7 (35.4)	41.9 (46.2)	+13.1 (+23.9)	+13.8 (+24.6)	+31.7 (+37.6)
(D9 + 2)Men	24.5 (31.9)	24.9 (32.3)	41.0 (43.8)	+16.6 (+25.4)	+17.9 (+26.6)	+33.6 (+37.8)
(D10 + L)O	7.8 (14.1)	8.6 (15.0)	21.1 (23.7)	-89.5 ^a (-87.6) ^a	-86.2 ^a (-84.2) ^a	-74.3 ^a (-76.0) ^a
(D10 + L)M	15.8 (20.2)	16.6 (21.1)	29.0 (29.7)	-43.1 ^a (-41.2) ^a	-40.8 ^a (-38.9) ^a	-29.5 ^a (-31.1) ^a
(D10 + 1)O	2.6 (13.6)	2.7 (13.7)	19.2 (25.6)	-40.0 (-26.1)	-37.1 (-23.2)	-22.1 (-12.5)
				-95.9 ^a (-86.5) ^a	-93.5 ^a (-84.1) ^a	-76.9 ^a (-72.2) ^a
(D10 + 1)M	13.5 (20.2)	14.4 (21.0)	27.5 (30.3)	-21.1 (-12.0)	-18.6 (-9.5)	-5.4 (-0.2)
(D10 + 2)O	1.6 (12.7)	1.7 (12.8)	17.1 (23.8)	-41.3 (-25.9)	-39.0 (-23.6)	-21.5 (-10.9)
				-96.9 ^a (-86.2) ^a	-94.7 ^a (-84.0) ^a	-79.0 ^a (-72.8) ^a
(D10 + 2)M	14.3 (20.5)	15.1 (21.3)	28.1 (30.5)	-21.6 (-11.1)	-19.0 (-8.5)	-4.5 (+1.8)
(D11 + L)	41.4 (50.3)	41.4 (50.3)	56.0 (60.7)	+24.5 (+35.9)	+25.5 (+37.0)	+40.6 (+47.7)
(D11 + 1)	33.3 (46.2)	33.2 (46.1)	48.9 (57.3)	+21.8 (+37.0)	+22.3 (+37.5)	+41.2 (+51.3)
(D11 + 2)	30.9 (44.5)	31.0 (44.5)	48.2 (56.9)	+20.2 (+35.6)	+20.8 (+36.2)	+39.9 (+50.1)
(D12 + L)	13.4 (18.6)	14.1 (19.3)	26.5 (28.0)	-26.9 (-19.0)	-24.8 (-16.9)	-12.8 (-8.6)
(D12 + 1)	13.2 (20.1)	13.7 (20.5)	27.6 (30.4)	-23.2 (-13.0)	-21.7 (-11.4)	-4.9 (+0.7)
(D12 + 2)	14.9 (22.5)	14.8 (22.3)	30.0 (33.2)	-23.6 (-13.1)	-22.0 (-11.5)	-4.9 (+0.9)

^a Energies corresponding to the formation of acyclic products.

TABLE 4S. Energies of FMOs of Dipoles and Nitriles (Hartree)

	E _{HOMO}	E _{LUMO}
D1	−0.14474	+0.01277
D2^a	−0.17433	−0.01948
D3	−0.18492	−0.00437
D4^a	−0.22169	−0.04712
D5	−0.21991	−0.01831
D6	−0.24799 ^b	−0.08890
D7	−0.22955	−0.02612
D8^a	−0.26338	−0.08251
D9	−0.26870	−0.04409
D10^a	−0.30261 ^b	−0.12881
D11	−0.31507 ^c	−0.06972
D12^a	−0.37180 ^c	−0.16909
CH ₃ CN	−0.32642	+0.03660
1^d	−0.31019	−0.03480
2^e	−0.35740	−0.04114

^a Instability of wavefunctions was found for the restricted methods. Hence, unrestricted approximation was used with following reoptimization of the wavefunctions to achieve a stable solution. Values are given for β -spin orbitals. ^b For 2nd-HOMO. ^c For 3rd-HOMO. ^d For the highest occupied π (CN) orbital (8-HOMO) and lowest unoccupied π^* (CN) orbital (2-LUMO). ^e For the highest occupied π (CN) orbital (11-HOMO) and lowest unoccupied π^* (CN) orbital (3-LUMO).

TABLE 5S. HOMO–LUMO Gaps and $\Delta\Delta E = |E(\text{HOMO}_{\text{dipole}}) - E(\text{LUMO}_{\text{nitrile}})| - |E(\text{HOMO}_{\text{nitrile}}) - E(\text{LUMO}_{\text{dipole}})|$ Difference (eV)

Dipole	HOMO _{dipole} –LUMO _{nitrile}	HOMO _{nitrile} –LUMO _{dipole}	$\Delta\Delta E$
MeCN			
D1	4.93	9.23	–4.30
D2	5.74	8.35	–2.61
D3	6.03	8.76	–2.73
D4	7.03	7.60	–0.57
D5	6.98	8.38	–1.40
D6	7.74	6.46	1.28
D7	7.24	8.17	–0.93
D8	8.16	6.64	1.52
D9	8.31	7.68	0.63
D10	9.23	5.38	3.85
D11	9.57	6.98	2.59
D12	11.11	4.28	6.83
1			
D1	2.99	8.79	–5.80
D2	3.80	7.91	–4.11
D3	4.08	8.32	–4.24
D4	5.09	7.16	–2.07
D5	5.04	7.94	–2.9
D6	5.80	6.02	–0.22
D7	5.30	7.73	–2.43
D8	6.22	6.20	0.02
D9	6.36	7.24	–0.88
D10	7.29	4.94	2.35
D11	7.63	6.54	1.09
D12	9.17	3.84	5.33
2			
D1	2.82	10.07	–7.25
D2	3.62	9.19	–5.57
D3	3.91	9.61	–5.70
D4	4.91	8.44	–3.53
D5	4.86	9.23	–4.37
D6	5.63	7.31	–1.68
D7	5.13	9.01	–3.88
D8	6.05	7.48	–1.43
D9	6.19	8.53	–2.34
D10	7.11	6.22	0.89
D11	7.45	7.83	–0.38
D12	9.00	5.12	3.88

TABLE 6S. NBO Atomic Charges

	$q_{X(5)}$	$q_{Z(3)}$
D1	−0.39	−0.39
D2	−0.16	−0.16
D3	−0.33	−0.59
D4	−0.03	−0.42
D5	−0.25	−0.51
D6	0.08	−0.38
D7	−0.53	−0.53
D8	−0.26	−0.26
D9	−0.45	−0.46
D10	−0.18	−0.21
D11	−0.37	−0.37
D12	−0.11	−0.11
	$q_{N(1)}$	$q_{C(2)}$
MeCN	−0.33	0.28
1	−0.35	0.47
2	−0.33	0.53

TABLE 7S. Dipole-to-Nitrile NBO Charge Transfer

	MeCN	1	2
D1	0.19	–	0.08
D2	0.09	–	0.04
D3, <i>ortho,exo</i>	0.15	0.31	0.16
D3, <i>ortho, endo</i>	0.16	–	0.10
D3, <i>meta, exo</i>	0.21	–	0.17
D3, <i>meta,endo</i>	0.18	0.27	0.17
D4, <i>ortho</i>	0.05	–	0.06
D4, <i>meta</i>	0.08	0.15	0.14
D5, <i>ortho</i>	0.06	0.27	0.33
D5, <i>meta</i>	0.12	0.25	0.32
D6, <i>ortho</i>	–0.02	0.14	0.15
D6, <i>meta</i>	0.01	0.06	0.14
D7, <i>exo,exo</i>	0.10	0.32	0.40
D7, <i>exo,endo</i>	0.08	0.27	0.38
D7, <i>endo,endo</i>	0.10	0.29	0.34
D8, <i>exo</i>	0.00	0.12	0.17
D8, <i>endo</i>	0.01	0.12	0.16
D9, <i>ortho,exo</i>	–0.01	0.20	0.27
D9, <i>ortho,endo</i>	–0.03	0.15	0.25
D9, <i>meta,exo</i>	–0.02	0.15	0.26
D9, <i>meta,endo</i>	0.02	0.21	0.21
D10, <i>ortho</i>	–0.09	0.04	0.10
D10, <i>meta</i>	–0.06	0.01	0.09
D11	–0.12	0.01	0.08
D12	–0.17	–0.13	–0.03

TABLE 8S. Total Energies of the Neutral Molecules of Dipoles, Corresponding Cations and Anions (Hartree) and NBO Atomic Charges in the Cations and Anions of Dipoles

	E_{neutral}	E_{cation}	E_{anion}	cation		anion	
				$q_{\text{X}(5)}$	$q_{\text{Z}(3)}$	$q_{\text{X}(5)}$	$q_{\text{Z}(3)}$
D1	−173.195281	−172.960506	−173.094886	0.01	0.01	−0.67	−0,67
D2	−153.713242	−153.445924	−153.641175	0.22	0.22	−0.51	−0,51
D3	−189.238036	−188.957735	−189.149312	0.06	−0.16	−0.65	−0,85
D4	−169.731465	−169.423983	−169.685378	0.37	−0.01	−0.41	−0,75
D5	−209.111685	−208.790354	−209.032555	0.12	−0.07	−0.61	−0,73
D6	−189.576819	−189.223627	−189.553559	0.33	0.21	−0.35	−0,66
D7	−205.277505	−204.946185	−205.203900	−0.10	−0.10	−0.82	−0,82
D8	−185.737271	−185.371479	−185.719444	0.13	0.13	−0.64	−0,64
D9	−225.150543	−224.773585	−225.089226	−0.04	−0.02	−0.78	−0,72
D10	−205.575525	−205.170079	−205.587018	0.12	0.32	−0.58	−0,59
D11	−245.009331	−244.596514	−244.966359	0.17	−0.11	−0.67	−0,67
D12	−225.408689	−224.917782	−225.454172	0.37	0.37	−0.54	−0,54

TABLE 9S. Local Softnesses (au) of the X(5) and Z(3) Atoms of Dipoles

	$s^+_{\text{X}(5)}$	$s^-_{\text{Z}(3)}$	$s^-_{\text{X}(5)}$	$s^+_{\text{Z}(3)}$
D1	0.847	1.181	1.181	0.847
D2	1.031	1.117	1.117	1.031
D3	0.862	1.173	1.046	0.705
D4	1.069	1.154	1.123	0.919
D5	0.904	1.111	0.934	0.547
D6	1.150	1.565	0.656	0.733
D7	0.716	1.057	1.057	0.716
D8	0.998	1.017	1.017	0.998
D9	0.753	1.011	0.945	0.593
D10	1.015	1.348	0.769	0.960
D11	0.658	0.577	1.191	0.658
D12	0.961	1.084	1.084	0.961

TABLE 10S. Distortion and Interaction Energies (kcal/mol) for the Reactions with MeCN

	$E_{\text{dist}}^{\text{D}}$	$E_{\text{dist}}^{\text{N}}$	E_{dist}	E_{int}
D1	5.65	8.74	14.39	−10.94
D2	3.24	3.24	6.48	−6.54
D3, <i>ortho,exo</i>	15.74	11.04	26.78	−15.42
D3, <i>ortho,endo</i>	13.32	11.04	24.36	−13.12
D3, <i>meta,exo</i>	11.83	14.57	26.41	−12.54
D3, <i>meta,endo</i>	14.79	13.19	27.98	−10.73
D4, <i>ortho</i>	4.25	4.31	8.57	−9.22
D4, <i>meta</i>	6.27	7.29	13.56	−4.32
D5, <i>ortho</i>	18.31	9.53	27.85	−13.86
D5, <i>meta</i>	18.49	17.02	35.51	−10.48
D6, <i>ortho</i>	5.27	2.86	8.13	−12.01
D6, <i>meta</i>	8.05	9.39	17.44	−2.67
D7, <i>exo,exo</i>	26.31	16.63	42.94	−17.43
D7, <i>exo,endo</i>	25.54	15.87	41.41	−14.5
D7, <i>endo,endo</i>	25.65	15.83	41.48	−11.01
D8, <i>exo</i>	8.55	8.85	17.4	−7.62
D8, <i>endo</i>	6.77	8.62	15.39	−4.72
D9, <i>ortho,exo</i>	28.42	16.01	44.43	−13.6
D9, <i>ortho,endo</i>	33.18	14.87	48.05	−10.94
D9, <i>meta,exo</i>	33.12	19.62	52.75	−14.4
D9, <i>meta,endo</i>	29.16	20.64	49.79	−9.64
D10, <i>ortho</i>	6.55	6.94	13.49	−5.74
D10, <i>meta</i>	5.41	11.07	16.48	−0.69
D11	31.51	19.43	50.93	−9.56
D12	6.51	9.3	15.81	−2.4

TABLE 11S. Total Energies, Enthalpies, and Gibbs Free Energies in Gas Phase and in CH₂Cl₂ Solution (kcal/mol) and Entropies in Solution (kcal/mol•K) at the B3LYP and CBS-Q (in parentheses) Levels of Theory

	E _g	E _s	H _g	H _s	S _s	G _g	G _s
D1	−173.195281 (−172.856601)	−173.261184	−173.093174 (−172.850238)	−173.159077	53.40	−173.127649 (−172.883925)	−173.184449
D2	−153.713242 (−153.469075)	−153.770618	−153.655076 (−153.464098)	−153.712452	46.77	−153.685545 (−153.493496)	−153.734674
D3 anti	−189.238036 (−188.905301)	−189.312437	−189.146430 (−188.899682)	−189.220831	51.61	−189.179822 (−188.932088)	−189.245353
D3 syn	−189.233220	−189.310720	−189.141833	−189.219333	50.33	−189.174451	−189.243246
D4	−169.731465 (−169.496796)	−169.797822	−169.683899 (−169.490999)	−169.750256	43.74	−169.712682 (−169.522662)	−169.771038
D5	−209.111685	−209.191670	−209.032366	−209.112351	49.13	−209.064260	−209.135694
D6	−189.576819 (−189.344023)	−189.651615	−189.541267 (−189.339443)	−189.616063	43.18	−189.569571 (−189.368395)	−189.636579
D7 anti,anti	−205.277505 (−204.952424)	−205.361098	−205.196718 (−204.946965)	−205.280311	50.51	−205.229445 (−204.979834)	−205.304310
D7 syn,anti	−205.275131	−205.360015	−205.194421	−205.279305	49.83	−205.226741	−205.302981
D7 syn,syn	−205.260495	−205.353664	−205.180117	−205.273286	50.80	−205.213019	−205.297423
D8 anti	−185.741067	−185.813844	−185.704710	−185.777487	43.04	−185.732931	−185.797937
D8 syn	−185.737271 (−185.509830)	−185.814553	−185.700776 (−185.505706)	−185.778058	43.07	−185.729017 (−185.533644)	−185.798522
D9 anti	−225.150543 (−224.829718)	−225.236953	−225.082108 (−224.824581)	−225.168518	48.87	−225.113849 (−224.856145)	−225.191738
D9 syn	−225.137934	−225.230861	−225.069811	−225.162738	49.31	−225.101814	−225.186167
D10	−205.575525 (−205.351945)	−205.655933	−205.551798 (−205.347881)	−205.632206	42.55	−205.579722 (−205.375727)	−205.652423
D11	−245.009331 (−244.695315)	−245.101293	−244.953846 (−244.690025)	−245.045808	52.04	−244.987499 (−244.723752)	−245.070534
D12	−225.408689 (−225.195324)	−225.486645	−225.397830 (−225.191453)	−225.475786	42.21	−225.425548 (−225.218933)	−225.495841
MeCN	−132.754929 (−132.527113)	−132.803056	−132.704747 (−132.522567)	−132.752874	43.60	−132.733302 (−132.551110)	−132.773590
1	−1305.410811	−1305.558393	−1305.298316	−1305.445898	96.23	−1305.358649	−1305.491620
2	−2225.788953	−2225.998292	−2225.670044	−2225.879383	106.73	−2225.736716	−2225.930094
P(1-L)	−306.032034 (−305.456840)	−306.132857	−305.873930 (−305.448511)	−305.974753	61.56	−305.913329 (−305.488034)	−306.004002
P(1-Pt^{II})	−1478.708151	−1478.904410	−1478.487636	−1478.683895	104.31	−1478.552847	−1478.733456
P(1-Pt^{IV})	−2399.093745	−2399.351319	−2398.866665	−2399.124239	112.44	−2398.936785	−2399.177663
P(2-L)	−286.590639 (−286.109500)	−286.688126	−286.474310 (−286.102619)	−286.571797	56.68	−286.510765 (−286.139049)	−286.598728
P(2-Pt^{II})	−1459.263424	−1459.456769	−1459.084260	−1459.277605	105.27	−1459.150048	−1459.327622
P(2-Pt^{IV})	−2379.647167	−2379.902364	−2379.462338	−2379.717535	106.96	−2379.529149	−2379.768355
P(3-L)Oex	−322.049483 (−321.483906)	−322.160661	−321.902828 (−321.475799)	−322.014006	61.74	−321.942340 (−321.515059)	−322.043341
P(3-L)Oen	−322.045836	−322.158706	−321.899150	−322.012020	60.29	−321.937785	−322.040666
P(3-L)Mex	−322.023636	−322.133658	−321.877461	−321.987483	61.58	−321.916872	−322.016742
P(3-L)Men	−322.020094	−322.131423	−321.873891	−321.985220	60.07	−321.912392	−322.013761
P(3-Pt^{II})Oex	−1494.727742	−1494.933653	−1494.519099	−1494.725010	103.93	−1494.584082	−1494.774390
P(3-Pt^{II})Oen	−1494.725738	−1494.932967	−1494.517011	−1494.724240	102.46	−1494.581106	−1494.772922
P(3-Pt^{II})Mex	−1494.695927	−1494.900024	−1494.487949	−1494.692046	102.80	−1494.552247	−1494.740890

	E _g	E _s	H _g	H _s	S _s	G _g	G _s
P(3-Pt ^{II})Men	-1494.693342	-1494.896734	-1494.484402	-1494.687794	106.73	-1494.551073	-1494.738505
P(3-Pt ^{IV})Oex	-2415.115543	-2415.383437	-2414.900353	-2415.168247	112.46	-2414.970484	-2415.221680
P(3-Pt ^{IV})Oen	-2415.114528	-2415.383017	-2414.899252	-2415.167741	112.06	-2414.969141	-2415.220984
P(3-Pt ^{IV})Mex	-2415.076573	-2415.342450	-2414.862252	-2415.128129	112.92	-2414.932663	-2415.181781
P(3-Pt ^{IV})Men	-2415.076045	-2415.340772	-2414.861664	-2415.126391	111.90	-2414.931454	-2415.179558
P(4-L)O	-302.583532 (-302.110909)	-302.691022	-302.479231 (-302.104173)	-302.586721	55.97	-302.515255 (-302.140228)	-302.613314
P(4-L)M	-302.561299	-302.667427	-302.457611	-302.563739	55.58	-302.493399	-302.590147
P(4-Pt ^{II})O	-1475.256946	-1475.458919	-1475.090698	-1475.292671	97.69	-1475.151910	-1475.339087
P(4-Pt ^{II})M	-1475.228488	-1475.427449	-1475.061918	-1475.260879	102.45	-1475.126007	-1475.309556
P(4-Pt ^{IV})O	-2395.643470	-2395.907375	-2395.469622	-2395.733527	112.61	-2395.539844	-2395.787032
P(4-Pt ^{IV})M	-2395.608480	-2395.869333	-2395.436416	-2395.697269	106.98	-2395.503237	-2395.748099
P(5-L)O	-341.904504	-342.016983	-341.770807	-341.883286	60.66	-341.809667	-341.912108
P(5-L)M	-341.858754	-341.971536	-341.726180	-341.838962	60.47	-341.764926	-341.867693
P(5-Pt ^{II})O	-1514.578577	-1514.784134	-1514.382992	-1514.588549	102.47	-1514.447092	-1514.637236
P(5-Pt ^{II})M	-1514.521867	-1514.730338	-1514.326777	-1514.535248	109.14	-1514.394902	-1514.587104
P(5-Pt ^{IV})O	-2434.965482	-2435.231741	-2434.761453	-2435.027712	120.28	-2434.836306	-2435.084861
P(5-Pt ^{IV})M	-2434.901094	-2435.171648	-2434.700539	-2434.971093	112.85	-2434.770905	-2435.024712
P(6-L)O	-322.424007 (-321.955372)	-322.531076	-322.332927 (-321.948494)	-322.439996	57.19	-322.369688 (-321.986081)	-322.467169
P(6-L)M	-322.383624	-322.490589	-322.293847	-322.400812	56.43	-322.330153	-322.427624
P(6-Pt ^{II})O	-1495.092159	-1495.293206	-1494.939304	-1495.140351	97.04	-1495.000123	-1495.186458
P(6-Pt ^{II})M	-1495.035003	-1495.238997	-1494.883500	-1495.087494	99.48	-1494.945796	-1495.134760
P(6-Pt ^{IV})O	-2415.477790	-2415.739506	-2415.318331	-2415.580047	106.16	-2415.384658	-2415.630487
P(6-Pt ^{IV})M	-2415.411969	-2415.678866	-2415.253959	-2415.520856	108.46	-2415.321675	-2415.572389
P(7-L)exex	-338.041262 (-337.485212)	-338.161744	-337.907050 (-337.477402)	-338.027532	60.02	-337.945524 (-337.515760)	-338.056049
P(7-L)exen	-338.035707	-338.158032	-337.901528	-338.023853	59.93	-337.939947	-338.052328
P(7-L)enen	-338.028483	-338.152664	-337.894352	-338.018533	59.46	-337.932482	-338.046784
P(7-Pt ^{II})exex	-1510.714366	-1510.926754	-1510.518391	-1510.730779	102.67	-1510.582608	-1510.779561
P(7-Pt ^{II})exen	-1510.710468	-1510.925860	-1510.514476	-1510.729868	103.46	-1510.579173	-1510.779025
P(7-Pt ^{II})enen	-1510.702898	-1510.917810	-1510.506966	-1510.721878	101.22	-1510.570311	-1510.769971
P(7-Pt ^{IV})exex	-2431.097065	-2431.373721	-2430.894662	-2431.171318	111.87	-2430.964434	-2431.224471
P(7-Pt ^{IV})exen	-2431.094150	-2431.371151	-2430.890802	-2431.167803	118.63	-2430.964660	-2431.224168
P(7-Pt ^{IV})enen	-2431.087542	-2431.364092	-2430.885219	-2431.161769	111.77	-2430.954931	-2431.214875
P(8-L)ex	-318.551725	-318.666522	-318.460341	-318.575138	55.12	-318.495854	-318.601327
P(8-L)en	-318.549927 (-318.086567)	-318.667016	-318.459192 (-318.080060)	-318.576281	55.35	-318.494844 (-318.115459)	-318.602580
P(8-Pt ^{II})ex	-1491.217275	-1491.424250	-1491.063316	-1491.270291	103.10	-1491.127796	-1491.319277
P(8-Pt ^{II})en	-1491.215311	-1491.426152	-1491.061879	-1491.272720	103.29	-1491.126475	-1491.321796
P(8-Pt ^{IV})ex	-2411.597727	-2411.866462	-2411.438359	-2411.707094	106.73	-2411.505029	-2411.757805
P(8-Pt ^{IV})en	-2411.594893	-2411.869283	-2411.435954	-2411.710344	106.64	-2411.502573	-2411.761012
P(9-L)Oex	-357.896361 (-357.344717)	-358.017367	-357.775102 (-357.337066)	-357.896108	59.65	-357.813347 (-357.375125)	-357.924450
P(9-L)Oen	-357.885393	-358.008236	-357.764468	-357.887311	59.63	-357.802701	-357.915643
P(9-L)Mex	-357.876379	-357.997609	-357.755736	-357.876966	59.73	-357.794033	-357.905346
P(9-L)Men	-357.866668	-357.991478	-357.746317	-357.871127	59.80	-357.784655	-357.899540
P(9-Pt ^{II})Oex	-1530.567177	-1530.779939	-1530.384302	-1530.597064	102.49	-1530.448415	-1530.645760
P(9-Pt ^{II})Oen	-1530.555439	-1530.767897	-1530.372805	-1530.585263	100.65	-1530.435808	-1530.633085
P(9-Pt ^{II})Mex	-1530.538281	-1530.754697	-1530.356180	-1530.572596	102.54	-1530.420321	-1530.621316
P(9-Pt ^{II})Men	-1530.530980	-1530.750718	-1530.349088	-1530.568826	103.86	-1530.414024	-1530.618173
P(9-Pt ^{IV})Oex	-2450.949944	-2451.224711	-2450.760654	-2451.035421	111.99	-2450.830498	-2451.088631
P(9-Pt ^{IV})Oen	-2450.938486	-2451.211078	-2450.749469	-2451.022061	111.38	-2450.818949	-2451.074981
P(9-Pt ^{IV})Mex	-2450.918608	-2451.197153	-2450.730109	-2451.008654	112.22	-2450.800096	-2451.061973
P(9-Pt ^{IV})Men	-2450.912995	-2451.194846	-2450.723664	-2451.005515	117.94	-2450.797101	-2451.061552
P(10-L)O,acyc	-338.473114	-338.598562	-338.393867	-338.519315	58.53	-338.431441	-338.547125
P(10-L)M,acyc	-338.399140	-338.524616	-338.321590	-338.447066	59.96	-338.360025	-338.475555

	E _g	E _s	H _g	H _s	S _s	G _g	G _s
P(10-Pt^{II})O	-1511.050146	-1511.255942	-1510.909313	-1511.115109	102.75	-1510.973582	-1511.163929
P(10-Pt^{II})O_{acyc}	-1511.139112	-1511.352139	-1510.999167	-1511.212194	98.60	-1511.060931	-1511.259042
P(10-Pt^{II})M	-1511.019961	-1511.233433	-1510.879816	-1511.093288	107.42	-1510.946906	-1511.144327
P(10-Pt^{IV})O	-2431.430323	-2431.695453	-2431.284002	-2431.549132	106.87	-2431.350758	-2431.599909
P(10-Pt^{IV})O_{acyc}	-2431.518955	-2431.791632	-2431.372833	-2431.645510	111.50	-2431.442384	-2431.698487
P(10-Pt^{IV})M	-2431.398866	-2431.671843	-2431.252167	-2431.525144	114.66	-2431.323625	-2431.579623
P(11-L)	-377.725260 (-377.177959)	-377.847116	-377.617917 (-377.170358)	-377.739773	59.65	-377.656163 (-377.208313)	-377.768115
P(11-Pt^{II})	-1550.385405	-1550.600774	-1550.216647	-1550.432016	101.97	-1550.280446	-1550.480465
P(11-Pt^{IV})	-2470.766031	-2471.042787	-2470.590799	-2470.867555	111.95	-2470.660618	-2470.920746
P(12-L)	-358.206460 (-357.748936)	-358.320043	-358.142037 (-357.742519)	-358.255620	57.95	-358.179257 (-357.777788)	-358.283154
P(12-Pt^{II})	-1530.856475	-1531.065696	-1530.730671	-1530.939892	97.93	-1530.792032	-1530.986422
P(12-Pt^{IV})	-2451.235294	-2451.505736	-2451.102996	-2451.373438	107.34	-2451.170033	-2451.424439
TS(1-L)	-305.944712 (-305.378272)	-306.050689	-305.790407 (-305.368929)	-305.896384	66.13	-305.832569 (-305.410690)	-305.927805
TS(1-Pt^{II})₁	-1478.616518	-1478.814764	-1478.401390	-1478.599636	113.31	-1478.472033	-1478.653473
I(1-Pt^{II})	-1478.668848	-1478.866058	-1478.449931	-1478.647141	102.01	-1478.513752	-1478.695609
TS(1-Pt^{II})₂	-1478.640617	-1478.838825	-1478.422230	-1478.620438	108.58	-1478.490020	-1478.672028
TS(1-Pt^{IV})	-2398.993292	-2399.253078	-2398.771767	-2399.031553	126.22	-2398.850203	-2399.091524
TS(2-L)	-286.468273 (-285.994956)	-286.567243	-286.357460 (-285.986930)	-286.456430	61.31	-286.396709 (-286.025392)	-286.485560
I(2-Pt^{II})	-1459.208185	-1459.400379	-1459.030978	-1459.223172	102.79	-1459.095267	-1459.272011
TS(2-Pt^{II})₂	-1459.172885	-1459.366576	-1458.997093	-1459.190784	101.52	-1459.060618	-1459.239019
TS(2-Pt^{IV})	-2379.508859	-2379.763105	-2379.329608	-2379.583854	126.42	-2379.408166	-2379.643920
TS(3-L)O_{ex}	-321.974858	-322.087603	-321.831382	-321.944127	64.00	-321.872257	-321.974536
TS(3-L)O_{en}	-321.975053 (-321.417849)	-322.090286	-321.831773 (-321.409025)	-321.947006	63.70	-321.872468 (-321.449515)	-321.977272
TS(3-L)Mex	-321.970864	-322.088686	-321.827513	-321.945335	64.56	-321.868726	-321.976010
TS(3-L)Men	-321.965483	-322.082506	-321.822402	-321.939425	64.22	-321.863409	-321.969938
TS(3-Pt^{II})O_{ex}	-1494.650152	-1494.858211	-1494.444412	-1494.652471	115.80	-1494.516556	-1494.707491
TS(3-Pt^{II})O_{ex1}	-1494.657113	-1494.862548	-1494.451576	-1494.657011	111.77	-1494.521289	-1494.710117
I(3-Pt^{II})O_{ex}	-1494.676758	-1494.883807	-1494.470366	-1494.677415	102.67	-1494.534586	-1494.726197
TS(3-Pt^{II})O_{ex2}	-1494.651619	-1494.858694	-1494.445557	-1494.652632	108.48	-1494.513285	-1494.704174
TS(3-Pt^{II})O_{en1}	-1494.655592	-1494.863865	-1494.450020	-1494.658293	112.42	-1494.520127	-1494.711707
I(3-Pt^{II})O_{en}	-1494.680265	-1494.888627	-1494.472476	-1494.680838	107.86	-1494.539832	-1494.732086
TS(3-Pt^{II})O_{en2}	-1494.655527	-1494.863422	-1494.449259	-1494.657154	109.02	-1494.517315	-1494.708953
TS(3-Pt^{II})Mex₁	-1494.647890	-1494.853205	-1494.442498	-1494.647813	112.69	-1494.512766	-1494.701356
I(3-Pt^{II})Mex	-1494.671624	-1494.876090	-1494.464872	-1494.669338	101.80	-1494.528569	-1494.717706
TS(3-Pt^{II})Mex₂	-1494.649141	-1494.858137	-1494.443898	-1494.652894	104.64	-1494.509307	-1494.702612
TS(3-Pt^{II})Men	-1494.643392	-1494.851308	-1494.437767	-1494.645683	113.97	-1494.508812	-1494.699834
TS(3-Pt^{II})Men₁	-1494.642537	-1494.850224	-1494.437127	-1494.644814	112.66	-1494.507377	-1494.698342
I(3-Pt^{II})Men	-1494.666944	-1494.873737	-1494.459429	-1494.666222	108.48	-1494.527157	-1494.717764
TS(3-Pt^{II})Men₂	-1494.645618	-1494.854411	-1494.439559	-1494.648352	110.27	-1494.508369	-1494.700745
TS(3-Pt^{IV})O_{ex}	-2415.038540	-2415.305999	-2414.827587	-2415.095046	122.76	-2414.903935	-2415.153373
TS(3-Pt^{IV})O_{en}	-2415.036964	-2415.307313	-2414.826172	-2415.096521	122.20	-2414.902181	-2415.154582
TS(3-Pt^{IV})Mex	-2415.024892	-2415.295600	-2414.813129	-2415.083837	129.10	-2414.893306	-2415.145177
TS(3-Pt^{IV})Men	-2415.025552	-2415.295528	-2414.813926	-2415.083902	127.68	-2414.893244	-2415.144567
TS(4-L)O	-302.487427 (-302.021144)	-302.595097	-302.387479 (-302.013636)	-302.495149	59.06	-302.425369 (-302.051003)	-302.523210
TS(4-L)M	-302.471668	-302.580891	-302.371928	-302.481151	59.34	-302.409990	-302.509345
TS(4-Pt^{II})O₁	-1475.153178	-1475.355031	-1474.991141	-1475.192994	107.41	-1475.058225	-1475.244028
I(4-Pt^{II})O	-1475.201029	-1475.402548	-1475.036871	-1475.238390	96.05	-1475.097098	-1475.284026
TS(4-Pt^{II})O₂	-1475.167639	-1475.369006	-1475.004969	-1475.206336	96.21	-1475.065288	-1475.252048
TS(4-Pt^{II})M	-1475.137034	-1475.339325	-1474.974848	-1475.177139	108.20	-1475.042408	-1475.228548
TS(4-Pt^{II})M₁	-1475.136072	-1475.337685	-1474.974433	-1475.176046	107.99	-1475.041867	-1475.227356

	E _g	E _s	H _g	H _s	S _s	G _g	G _s
I(4-Pt ^{II})M	-1475.183789	-1475.382117	-1475.019898	-1475.218226	96.44	-1475.080357	-1475.264048
TS(4-Pt ^{II})M ₂	-1475.150666	-1475.350701	-1474.987408	-1475.187443	101.93	-1475.051183	-1475.235873
TS(4-Pt ^{IV})O	-2395.532944	-2395.797295	-2395.364624	-2395.628975	122.55	-2395.440848	-2395.687202
TS(4-Pt ^{IV})M	-2395.516369	-2395.781357	-2395.348064	-2395.613052	120.29	-2395.422925	-2395.670206
TS(5-L)O	-341.844317	-341.960170	-341.713371	-341.829224	62.77	-341.753500	-341.859048
TS(5-L)M	-341.826721	-341.948598	-341.696178	-341.818055	63.21	-341.736576	-341.848088
TS(5-Pt ^{II})O	-1514.517675	-1514.729562	-1514.325439	-1514.537326	105.71	-1514.391493	-1514.587552
TS(5-Pt ^{II})O ₁	-1514.524400	-1514.735040	-1514.331644	-1514.542284	108.57	-1514.399427	-1514.593869
I(5-Pt ^{II})O	-1514.528770	-1514.737387	-1514.334642	-1514.543259	106.99	-1514.401468	-1514.594093
TS(5-Pt ^{II})M	-1514.498749	-1514.713990	-1514.305815	-1514.521056	112.78	-1514.376140	-1514.574641
TS(5-Pt ^{II})M ₁	-1514.501597	-1514.714777	-1514.309035	-1514.522215	110.30	-1514.377862	-1514.574622
I(N-Pt ^{II})M	-1514.510963	-1514.720148	-1514.316900	-1514.526085	107.31	-1514.383924	-1514.577071
TS(5-Pt ^{IV})O	-2434.909273	-2435.181023	-2434.708673	-2434.980423	127.96	-2434.788163	-2435.041221
TS(5-Pt ^{IV})M	-2434.881358	-2435.157402	-2434.682093	-2434.958137	125.02	-2434.759806	-2435.017538
TS(6-L)O	-322.337927 (-321.875990)	-322.451483	-322.250400 (-321.868769)	-322.363956	58.30	-322.287830 (-321.905668)	-322.391656
TS(6-L)M	-322.308207	-322.424532	-322.221106	-322.337431	58.46	-322.258635	-322.365207
TS(6-Pt ^{II})O	-1494.999613	-1495.205878	-1494.850178	-1495.056443	105.23	-1494.915946	-1495.106441
TS(6-Pt ^{II})O ₁	-1495.003625	-1495.212047	-1494.855324	-1495.063746	100.45	-1494.918204	-1495.111473
I(6-Pt ^{II})O	-1495.034172	-1495.236217	-1494.883028	-1495.085073	101.10	-1494.946302	-1495.133109
TS(6-Pt ^{II})O ₂	-1495.001573	-1495.203512	-1494.851761	-1495.053700	99.97	-1494.914349	-1495.101199
TS(6-Pt ^{II})M	-1494.967109	-1495.177044	-1494.817796	-1495.027731	107.06	-1494.884666	-1495.078599
TS(6-Pt ^{II})M ₁	-1494.969147	-1495.177187	-1494.820559	-1495.028599	108.14	-1494.888082	-1495.079980
I(6-Pt ^{II})M	-1495.002060	-1495.202675	-1494.850915	-1495.051530	101.45	-1494.914400	-1495.099732
TS(6-Pt ^{II})M ₂	-1494.971940	-1495.178494	-1494.822058	-1495.028612	102.93	-1494.886432	-1495.077517
TS(6-Pt ^{IV})O	-2415.383808	-2415.650897	-2415.227951	-2415.495040	118.12	-2415.301497	-2415.551163
TS(6-Pt ^{IV})M	-2415.343720	-2415.617186	-2415.188074	-2415.461540	118.63	-2415.261931	-2415.517905
TS(7-L)exex	-337.991789 (-337.443409)	-338.114599	-337.859741 (-337.434969)	-337.982551	62.48	-337.899700 (-337.474784)	-338.012237
TS(7-L)exen	-337.989545	-338.111063	-337.857768	-337.979286	62.38	-337.897662	-338.008925
TS(7-L)enen	-337.983876	-338.111815	-337.852363	-337.980302	62.39	-337.892266	-338.009946
TS(7-Pt ^{II})exex	-1510.666697	-1510.883932	-1510.473450	-1510.690685	106.58	-1510.540033	-1510.741325
TS(7-Pt ^{II})exen	-1510.667438	-1510.881932	-1510.473280	-1510.687774	110.69	-1510.542344	-1510.740366
TS(7-Pt ^{II})enen	-1510.665611	-1510.885675	-1510.471424	-1510.691488	112.16	-1510.541372	-1510.744779
TS(7-Pt ^{II})exen ₁	-1510.679782		-1510.485713			-1510.554275	
I(7-Pt ^{II})exen	-1510.678889		-1510.483731			-1510.550950	
TS(7-Pt ^{IV})exex	-2431.056095	-2431.336486	-2430.856478	-2431.136869	120.85	-2430.931676	-2431.194289
TS(7-Pt ^{IV})exen	-2431.055285	-2431.332349	-2430.854645	-2431.131709	123.85	-2430.931651	-2431.190554
TS(7-Pt ^{IV})enen	-2431.052780	-2431.333452	-2430.852111	-2431.132783	125.79	-2430.930290	-2431.192550
TS(8-L)ex	-318.476621	-318.589539	-318.388337	-318.501255	57.56	-318.425323	-318.528604
TS(8-L)en	-318.475190 (-318.020568)	-318.592003	-318.386921 (-318.013523)	-318.503734	57.68	-318.423977 (-318.050103)	-318.531140
TS(8-Pt ^{II})ex	-1491.141390	-1491.347863	-1490.990907	-1491.197380	107.24	-1491.057884	-1491.248333
TS(8-Pt ^{II})ex ₁	-1491.147322	-1491.354524	-1490.997244	-1491.204446	104.46	-1491.062542	-1491.254078
I(8-Pt ^{II})ex	-1491.174113	-1491.379957	-1491.023126	-1491.228970	96.30	-1491.083499	-1491.274725
TS(8-Pt ^{II})ex ₂	-1491.138232	-1491.345136	-1490.987783	-1491.194687	103.65	-1491.052598	-1491.243934
TS(8-Pt ^{II})en	-1491.142357	-1491.352409	-1490.991728	-1491.201780	106.31	-1491.058166	-1491.252291
TS(8-Pt ^{IV})ex	-2411.522335	-2411.790293	-2411.365421	-2411.633379	121.24	-2411.440855	-2411.690984
TS(8-Pt ^{IV})en	-2411.523394	-2411.794991	-2411.366313	-2411.637910	117.79	-2411.439660	-2411.693876
TS(9-L)Oex	-357.856348 (-357.309473)	-357.979400	-357.737023 (-357.301343)	-357.860075	61.29	-357.776263 (-357.340453)	-357.889196
TS(9-L)Oen	-357.846326	-357.971997	-357.727651	-357.853322	61.36	-357.766933	-357.882476
TS(9-L)Mex	-357.844358	-357.968506	-357.725343	-357.849491	61.60	-357.764766	-357.878759
TS(9-L)Men	-357.841496	-357.970931	-357.722820	-357.852255	61.59	-357.762242	-357.881518
TS(9-Pt ^{II})Oex	-1530.527491	-1530.744955	-1530.346132	-1530.563596	111.47	-1530.415667	-1530.616559
TS(9-Pt ^{II})Oen	-1530.522441	-1530.739023	-1530.342413	-1530.558995	103.13	-1530.406911	-1530.607995
TS(9-Pt ^{II})Mex	-1530.514001	-1530.733116	-1530.332811	-1530.551926	108.52	-1530.400566	-1530.603487

	E _g	E _s	H _g	H _s	S _s	G _g	G _s
TS(9-Pt ^{II})Men	-1530.516418	-1530.740116	-1530.335113	-1530.558811	109.60	-1530.403517	-1530.610885
TS(9-Pt ^{IV})Oex	-2450.915690	-2451.195396	-2450.727723	-2451.007429	118.78	-2450.801671	-2451.063865
TS(9-Pt ^{IV})Oen	-2450.909142	-2451.187475	-2450.721701	-2451.000034	122.08	-2450.797638	-2451.058038
TS(9-Pt ^{IV})Mex	-2450.897257	-2451.179202	-2450.709625	-2450.991570	119.10	-2450.783764	-2451.048158
TS(9-Pt ^{IV})Men	-2450.900495	-2451.184464	-2450.712528	-2450.996497	116.78	-2450.785266	-2451.051983
TS(10-L)O	-338.318108 (-337.864037)	-338.436485	-338.242793 (-337.857161)	-338.361170	56.95	-338.279411 (-337.893408)	-338.388229
TS(10-L)M	-338.305285	-338.426729	-338.230035	-338.351479	57.29	-338.266857	-338.378699
TS(10-Pt ^{II})O	-1510.982175	-1511.192653	-1510.845813	-1511.056291	98.96	-1510.907795	-1511.103310
I(10-Pt ^{II})O	-1511.018401		-1510.880139			-1510.944029	
TS(10-Pt ^{II})M	-1510.964756	-1511.182080	-1510.827245	-1511.044569	107.76	-1510.894539	-1511.095769
TS(10-Pt ^{IV})O	-2431.361973	-2431.634057	-2431.219169	-2431.491253	112.27	-2431.289185	-2431.544596
TS(10-Pt ^{IV})M	-2431.341768	-2431.621564	-2431.197838	-2431.477634	118.60	-2431.271672	-2431.533985
TS(11-L)	-377.698340 (-377.160149)	-377.824263	-377.592659 (-377.152170)	-377.718582	60.77	-377.631585 (-377.191002)	-377.747456
TS(11-Pt ^{II})	-1550.367154	-1550.586130	-1550.199297	-1550.418273	110.58	-1550.268293	-1550.470813
TS(11-Pt ^{IV})	-2470.748998	-2471.028737	-2470.574560	-2470.854299	117.00	-2470.647431	-2470.909889
TS(12-L)	-358.142246 (-357.703672)	-358.260059	-358.080117 (-357.696927)	-358.197930	56.72	-358.116593 (-357.732986)	-358.224880
TS(12-Pt ^{II})	-1530.798415	-1531.012991	-1530.674381	-1530.888957	105.25	-1530.740158	-1530.938965
TS(12-Pt ^{II}) ₁	-1530.816706	-1531.030444	-1530.692852	-1530.906591	103.15	-1530.757364	-1530.955601
I(12-Pt ^{II})	-1530.834253	-1531.042655	-1530.709176	-1530.917578	101.32	-1530.772582	-1530.965718
TS(12-Pt ^{II}) ₂	-1530.801615	-1531.011626	-1530.677909	-1530.887920	102.72	-1530.742162	-1530.936726
TS(12-Pt ^{IV})	-2451.173922	-2451.449146	-2451.044344	-2451.319564	112.47	-2451.114483	-2451.373002
³ I(1-L) ₁	-305.926239						
³ I(1-L) ₂	-305.909154						
³ I(1-L) ₃	-305.902462						
¹ I(2-L)	-286.440904						
³ I(2-L) ₁	-286.474568						
³ I(2-L) ₂	-286.456740						
³ I(2-L) ₃	-286.451077						
³ TS(2-L) ₁	-286.435595						
³ I(3-L) ₁	-321.937186						
³ I(3-L) ₂	-321.943082						
¹ I(4-L)	-302.435152						
³ I(4-L) ₁	-302.462681						
³ I(4-L) ₂	-302.475205						
³ I(4-L) ₃	-302.468279						
³ I(6-L) ₁	-322.310209						
³ I(6-L) ₂	-322.303490						
³ I(7-L) ₁	-337.973204						
³ I(7-L) ₂	-337.928340						
³ I(8-L) ₁	-318.479071						
³ I(8-L) ₂	-318.443703						
³ I(8-L) ₃	-318.437414						
³ TS(8-L) ₁	-318.455814						
³ I(9-L) ₁	-357.821662						
³ I(9-L) ₂	-357.797721						
³ I(9-L) ₃	-357.790132						
³ I(11-L) ₁	-377.691551						
³ I(11-L) ₂	-377.631760						
³ I(12-L)	-358.170555						
³ TS(12-L)	-358.130272						

TABLE 12S. Atomic Cartesian Coordinates (Å) for the Equilibrium Geometries of the Calculated Structures. The Element Symbol or Nuclear Charge is Indicated in the First Column while x, y, and z Coordinated are Given in the Second–Fourth Columns (imaginary frequencies are included in parentheses near the structure name)

D1 (no)

6	0.988908	-0.975239	-0.181417
7	0.080752	0.005021	-0.107183
6	-0.263231	0.904233	-1.036806
6	-0.690505	0.065075	1.153726
1	-1.578775	-0.565042	1.067784
1	-0.063236	-0.286475	1.973617
1	-0.984378	1.097867	1.344208
1	1.131762	-1.621417	0.669051
1	1.533065	-1.113218	-1.104700
1	-1.030918	1.625151	-0.808380
1	0.216189	0.863575	-2.004320

D2 (no)

6	0.877003	-0.811542	-0.078192
8	-0.003858	0.029194	0.388484
6	-0.873803	0.789762	-0.215821
1	-0.940160	0.779003	-1.298014
1	-1.485869	1.392790	0.435029
1	1.473594	-1.311472	0.667489
1	0.964103	-0.963196	-1.148298

D3anti (no)

N	0.653413	-0.942664	-0.762589
N	0.005347	0.003749	-0.127161
C	-0.646480	1.060117	-0.586266
H	-1.124050	1.736338	0.104816
C	0.049277	-0.203625	1.336759
H	1.096711	-0.215756	1.640457
H	-0.395062	-1.176753	1.549066
H	-0.493225	0.589719	1.849903
H	0.571058	-0.719543	-1.763036
H	-0.683538	1.219444	-1.655908

D3syn (no)

N	0.659597	-0.868338	-0.876897
N	0.004932	0.008033	-0.146952
C	-0.653949	1.035234	-0.650895
H	-1.162741	1.716144	0.011604
C	-0.001142	-0.152216	1.327288
H	1.034308	-0.122820	1.675614
H	-0.436797	-1.127066	1.559902

H	-0.578528	0.638792	1.805357
H	1.071857	-1.536587	-0.219669
H	-0.649256	1.155563	-1.724223

D4

N	0.688445	-0.961599	-0.165528
O	0.055912	0.089102	0.398498
C	-0.732213	0.840343	-0.273376
H	-0.900585	0.631534	-1.324578
H	-1.181086	1.650328	0.283302
H	1.208538	-1.305542	0.652243

D5 (no)

8	-1.537747	0.649110	0.462852
7	-0.347954	1.002814	0.206514
6	0.713018	0.656107	0.887929
1	0.567398	0.012756	1.744225
1	1.685113	1.014322	0.583749
6	-0.210874	1.885059	-0.979230
1	-0.820683	2.770337	-0.791857
1	-0.621850	1.341820	-1.831669
1	0.830189	2.159269	-1.156802

D6 (no)

8	0.779661	-0.808560	-0.406095
8	0.149951	0.031534	0.431694
6	-0.832675	0.708894	0.012397
1	-1.148052	0.597837	-1.021240
1	-1.292795	1.365010	0.742061

D7anti,anti (no)

7	-0.663688	1.171464	-0.051077
7	-0.126423	-0.001952	0.012505
7	-0.622418	-1.194505	0.050526
1	-1.645361	-1.083586	0.012572
6	1.356397	0.024051	0.001974
1	1.679837	0.942183	0.488931
1	1.685281	0.013383	-1.038935
1	1.711749	-0.864424	0.519944
1	-1.682181	1.023083	-0.078040

D7syn,anti (no)

7	1.163427	-0.192427	-0.682214
7	0.010113	-0.005303	-0.145214
7	-1.103560	0.145538	-0.788141
1	-1.839647	0.274181	-0.087242
6	0.040439	0.028494	1.340784
1	1.068042	-0.118472	1.663746
1	-0.605381	-0.769302	1.714597
1	-0.338060	0.999258	1.668904
1	0.982552	-0.191278	-1.695723

D7 syn,syn (no)

7	0.982407	-0.978426	-0.062998
7	0.178179	0.028955	0.016727
7	0.632935	1.236899	0.056425
1	-0.181108	1.853508	0.112752
6	-1.302763	-0.208369	-0.008911
1	-1.520746	-1.145003	0.506164
1	-1.623657	-0.266082	-1.051518
1	-1.809492	0.613081	0.498847
1	0.396935	-1.817279	-0.083855

D8 anti (no)

7	0.843605	0.823798	0.115918
8	0.065325	-0.044851	-0.430728
7	-0.821365	-0.704924	0.280306
1	-1.252178	-1.290929	-0.448747
1	0.573895	0.817621	1.121007

D8 syn (no)

7	1.106900	0.325315	-0.000096
8	0.012237	-0.385730	0.000197
7	-1.125282	0.254821	-0.000114
1	-1.776613	-0.544280	-0.000120
1	1.807387	-0.430834	0.000015

D9 anti (no)

8	3.514883	-0.200151	0.010536
7	3.186754	0.969412	0.301781
7	2.573818	1.809470	-0.429114
6	3.554853	1.436957	1.662817
1	3.080849	0.759296	2.374446
1	4.639162	1.352437	1.749276
1	3.217348	2.462645	1.794492
1	2.408443	1.310240	-1.314752

D9 syn (no)

8	0.589063	-1.059167	-0.547217
7	0.015261	-0.022870	-0.175048
7	-0.448832	0.848605	-0.979603
1	-0.864539	1.590680	-0.409076
6	-0.086405	0.118716	1.315685
1	0.932159	0.101358	1.704708
1	-0.630131	-0.753763	1.679342
1	-0.596566	1.042626	1.591211

D10 (no)

7	-0.304940	-0.001089	0.000000
1	-0.983713	0.780017	0.000000
8	0.797776	0.652476	0.000000
8	1.890877	-0.031403	0.000000

D11 (no)

8	0.722282	1.091802	0.045617
7	0.174001	-0.005021	0.003016

8	0.740505	-1.091191	-0.054989
6	-1.325530	-0.001907	0.007298
1	-1.671747	-1.030422	0.079863
1	-1.647487	0.467649	-0.923973
1	-1.647888	0.604466	0.854183

D12 (no)

8	0.738322	-0.709036	-0.415090
8	0.147154	0.048875	0.406080
8	-0.885476	0.660161	0.009010

P(1-L) (no)

C	0.863460	-0.500804	0.017678
N	-1.435525	-0.050534	0.126677
N	0.694925	0.939660	0.157885
C	-0.564123	-0.982054	0.203809
C	-0.727582	1.200880	-0.110427
H	-1.114566	1.992283	0.544746
C	-0.914129	-2.422378	0.414376
C	1.631915	1.767776	-0.572392
H	-0.919903	1.514499	-1.156089
H	-1.998159	-2.541929	0.474809
H	-0.458958	-2.802272	1.338095
H	-0.530195	-3.041143	-0.407358
H	1.592238	1.614968	-1.669903
H	2.654681	1.561026	-0.238563
H	1.426022	2.824907	-0.370427
H	1.231402	-0.814042	-0.983452
H	1.564391	-0.912694	0.757950

P(1-Pt^{II}) (-13i)

Pt	-0.826744	-0.012395	-0.086133
Cl	-1.375195	-0.923780	2.030935
Cl	-0.238099	0.907531	-2.191836
C	3.293021	-0.372230	1.069426
N	1.119169	0.028957	0.431667
N	3.218301	1.058121	0.744881
C	1.950711	-0.930275	0.625989
C	1.786602	1.332345	0.730759
H	1.418790	1.653997	1.712918
C	1.656732	-2.382652	0.483457
C	3.863081	1.373496	-0.538047
H	1.508328	2.069389	-0.023517
H	0.605342	-2.553434	0.249558
H	1.905840	-2.905228	1.415062
H	2.284903	-2.811034	-0.308087
H	3.438144	0.828337	-1.397842
H	4.930323	1.143149	-0.464450
H	3.766087	2.445543	-0.729896
N	-2.741946	-0.006269	-0.599703

C	-3.855171	0.008005	-0.899036
C	-5.261546	0.029784	-1.275894
H	-5.869896	0.351432	-0.424932
H	-5.581653	-0.970399	-1.584015
H	-5.412815	0.724643	-2.107662
H	4.140816	-0.859639	0.577306
H	3.403939	-0.533920	2.153450

P(1-Pt^{IV}) (13i)

78	-0.452659	-0.022827	-0.094422
17	-0.511561	1.722589	-1.734566
17	-0.505852	1.598308	1.669598
6	3.854913	-0.275181	-0.019814
7	1.582267	0.036949	-0.073734
7	3.633545	1.135566	0.296049
6	2.464868	-0.899537	-0.008900
6	2.296632	1.374176	-0.198330
1	2.288056	1.618547	-1.264184
6	2.290831	-2.375783	0.039877
6	3.778317	1.423266	1.731105
1	1.758786	2.137211	0.359590
1	1.307523	-2.699465	-0.291804
1	3.068039	-2.840204	-0.579158
1	2.445958	-2.715179	1.071467
1	3.103919	0.835803	2.375849
1	4.813039	1.225717	2.026884
1	3.577106	2.484152	1.899784
17	-0.486317	-1.624389	-1.871360
17	-0.536118	-1.737464	1.573980
7	-2.472552	-0.020502	-0.105401
6	-3.621126	-0.008636	-0.113824
6	-5.075562	0.009012	-0.124930
1	-5.436656	0.857781	0.463587
1	-5.458226	-0.920244	0.307586
1	-5.433808	0.103932	-1.154382
1	4.534196	-0.759503	0.688365
1	4.280865	-0.399794	-1.028265

P(2-L) (no)

6	1.179887	-0.081421	0.019013
7	-1.127490	0.238153	-0.018230
8	0.955358	1.317246	0.013035
6	-0.222437	-0.661208	-0.002725
6	-0.464932	1.526037	-0.009182
1	-0.770803	2.100058	0.877241
6	-0.501229	-2.131366	-0.005237
1	-0.742980	2.098469	-0.905716
1	-1.578082	-2.311842	-0.023231
1	-0.072347	-2.609911	0.884576

1	-0.042345	-2.612711	-0.878408
1	1.768608	-0.392058	-0.859461
1	1.739792	-0.389288	0.917120

P(2-Pt^{II}) (no)

78	-0.384966	0.049109	-0.005048
17	-0.358576	-0.664887	2.253813
17	-0.367468	0.762794	-2.262953
6	3.893543	-0.182343	0.092305
7	1.629958	0.147989	0.011033
8	3.677021	1.203862	-0.112221
6	2.510389	-0.784522	0.040755
6	2.291559	1.462704	0.036808
1	2.063519	1.945509	0.997275
6	2.236915	-2.246782	0.043212
1	1.927887	2.074983	-0.791896
1	1.164981	-2.442868	0.086316
1	2.724182	-2.717193	0.905492
1	2.658228	-2.702299	-0.861899
7	-2.363735	-0.008813	-0.019579
6	-3.516085	-0.033870	-0.027115
6	-4.971815	-0.062331	-0.035119
1	-5.354606	0.224439	0.949191
1	-5.324335	-1.070373	-0.274576
1	-5.352997	0.636471	-0.786048
1	4.552327	-0.577545	-0.691304
1	4.364131	-0.388343	1.069067

P(2-Pt^{IV}) (15i)

78	-0.308330	0.048688	-0.020130
17	-0.296822	1.692596	-1.762876
17	-0.311877	1.775951	1.636443
6	3.977915	-0.364684	0.085145
7	1.732129	0.026664	0.005139
8	3.790799	1.027235	0.233840
6	2.577352	-0.934810	0.140546
6	2.478220	1.308444	-0.193291
1	2.423906	1.560203	-1.259151
6	2.352097	-2.394265	0.307212
1	2.043757	2.100531	0.413556
1	1.380817	-2.711162	-0.065467
1	3.151376	-2.937519	-0.210159
1	2.415774	-2.640465	1.373982
17	-0.383591	-1.661374	-1.695317
17	-0.466513	-1.557172	1.746840
7	-2.318143	0.118902	-0.045419
6	-3.465674	0.163964	-0.059092
6	-4.918838	0.222304	-0.075330
1	-5.255916	1.114426	0.461001

1	-5.327592	-0.668586	0.410822
1	-5.273162	0.265811	-1.109577
1	4.617355	-0.741458	0.890502
1	4.442388	-0.632022	-0.881800

P(3-L)Oex (no)

7	0.859011	-0.484741	0.017851
7	-1.342480	-0.003423	0.389238
7	0.831759	0.956024	0.175956
6	-0.475296	-0.919344	0.180183
6	-0.592592	1.242708	0.525190
1	-0.684071	1.607730	1.558813
6	-0.778645	-2.379996	0.057090
6	1.224171	1.566229	-1.097730
1	-0.994307	2.017164	-0.140636
1	-1.841158	-2.550073	0.237828
1	-0.197934	-2.962106	0.784222
1	-0.512268	-2.746925	-0.940291
1	0.563591	1.289858	-1.936678
1	2.244364	1.259021	-1.342472
1	1.211318	2.654549	-0.977086
1	1.506608	-0.901817	0.686591

P(3-L)Oen (no)

7	0.937988	-0.396658	0.243268
7	-1.279650	-0.026616	0.470911
7	0.823993	1.048989	0.132792
6	-0.376971	-0.895841	0.199343
6	-0.530189	1.214069	0.722541
1	-0.430698	1.355317	1.807952
6	-0.619201	-2.353722	-0.037026
6	0.842310	1.443133	-1.286615
1	-1.026361	2.090894	0.296361
1	-1.688818	-2.559308	0.028871
1	-0.092483	-2.955507	0.712845
1	-0.255464	-2.664839	-1.024431
1	0.076145	0.937797	-1.897518
1	1.832396	1.228262	-1.703593
1	0.687670	2.524961	-1.342471
1	1.625602	-0.783415	-0.396268

P(3-L)Mex (no)

7	-0.856616	1.076851	-0.196028
7	-1.366021	-0.148729	0.220945
7	0.608488	1.066640	0.039166
6	-0.404894	-0.984389	0.368995
6	0.946077	-0.362489	0.094453
1	1.686669	-0.577952	0.877180
6	-0.618565	-2.423731	0.703424
6	1.269664	1.778005	-1.048684

1	1.359923	-0.741310	-0.863035
1	-1.682283	-2.621984	0.855415
1	-0.252401	-3.075862	-0.101443
1	-0.070158	-2.701419	1.613111
1	1.097945	1.312531	-2.034212
1	0.908843	2.810270	-1.083403
1	2.345828	1.802273	-0.847274
1	-1.249008	1.785739	0.425953

P(3-L)Men (no)

N	-0.647214	0.987818	0.886824
N	-1.275117	-0.114484	0.265380
N	0.756209	1.032341	0.463941
C	-0.357758	-0.955017	-0.046636
C	1.018573	-0.408532	0.316224
H	1.350947	-0.825909	1.278968
C	-0.635483	-2.306314	-0.617364
C	0.881147	1.738447	-0.823481
H	1.798462	-0.598658	-0.427512
H	-1.710721	-2.448785	-0.751404
H	-0.137267	-2.437679	-1.586894
H	-0.258106	-3.098704	0.043677
H	0.241307	1.327846	-1.621956
H	0.629124	2.793254	-0.671542
H	1.926486	1.692814	-1.144936
H	-1.116254	1.844597	0.596126

P(3-Pt^{II})Oex (12i)

78	-0.567682	-0.013582	0.047529
17	-0.747717	-1.162154	2.116197
17	-0.352721	1.139207	-2.013827
7	3.610757	-0.415025	0.180040
7	1.439394	0.060374	0.247040
7	3.576960	1.026742	0.246072
6	2.316019	-0.889528	0.182873
6	2.150427	1.331585	0.490449
1	1.964371	1.637481	1.527388
6	2.032611	-2.348926	0.063833
6	4.052509	1.557534	-1.042221
1	1.791864	2.105010	-0.191804
1	1.205938	-2.622761	0.722951
1	2.922690	-2.936277	0.307617
1	1.743414	-2.577706	-0.968154
1	3.436239	1.235339	-1.894787
1	5.082601	1.227342	-1.197438
1	4.043671	2.649645	-0.981842
7	-2.536464	-0.041916	-0.151746
6	-3.683605	-0.047508	-0.267826
6	-5.132606	-0.050955	-0.412497

1	-5.603612	0.176673	0.548801
1	-5.472410	-1.034872	-0.750508
1	-5.434909	0.702067	-1.146762
1	4.260102	-0.836877	0.839460

P(3-Pt^{II})Oen (8i)

78	-0.812090	-0.041160	0.136793
17	-0.818057	-1.404778	2.077063
17	-0.772863	1.329662	-1.801277
7	3.370594	-0.264283	0.193864
7	1.199033	0.106525	0.213034
7	3.279946	1.172219	0.052186
6	2.113921	-0.801485	0.058192
6	1.900775	1.374556	0.527499
1	1.893067	1.511139	1.615456
6	1.890651	-2.257361	-0.176520
6	3.434524	1.541040	-1.370411
1	1.427123	2.220644	0.030571
1	1.178315	-2.640227	0.559116
1	2.829402	-2.813987	-0.106177
1	1.458814	-2.405870	-1.172122
1	2.701295	1.055756	-2.031249
1	4.449774	1.284253	-1.690000
1	3.322609	2.625611	-1.447587
7	-2.785780	-0.139721	0.051861
6	-3.936942	-0.188165	0.005372
6	-5.390935	-0.246085	-0.051271
1	-5.808885	-0.109868	0.951005
1	-5.711828	-1.217255	-0.440775
1	-5.769555	0.543671	-0.707414
1	4.174623	-0.694212	-0.245229

P(3-Pt^{II})Mex (15i)

78	-0.561454	-0.025817	0.046902
17	-0.536317	1.291556	2.029276
7	2.022458	1.363529	-0.082044
7	1.451392	0.061685	0.057095
7	3.453982	1.201892	-0.111759
6	2.353107	-0.838471	0.226724
6	3.709625	-0.179125	0.330381
1	4.064913	-0.230900	1.371749
6	2.101422	-2.298069	0.365640
6	3.910555	1.443894	-1.488361
1	4.464774	-0.659496	-0.301103
1	1.034439	-2.508853	0.446672
1	2.495101	-2.834346	-0.506354
1	2.624892	-2.678730	1.251679
1	3.484748	0.736938	-2.218105
1	3.623435	2.456961	-1.774357

1	5.002493	1.370274	-1.504842
17	-0.542037	-1.338795	-1.919965
7	-2.538188	-0.067645	0.060058
6	-3.690718	-0.081899	0.060486
6	-5.146607	-0.098392	0.058437
1	-5.528579	0.728400	0.665065
1	-5.510130	-1.043493	0.473656
1	-5.517846	0.006762	-0.965673
1	1.735378	1.869436	0.761677

P(3-Pt^{II})Men (no)

78	-0.546770	0.023816	-0.046153
17	-0.219177	-2.300677	0.352536
7	2.145248	-0.558289	-1.151878
7	1.461628	0.224567	-0.157775
7	3.521979	-0.640433	-0.723769
6	2.308664	0.983287	0.445654
6	3.688632	0.688068	-0.119875
1	3.928612	1.427403	-0.898688
6	1.999161	1.999966	1.485626
6	3.721218	-1.729762	0.254457
1	4.486245	0.693088	0.627082
1	0.935863	2.017960	1.725130
1	2.581256	1.790658	2.392186
1	2.290772	2.997563	1.133476
1	3.057987	-1.673146	1.130637
1	3.552367	-2.684081	-0.251700
1	4.765063	-1.702166	0.580831
17	-0.872377	2.319546	-0.496180
7	-2.506435	-0.217652	0.054221
6	-3.649073	-0.359857	0.104397
6	-5.092796	-0.538240	0.165736
1	-5.341779	-1.314128	0.896204
1	-5.472666	-0.837807	-0.816011
1	-5.570745	0.400663	0.461625
1	1.713505	-1.486134	-1.140495

P(3-Pt^{IV})Oex (2i)

Pt	-0.448388	-0.010762	-0.118709
Cl	-0.409834	1.711626	-1.783807
Cl	-0.479103	1.640845	1.615910
N	3.696985	-0.454802	0.375615
N	1.583814	-0.002130	-0.063412
N	3.659758	0.981181	0.387927
C	2.449886	-0.960023	0.133364
C	2.352216	1.272776	-0.208240
H	2.429236	1.493951	-1.276534
C	2.253478	-2.437637	0.144887
C	3.776465	1.441026	1.784523

H	1.852120	2.091553	0.305595
H	1.400436	-2.724617	-0.467580
H	3.163097	-2.922192	-0.227433
H	2.079043	-2.773643	1.170760
H	2.966841	1.070946	2.429634
H	4.738099	1.105190	2.180225
H	3.764838	2.534230	1.779056
Cl	-0.490424	-1.645688	-1.867525
Cl	-0.613496	-1.702121	1.566603
N	-2.465095	0.047887	-0.174494
C	-3.612725	0.088919	-0.203165
C	-5.065925	0.142398	-0.240021
H	-5.414959	1.022922	0.307688
H	-5.478991	-0.758753	0.222962
H	-5.405313	0.204156	-1.278336
H	4.509755	-0.873267	-0.064390

P(3-Pt^{IV})Oen (11i)

Pt	-0.449525	0.024056	0.099515
Cl	-0.567850	-1.306570	2.085237
Cl	-0.399168	1.374157	-1.879615
N	3.711523	-0.493787	0.047605
N	1.579477	-0.000817	0.095539
N	3.686815	0.856450	-0.445396
C	2.443588	-0.983489	0.141379
C	2.377059	1.266413	0.065920
H	2.467052	1.629228	1.093466
C	2.223294	-2.447267	0.320775
C	3.755285	0.854048	-1.922006
H	1.908680	2.015771	-0.567427
H	1.342478	-2.634604	0.933899
H	3.105753	-2.887795	0.795860
H	2.067091	-2.918266	-0.654121
H	2.958558	0.264845	-2.398084
H	4.732842	0.465232	-2.224124
H	3.685337	1.891433	-2.258246
N	-2.464756	0.117760	0.086655
C	-3.611847	0.178821	0.084314
C	-5.064342	0.258049	0.082533
H	-5.420783	0.489503	1.090759
H	-5.484742	-0.699478	-0.239095
H	-5.388552	1.044785	-0.605245
H	4.503957	-1.068031	-0.205387
Cl	-0.596189	-1.917623	-1.294837
Cl	-0.421752	1.992054	1.462583

P(3-Pt^{IV})Mex (14i)

Pt	-0.631850	-0.031356	0.055815
Cl	-0.729657	1.519251	-1.754417

Cl	-0.691694	1.765698	1.651254
N	1.979755	1.342241	0.013077
N	1.407909	0.033733	0.086160
N	3.399104	1.184950	-0.054963
C	2.313865	-0.877920	0.200790
C	3.659015	-0.199151	0.358081
H	3.978733	-0.277068	1.409596
C	2.166988	-2.356599	0.201833
C	3.827271	1.455413	-1.437393
H	4.435612	-0.657536	-0.261884
H	1.136255	-2.681757	0.310786
H	2.570237	-2.754335	-0.738569
H	2.773961	-2.768262	1.017581
H	3.387079	0.762823	-2.171567
H	3.528937	2.472312	-1.695078
H	4.918699	1.384755	-1.475882
Cl	-0.662089	-1.808102	-1.540436
Cl	-0.674439	-1.574263	1.898447
N	-2.639030	-0.051248	0.055526
C	-3.787382	-0.052795	0.053284
C	-5.241737	-0.052505	0.049683
H	-5.609273	0.833996	0.575227
H	-5.611009	-0.951066	0.552953
H	-5.605949	-0.038818	-0.981960
H	1.691691	1.829038	0.865450

P(3-Pt^{IV})Men (15i)

Pt	-0.609744	0.013772	0.110477
Cl	-0.456634	1.373542	-1.866720
N	2.092308	1.312858	0.130537
N	1.424324	0.028670	0.236859
N	3.406742	1.023249	-0.354103
C	2.308049	-0.888587	0.437902
C	3.674390	-0.217042	0.378921
H	4.003365	0.014561	1.402819
C	2.125356	-2.334830	0.721571
C	3.440713	0.837484	-1.820796
H	4.437114	-0.825589	-0.112099
H	1.084318	-2.611190	0.863671
H	2.543149	-2.917967	-0.108640
H	2.699025	-2.592520	1.621534
H	2.745101	0.070312	-2.191225
H	3.198073	1.792225	-2.293972
H	4.464247	0.571568	-2.100407
Cl	-0.850505	-1.300371	2.086695
N	-2.611655	0.037584	-0.056221
C	-3.756645	0.059975	-0.142524
C	-5.206763	0.089984	-0.249624

H	-5.494841	0.472394	-1.233424
H	-5.617656	0.741959	0.527112
H	-5.605635	-0.920889	-0.122671
H	1.566733	1.879542	-0.539295
Cl	-0.760283	1.983623	1.451401
Cl	-0.564357	-1.940366	-1.280445

P(4-L)O (no)

N	1.105548	-0.140885	0.105454
N	-1.101905	0.241317	-0.257740
O	0.940072	1.294760	0.150118
C	-0.218237	-0.629673	0.045390
C	-0.386888	1.495383	-0.391058
H	-0.324348	1.780174	-1.454279
C	-0.459987	-2.094134	0.234021
H	-0.861544	2.306481	0.173259
H	-1.522483	-2.303475	0.102151
H	0.117541	-2.673888	-0.494501
H	-0.153731	-2.421898	1.235211
H	1.589156	-0.377955	0.973104

P(4-L)M (no)

7	-0.600271	1.470108	0.098925
7	-1.115739	0.184869	0.091508
8	0.820505	1.373391	-0.324674
6	-0.157685	-0.662897	0.063067
6	1.185793	0.036656	-0.023232
1	1.735798	-0.033147	0.933616
6	-0.348277	-2.138784	0.167504
1	1.830711	-0.357161	-0.820451
1	-1.411550	-2.381691	0.228502
1	0.085815	-2.651990	-0.700150
1	0.154737	-2.536326	1.059221
1	-1.026463	1.978487	-0.680416

P(4-Pt^{II})O (15i)

Pt	-0.571904	0.101746	-0.024330
Cl	-0.523455	1.538827	1.859006
N	3.601801	-0.394752	-0.064538
N	1.448713	0.125624	-0.037751
O	3.545446	1.038238	0.039161
C	2.301030	-0.831690	0.122006
C	2.203760	1.342682	-0.360255
H	2.145450	1.529925	-1.442845
C	2.004036	-2.263038	0.413218
H	1.849468	2.198808	0.214383
H	1.223947	-2.613614	-0.268036
H	2.899970	-2.878398	0.297705
H	1.628983	-2.356757	1.438402
Cl	-0.591672	-1.327259	-1.918203

N	-2.547437	0.123433	-0.008876
C	-3.699881	0.150101	-0.002608
C	-5.155452	0.188775	0.000813
H	-5.502271	1.064624	0.557717
H	-5.552488	-0.714801	0.473742
H	-5.528539	0.246062	-1.026438
H	4.280849	-0.710940	0.625479

P(4-Pt^{II})M (no)

Pt	-0.574047	0.065250	0.033653
Cl	-0.540605	1.424841	-1.916439
N	2.035951	1.407907	0.085918
N	1.449213	0.115672	0.023846
O	3.383589	1.207281	-0.403994
C	2.359177	-0.792490	0.007562
C	3.706556	-0.107482	0.028004
H	4.129003	-0.116532	1.049527
C	2.142424	-2.262179	0.021864
H	4.433319	-0.536307	-0.667873
H	1.080667	-2.507628	0.004354
H	2.645771	-2.715965	-0.840993
H	2.584127	-2.697074	0.927335
Cl	-0.593805	-1.251109	1.995426
N	-2.547593	0.051179	0.018168
C	-3.699935	0.051502	0.015903
C	-5.155731	0.053083	0.015092
H	-5.526537	0.943937	0.531540
H	-5.528245	-0.838292	0.529048
H	-5.527523	0.056746	-1.014115
H	1.580569	1.947013	-0.661488

P(4-Pt^{IV})O (no)

Pt	-0.309621	0.049726	-0.019610
Cl	-0.312592	1.678453	-1.774282
Cl	-0.288028	1.796860	1.615513
N	3.878225	-0.399058	-0.004265
N	1.724774	0.056203	-0.010663
O	3.780448	1.009781	0.228082
C	2.598564	-0.898535	0.112873
C	2.480923	1.304581	-0.278913
H	2.504353	1.481581	-1.360974
C	2.412802	-2.363413	0.306916
H	2.070176	2.152710	0.264010
H	1.525713	-2.710156	-0.222692
H	3.297506	-2.892268	-0.059969
H	2.276289	-2.573654	1.372127
Cl	-0.388610	-1.682999	-1.671105
Cl	-0.431345	-1.548797	1.758154
N	-2.316723	0.105786	-0.022180

C	-3.464630	0.143136	-0.020754
C	-4.918271	0.191635	-0.018326
H	-5.253798	1.107562	0.477307
H	-5.313711	-0.676035	0.518246
H	-5.288077	0.180521	-1.047990
H	4.577890	-0.771909	0.633070

P(4-Pt^{IV})M (5i)

Pt	-0.431986	0.052684	0.040453
Cl	-0.418023	1.646706	-1.755856
Cl	-0.510488	1.834583	1.627711
N	2.221611	1.382882	0.061013
N	1.610692	0.086358	0.035758
O	3.507470	1.151526	-0.538478
C	2.517626	-0.827978	0.025037
C	3.859566	-0.127320	-0.034484
H	4.301716	-0.069511	0.976677
C	2.377240	-2.302257	0.120806
H	4.568967	-0.593838	-0.722265
H	1.352040	-2.616846	0.296382
H	2.742426	-2.755866	-0.808734
H	3.017324	-2.663625	0.936457
Cl	-0.469653	-1.711417	-1.583634
Cl	-0.510320	-1.507394	1.844261
N	-2.430956	0.056791	0.011672
C	-3.579164	0.061710	-0.000335
C	-5.033261	0.068465	-0.014922
H	-5.400505	0.965881	0.491981
H	-5.409130	-0.819477	0.502253
H	-5.390156	0.064050	-1.049212
H	1.716080	1.948639	-0.631781

P(5-L)O (no)

O	-0.129339	-0.777917	-0.629987
N	-0.551406	1.212697	0.359422
N	1.191462	-0.134399	-0.535354
C	-0.993736	0.070860	0.012204
C	0.821815	1.253206	-0.137605
H	0.875346	1.915082	-1.011875
C	-2.376714	-0.460025	0.193742
C	1.891764	-0.855611	0.531166
H	1.518705	1.622800	0.623318
H	-2.995910	0.295849	0.678454
H	-2.810659	-0.718835	-0.778286
H	-2.362788	-1.371364	0.801154
H	1.386654	-0.794595	1.508045
H	1.991117	-1.903210	0.238583
H	2.893084	-0.421051	0.614982

P(5-L)M (no)

6	1.029986	0.420477	0.163978
7	-0.878781	-0.847856	0.491744
7	-0.109820	1.341609	0.153045
6	0.360490	-0.940799	0.190438
8	-1.209844	0.499794	0.670948
6	1.041256	-2.250598	-0.035846
1	0.338093	-3.074499	0.106867
1	1.454092	-2.310709	-1.050896
1	1.879797	-2.378244	0.661160
1	1.641752	0.563551	1.066828
1	1.671614	0.575753	-0.710690
6	-0.519136	1.715583	-1.205493
1	-1.453112	2.276879	-1.139198
1	-0.662812	0.852938	-1.874420
1	0.253960	2.371731	-1.619220

P(5-Pt^{II})O

Pt	-0.562105	0.018765	-0.059999
Cl	-0.858252	2.316210	-0.550373
Cl	-0.230629	-2.281089	0.426471
O	3.567844	0.701829	0.223527
N	1.446644	0.218546	-0.196275
N	3.624728	-0.406658	-0.759361
C	2.273096	0.874052	0.542849
C	2.234913	-0.449302	-1.246978
H	2.133098	0.119259	-2.177458
C	1.977705	1.776290	1.687980
C	3.993356	-1.592270	0.025813
H	1.899421	-1.478124	-1.388271
H	1.024303	2.281373	1.524560
H	2.782953	2.507130	1.795468
H	1.918361	1.186209	2.610019
H	3.252677	-1.855582	0.794071
H	4.966704	-1.410119	0.485424
H	4.089843	-2.421376	-0.681366
N	-2.518941	-0.221102	0.050757
C	-3.660744	-0.369556	0.108487
C	-5.102777	-0.558932	0.178711
H	-5.537952	-0.482142	-0.822599
H	-5.548803	0.207805	0.819653
H	-5.328508	-1.546952	0.591518

P(5-Pt^{II})M (no)

78	1.001458	-1.175962	-0.039830
17	1.353176	-2.278242	-2.105897
6	4.219482	1.464866	-1.015343
7	2.422050	0.158735	-0.510717
7	3.070658	2.351794	-0.806563
6	3.700587	0.118974	-0.553826

8	1.952409	1.441687	-0.923332
6	4.520084	-1.081425	-0.236003
6	3.014138	2.923837	0.548577
1	3.883394	-1.935954	-0.001646
1	5.153686	-1.334070	-1.094992
1	5.180545	-0.873562	0.614646
1	3.057159	2.169176	1.346016
1	3.853716	3.620131	0.641777
1	2.081532	3.482299	0.638615
17	0.726700	-0.107040	2.057210
7	-0.405584	-2.477438	0.429485
6	-1.239976	-3.224911	0.699405
6	-2.296006	-4.168801	1.035865
1	-2.077042	-4.646994	1.995567
1	-2.368481	-4.937065	0.260009
1	-3.253355	-3.643712	1.110371
1	5.090412	1.810607	-0.451213
1	4.486040	1.413861	-2.080401

P(5-Pt^{IV})O (no)

Pt	-0.612360	-0.054716	0.163717
Cl	-0.510554	-2.135834	1.343566
Cl	-0.653912	-1.224845	-1.927661
O	3.534810	0.595079	-0.100883
N	1.420317	-0.012699	0.063718
N	3.500227	-0.787092	-0.633441
C	2.268792	0.964126	0.140837
C	2.210401	-1.257474	-0.128823
H	2.324943	-1.744406	0.842147
C	2.086781	2.402431	0.467743
C	3.551304	-0.643241	-2.094692
H	1.723293	-1.926728	-0.836779
H	1.184680	2.557998	1.056038
H	2.970248	2.742054	1.015999
H	2.010449	2.974931	-0.461866
H	2.696602	-0.095238	-2.514588
H	4.485508	-0.142126	-2.355195
H	3.569892	-1.655753	-2.507872
Cl	-0.629452	1.095579	2.259691
Cl	-0.820662	2.001085	-1.043072
N	-2.617091	-0.156321	0.239602
C	-3.762960	-0.220039	0.285920
C	-5.213893	-0.301981	0.345456
H	-5.572872	-1.009703	-0.407806
H	-5.645904	0.684215	0.150828
H	-5.521711	-0.642873	1.338540

P(5-Pt^{IV})M (8i)

Pt	0.810767	-0.164017	-0.156671
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Cl	0.564404	-1.335894	-2.236493
C	5.089813	-0.409469	-0.501249
N	2.836785	-0.191242	-0.310301
N	4.825107	0.814296	0.252114
C	3.727153	-1.077574	-0.569305
O	3.459791	1.084904	-0.088712
C	3.537058	-2.512465	-0.907597
C	4.897337	0.640222	1.711908
H	2.499134	-2.756847	-1.119112
H	4.159899	-2.749930	-1.778948
H	3.889329	-3.127991	-0.070927
H	4.285441	-0.192191	2.086272
H	5.949121	0.475181	1.965378
H	4.559944	1.567234	2.175960
Cl	0.957104	1.010265	1.917900
N	-1.177468	-0.120178	0.010178
C	-2.321175	-0.082744	0.103149
C	-3.769834	-0.031318	0.218687
H	-4.097311	-0.683177	1.034109
H	-4.224672	-0.365913	-0.718496
H	-4.083762	0.995886	0.427283
H	5.843513	-1.029130	-0.007973
H	5.429231	-0.178313	-1.520634
Cl	0.830773	-2.227538	1.075733
Cl	0.693946	1.894892	-1.354594

P(6-L)O (no)

8	1.041989	-0.192205	0.307488
7	-1.071484	0.252044	-0.346215
8	0.996696	1.256244	0.075362
6	-0.234180	-0.609044	0.068096
6	-0.337490	1.488999	-0.464974
1	-0.258421	1.796856	-1.518199
6	-0.462681	-2.062048	0.326891
1	-0.796371	2.293805	0.123052
1	-1.497577	-2.307649	0.086453
1	0.211094	-2.668298	-0.287509
1	-0.261713	-2.298784	1.376829

P(6-L)M (no)

6	0.827134	0.854475	0.007574
7	-0.942061	-0.623885	0.013605
8	-0.346166	1.623896	0.120703
6	0.331852	-0.582445	-0.055087
8	-1.495358	0.578561	0.120010
6	1.201447	-1.787076	-0.179245
1	0.593301	-2.693919	-0.202858
1	1.802661	-1.741390	-1.096094
1	1.900051	-1.852582	0.664460

1	1.483491	1.006789	0.880452
1	1.384514	1.118923	-0.906352

P(6-Pt^{II})O (13i)

78	-0.385613	-0.025577	-0.042849
17	-0.352241	2.289840	-0.548726
17	-0.395853	-2.344043	0.441171
8	3.804435	0.187249	0.198428
7	1.637520	-0.102507	-0.148901
8	3.679860	-0.968094	-0.703503
6	2.542383	0.503860	0.533689
6	2.319600	-0.908523	-1.161000
1	2.244462	-0.415864	-2.140093
6	2.391299	1.485140	1.641181
1	1.929795	-1.927876	-1.184543
1	1.483096	2.069548	1.486144
1	3.264588	2.141008	1.677308
1	2.322062	0.943192	2.591387
7	-2.355176	0.011453	0.034865
6	-3.507082	0.024527	0.071872
6	-4.962339	0.038774	0.114664
1	-5.356034	0.531388	-0.779803
1	-5.304259	0.583109	1.000379
1	-5.342255	-0.986604	0.156253

P(6-Pt^{II})M (15i)

Pt	-0.568007	0.114997	-0.012866
Cl	-0.522953	-0.056983	2.349658
O	2.026951	1.342875	-0.130748
N	1.445910	0.085922	-0.028566
O	3.457870	1.087695	-0.395944
C	2.321234	-0.838789	0.100032
C	3.691099	-0.210101	0.135434
H	4.077165	-0.181701	1.168942
C	2.010972	-2.282896	0.264621
H	4.414932	-0.710131	-0.516688
H	0.932316	-2.447381	0.260008
H	2.471499	-2.861110	-0.545290
H	2.423123	-2.646506	1.213926
Cl	-0.591839	0.200807	-2.373558
N	-2.536605	0.148843	0.010369
C	-3.688065	0.183770	0.019385
C	-5.142793	0.232794	0.030321
H	-5.489687	0.754145	0.927761
H	-5.549911	-0.783061	0.027572
H	-5.502227	0.764206	-0.856197

P(6-Pt^{IV})O (10i)

Pt	-0.433268	0.070142	-0.036227
Cl	-0.415879	1.684612	-1.805216

Cl	-0.421471	1.833739	1.580253
O	3.741414	-0.429621	0.156117
N	1.604634	0.080348	-0.016421
O	3.646602	1.032439	0.274138
C	2.472133	-0.863305	0.147961
C	2.363654	1.318804	-0.279919
H	2.410462	1.496134	-1.359677
C	2.328697	-2.332700	0.316631
H	1.948263	2.168601	0.261327
H	1.401996	-2.679775	-0.136821
H	3.192847	-2.822597	-0.141148
H	2.317127	-2.564553	1.386151
Cl	-0.489363	-1.679106	-1.669507
Cl	-0.547367	-1.514217	1.750349
N	-2.433310	0.119035	-0.053733
C	-3.581296	0.150624	-0.060055
C	-5.035002	0.191581	-0.066893
H	-5.378681	1.092127	0.450887
H	-5.429175	-0.692430	0.443343
H	-5.397179	0.206235	-1.099242

P(6-Pt^{IV})M (14i)

78	-0.312758	0.054546	0.001860
17	-0.327439	-0.780901	2.254682
8	2.294549	1.199991	-0.506266
7	1.730334	0.000491	-0.048868
8	3.660156	0.842634	-0.880225
6	2.634841	-0.857874	0.254425
6	3.981080	-0.216654	0.007297
1	4.414872	0.136846	0.958271
6	2.468058	-2.228787	0.799994
1	4.686282	-0.877088	-0.505455
1	1.450997	-2.420985	1.132902
1	2.738937	-2.956282	0.025044
1	3.163909	-2.358246	1.638082
17	-0.385040	0.897240	-2.226700
7	-2.296054	0.120367	0.043946
6	-3.442907	0.166281	0.061287
6	-4.895430	0.227140	0.081147
1	-5.232780	0.623891	1.043391
1	-5.306775	-0.776517	-0.062466
1	-5.244622	0.881006	-0.723700
17	-0.270728	2.276391	0.872828
17	-0.453683	-2.171250	-0.886087

P(7-L)exex (no)

7	0.891227	-0.003038	0.512215
7	-1.333377	0.207627	0.066637
7	0.802407	0.709551	-0.742352

6	-0.457335	-0.305586	0.847192
7	-0.629407	0.964625	-0.922741
6	-0.765059	-1.174524	2.020515
6	1.207624	-0.217325	-1.809709
1	-1.845073	-1.226955	2.169806
1	-0.299661	-0.774584	2.930758
1	-0.368906	-2.185249	1.871164
1	0.610841	-1.140431	-1.819593
1	2.261020	-0.467711	-1.660154
1	1.085819	0.299085	-2.764560
1	1.336396	0.581569	1.223803
1	-0.807767	1.947527	-0.695527

P(7-L)exen (no)

7	3.285566	-0.366639	0.520275
7	1.124103	0.020172	0.021113
7	3.236424	1.034405	0.116516
6	2.024099	-0.881399	0.175703
7	1.814760	1.298263	0.174770
6	1.771205	-2.352266	0.122189
6	3.658904	1.173634	-1.289457
1	0.705906	-2.534075	-0.030360
1	2.086498	-2.825908	1.059059
1	2.330861	-2.825948	-0.694080
1	3.095268	0.525397	-1.976640
1	4.727702	0.942709	-1.354348
1	3.506978	2.216472	-1.573878
1	4.106464	-0.837605	0.151169
1	1.625953	1.580608	1.141189

P(7-L)enen (no)

7	3.687722	-0.188267	0.445358
7	1.459008	0.013481	0.299345
7	3.457096	1.226785	0.197840
6	2.438342	-0.808088	0.198699
7	2.066016	1.258040	0.673908
6	2.319488	-2.278527	-0.017338
6	3.525920	1.507587	-1.259823
1	1.266308	-2.551461	-0.106509
1	2.756477	-2.826993	0.826073
1	2.846796	-2.595122	-0.926279
1	2.856204	0.876024	-1.861545
1	4.561532	1.366401	-1.586960
1	3.273309	2.562229	-1.408381
1	4.481106	-0.525544	-0.093329
1	1.585298	2.007804	0.175669

P(7-Pt^{II})exex (15i)

78	-0.559268	0.023549	-0.004538
17	-0.606462	2.368901	0.407050

17	-0.454358	-2.309521	-0.374361
7	3.609071	0.008898	0.612034
7	1.447782	0.131463	0.098764
7	3.533370	0.699437	-0.659989
6	2.302424	-0.345993	0.941450
7	2.133208	0.963388	-0.857832
6	1.997012	-1.197090	2.122637
6	3.969864	-0.243435	-1.705455
1	0.927406	-1.183136	2.333025
1	2.552002	-0.832503	2.995317
1	2.308283	-2.229053	1.930837
1	3.372761	-1.165142	-1.716719
1	5.019213	-0.485051	-1.520642
1	3.873248	0.264655	-2.666616
7	-2.529859	-0.033502	-0.118180
6	-3.679405	-0.064589	-0.198071
6	-5.131144	-0.104216	-0.302466
1	-5.518819	0.903869	-0.478473
1	-5.561892	-0.495471	0.624443
1	-5.426762	-0.752187	-1.133405
1	4.095668	0.549923	1.327651
1	1.908269	1.921967	-0.569295

P(7-Pt^{II})_{exen} (15i)

Pt	-0.814484	0.027186	0.049857
Cl	-0.798928	0.952600	2.239935
Cl	-0.777720	-0.940413	-2.114388
N	3.323566	-0.394670	0.427193
N	1.195757	0.045814	0.104345
N	3.272335	1.019588	0.083962
C	2.070925	-0.907384	0.181592
N	1.891808	1.316584	0.296592
C	1.775260	-2.367125	0.132641
C	3.578442	1.202256	-1.350201
H	0.947739	-2.542870	-0.558452
H	1.475687	-2.713610	1.128208
H	2.651421	-2.938330	-0.187734
H	2.936062	0.599284	-2.006475
H	4.630044	0.943388	-1.509627
H	3.436717	2.260299	-1.574996
N	-2.788850	0.042255	0.024914
C	-3.941388	0.064991	0.009507
C	-5.396993	0.095903	-0.011554
H	-5.757235	0.989167	0.508003
H	-5.797310	-0.791775	0.488064
H	-5.754123	0.114473	-1.045839
H	4.151825	-0.878879	0.102874
H	1.763102	1.523475	1.293299

P(7-Pt^{II})enen (15i)

78	-0.544875	-0.039679	0.067996
17	-0.744790	-1.833205	1.592287
17	-0.362947	1.793941	-1.445314
7	3.639760	-0.187156	0.452955
7	1.463988	0.040392	0.295138
7	3.437166	1.223688	0.189473
6	2.426503	-0.819539	0.209047
7	2.075387	1.303120	0.684872
6	2.326868	-2.283863	-0.034553
6	3.523007	1.495557	-1.270589
1	1.284239	-2.599830	-0.038005
1	2.852376	-2.824197	0.760830
1	2.798644	-2.541606	-0.990859
1	2.833417	0.892921	-1.875946
1	4.557665	1.317296	-1.580729
1	3.303616	2.555978	-1.419319
7	-2.501675	-0.063007	-0.177456
6	-3.646194	-0.068849	-0.314291
6	-5.092234	-0.073806	-0.484066
1	-5.578737	0.192397	0.459504
1	-5.428366	-1.069769	-0.788611
1	-5.379109	0.651437	-1.251656
1	4.478162	-0.556128	0.018574
1	1.579824	2.027716	0.155839

P(7-Pt^{IV})exex (13i)

Pt	-0.613680	-0.030219	-0.127057
Cl	-0.596153	1.622624	-1.867047
Cl	-0.752862	1.663372	1.544421
N	3.582882	-0.289314	0.197393
N	1.416830	0.037973	-0.068758
N	3.392421	1.143694	0.235835
C	2.337920	-0.871223	0.079054
N	2.045121	1.334898	-0.186457
C	2.201943	-2.350301	0.170859
C	3.513293	1.580519	1.640090
H	1.306736	-2.699463	-0.340051
H	3.092353	-2.813322	-0.269264
H	2.150844	-2.644486	1.223692
H	2.795318	1.076663	2.299481
H	4.534203	1.369649	1.967396
H	3.332330	2.656199	1.662064
Cl	-0.573750	-1.730274	-1.828546
Cl	-0.715260	-1.675407	1.605619
N	-2.619385	-0.048582	-0.211488
C	-3.766841	-0.049065	-0.258996
C	-5.220063	-0.047574	-0.318290

H	-5.607987	0.822092	0.220561
H	-5.607654	-0.961266	0.142162
H	-5.545246	-0.001728	-1.361962
H	4.309497	-0.610404	-0.440370
H	2.009684	1.559837	-1.184273

P(7-Pt^{IV})exen (no)

78	-0.453903	0.021965	0.024451
17	-0.532191	2.047456	1.300561
17	-0.440502	-1.997671	-1.267663
7	3.691396	-0.304024	0.560636
7	1.566201	0.031212	0.198165
7	3.629386	0.942981	-0.173989
6	2.451047	-0.869917	0.537645
7	2.267502	1.299379	-0.000443
6	2.237361	-2.289028	0.936440
6	3.894008	0.703243	-1.608759
1	1.405385	-2.714595	0.374758
1	1.979731	-2.331145	1.998548
1	3.145523	-2.872593	0.758977
1	3.231587	-0.055256	-2.045730
1	4.940156	0.399376	-1.713632
1	3.743939	1.653902	-2.121608
7	-2.454157	0.071160	-0.135082
6	-3.598629	0.109397	-0.222446
6	-5.048103	0.159921	-0.331716
1	-5.374604	1.202205	-0.396404
1	-5.499456	-0.306733	0.548981
1	-5.368368	-0.376065	-1.230164
1	4.538316	-0.848884	0.468975
1	2.176459	1.788836	0.894564
17	-0.323918	1.259343	-2.010536
17	-0.705190	-1.216127	2.068436

P(7-Pt^{IV})enen (11i)

Pt	-0.602685	-0.053564	0.125015
Cl	-0.698150	0.326620	2.476752
Cl	-0.581463	-0.391883	-2.255025
N	3.566490	-0.453427	-0.029961
N	1.423242	-0.147606	0.200870
N	3.430151	0.949940	0.281646
C	2.312837	-0.942764	-0.319889
N	2.173244	0.841723	0.978702
C	2.122579	-2.243022	-1.018896
C	3.341524	1.751512	-0.970573
H	1.203652	-2.232080	-1.604555
H	2.045855	-3.045464	-0.278463
H	2.976181	-2.443072	-1.673785
H	2.544555	1.422753	-1.649576

H	4.314106	1.692797	-1.468962
H	3.171268	2.790854	-0.679367
N	-2.603414	0.095200	0.056041
C	-3.748452	0.178669	0.023911
C	-5.198518	0.284278	-0.014839
H	-5.541091	0.928185	0.800751
H	-5.641705	-0.709671	0.098337
H	-5.511023	0.713675	-0.971422
H	4.355845	-0.685285	-0.619123
H	1.666829	1.728155	0.894984
Cl	-0.847695	-2.392084	0.514811
Cl	-0.439984	2.317963	-0.248800

P(8-L)ex (no)

7	1.143112	-0.064952	-0.100064
7	-1.100825	0.221628	0.173075
8	0.876869	1.323764	-0.219260
6	-0.177695	-0.634428	-0.037986
7	-0.505255	1.468348	0.378493
6	-0.362398	-2.104764	-0.177309
1	0.009398	-2.444953	-1.149894
1	-1.419656	-2.357129	-0.077844
1	0.202612	-2.644099	0.594346
1	1.596916	-0.195567	0.817738
1	-0.922885	2.111627	-0.299025

P(8-L)en (no)

7	1.134827	0.009991	-0.138105
7	-1.120560	-0.165846	0.144220
8	0.797068	-1.368120	-0.296364
6	-0.139442	0.640463	0.003413
7	-0.640416	-1.483062	0.079901
6	-0.234294	2.127565	-0.004856
1	-1.257711	2.433960	0.218076
1	0.440741	2.563262	0.742699
1	0.061626	2.525173	-0.981792
1	1.659599	0.115995	0.744821
1	-0.655346	-1.829179	1.053659

P(8-Pt^{II})ex (no)

78	-0.381093	0.051036	0.035809
17	-0.380697	-1.248944	2.010100
17	-0.374423	1.395588	-1.923738
7	3.849936	-0.258746	-0.170924
7	1.643382	0.079766	-0.017040
8	3.573294	1.056927	-0.632629
6	2.555096	-0.827771	-0.025335
7	2.269577	1.366360	-0.031161
6	2.390539	-2.297778	0.089429
1	2.707918	-2.768019	-0.848108

1	1.357435	-2.554964	0.319898
1	3.037720	-2.682614	0.887129
7	-2.352102	0.061405	0.057419
6	-3.504223	0.077085	0.070113
6	-4.959674	0.100622	0.087988
1	-5.314528	0.352357	1.092175
1	-5.351647	-0.881854	-0.192729
1	-5.327204	0.848702	-0.621045
1	4.301155	-0.173191	0.752948
1	1.799122	1.875984	-0.791731

P(8-Pt^{II})en (no)

Pt	-0.578931	-0.056829	-0.053757
Cl	-0.494851	-1.344745	1.951347
N	3.645454	0.050230	0.067428
N	1.432739	-0.211545	-0.123424
O	3.392026	-1.306380	-0.336063
C	2.376164	0.649276	0.044241
N	1.974678	-1.534005	-0.177005
C	2.226129	2.118889	0.203569
H	1.174984	2.380764	0.323413
H	2.797646	2.459083	1.075579
H	2.626761	2.626071	-0.680145
Cl	-0.606761	1.263915	-2.008050
N	-2.544164	0.049186	0.048587
C	-3.694557	0.100918	0.094068
C	-5.148023	0.165762	0.146090
H	-5.564192	-0.845938	0.176996
H	-5.527536	0.682264	-0.740889
H	-5.466181	0.709286	1.041095
H	4.047652	0.062207	1.015729
H	1.803591	-1.911810	0.771397

P(8-Pt^{IV})ex (15i)

Pt	-0.432191	0.055678	0.062722
Cl	-0.520733	-1.695768	1.683482
Cl	-0.387069	1.837439	-1.543515
N	3.788551	-0.253753	-0.242999
N	1.607433	0.066251	0.053427
O	3.502105	1.113657	-0.503443
C	2.507859	-0.842137	-0.116799
N	2.273563	1.334279	0.244703
C	2.384365	-2.318332	-0.178894
H	2.513337	-2.640407	-1.217462
H	1.420834	-2.656110	0.195437
H	3.194669	-2.763582	0.411649
N	-2.428103	0.094134	0.043528
C	-3.575992	0.119475	0.026815
C	-5.029590	0.152758	0.005658

H	-5.410692	0.183512	1.030829
H	-5.409632	-0.742081	-0.496362
H	-5.367864	1.042505	-0.533914
H	4.309335	-0.309995	0.645177
H	1.766886	2.001263	-0.353140
Cl	-0.490745	-1.528181	-1.733530
Cl	-0.464056	1.658066	1.835035

P(8-Pt^{IV})en (15i)

78	-0.313621	-0.030379	-0.010423
17	-0.409845	-1.821874	1.586040
17	-0.479509	-1.573870	-1.812969
7	3.928058	0.078241	-0.006680
7	1.720418	-0.179282	-0.023386
8	3.647200	-1.304843	-0.272164
6	2.677157	0.693992	0.006053
7	2.266809	-1.508280	0.036658
6	2.615619	2.178761	0.004894
1	1.678688	2.539934	0.422803
1	3.464824	2.568954	0.576622
1	2.714177	2.531463	-1.027135
17	-0.243408	1.517646	1.834189
17	-0.293006	1.757253	-1.593531
7	-2.306318	0.072032	0.024078
6	-3.453556	0.118748	0.033368
6	-4.906542	0.176109	0.043270
1	-5.313287	-0.827539	-0.113214
1	-5.252659	0.836134	-0.757826
1	-5.252939	0.561956	1.006718
1	4.439971	0.187661	0.879140
1	2.185298	-1.780535	1.029615

P(9-L)Oex (no)

8	3.590865	0.111766	0.655840
7	1.404026	0.178627	0.107614
7	3.515548	0.682107	-0.723041
6	2.299675	-0.235222	0.921993
7	2.125281	0.963426	-0.881306
6	2.065909	-1.037553	2.155052
6	3.880989	-0.438997	-1.601025
1	0.994511	-1.185289	2.298076
1	2.482302	-0.514666	3.022946
1	2.564178	-2.010497	2.084695
1	3.207468	-1.299524	-1.498298
1	4.906368	-0.730506	-1.365068
1	3.834330	-0.061944	-2.625244
1	1.992232	1.936480	-0.592071

P(9-L)Oen (no)

8	3.657047	0.618236	0.025750
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7	1.458226	0.264263	-0.239176
7	3.554315	-0.677363	-0.631326
6	2.354888	0.956139	0.343774
7	2.172133	-0.577870	-1.144992
6	2.167063	2.103493	1.269641
6	3.661076	-1.685533	0.444786
1	1.100832	2.288477	1.410314
1	2.635730	3.003733	0.855364
1	2.637072	1.902164	2.238460
1	2.888227	-1.577704	1.218349
1	4.652981	-1.591513	0.892103
1	3.583673	-2.669492	-0.028821
1	1.761991	-1.512767	-1.088769

P(9-L)Mex (no)

8	1.791600	1.382376	-0.193621
7	1.227302	0.101143	-0.249239
7	3.193788	1.218426	0.294143
6	2.176931	-0.750108	-0.146536
7	3.470106	-0.150889	0.027431
6	2.007981	-2.228008	-0.213746
6	3.105969	1.415708	1.748794
1	0.961720	-2.475716	-0.403409
1	2.330781	-2.696568	0.722565
1	2.621174	-2.651983	-1.019512
1	2.413445	0.715894	2.234486
1	2.776635	2.441865	1.922455
1	4.111346	1.280065	2.155886
1	4.000187	-0.203584	-0.846876

P(9-L)Men (no)

8	2.006617	1.549386	0.012582
7	1.448676	0.253042	-0.292415
7	3.382370	1.358236	0.420638
6	2.461834	-0.510364	-0.471774
7	3.692687	0.159795	-0.340021
6	2.375187	-1.938334	-0.894008
6	3.365465	1.071608	1.871988
1	1.329475	-2.215914	-1.038199
1	2.818171	-2.604782	-0.143754
1	2.916738	-2.086779	-1.835267
1	2.735001	0.211444	2.133944
1	2.993884	1.967916	2.372176
1	4.398860	0.895354	2.189995
1	4.445800	-0.363633	0.100469

P(9-Pt^{II})Oex (15i)

78	-0.554552	0.026260	-0.011209
17	-0.627884	2.377362	0.338118
17	-0.413292	-2.313917	-0.327333

8	3.583215	0.115216	0.666526
7	1.453812	0.156291	0.067002
7	3.507098	0.691944	-0.744587
6	2.325203	-0.252031	0.930867
7	2.148192	0.999676	-0.884847
6	2.066762	-1.041447	2.162256
6	3.864141	-0.448001	-1.604771
1	0.997881	-1.225313	2.268847
1	2.442062	-0.483773	3.027224
1	2.600428	-1.995537	2.112686
1	3.171546	-1.292699	-1.507066
1	4.881184	-0.749780	-1.349534
1	3.840078	-0.072270	-2.630008
7	-2.522389	-0.060947	-0.102458
6	-3.672309	-0.109312	-0.165499
6	-5.124636	-0.171310	-0.247722
1	-5.514478	0.768866	-0.649770
1	-5.548300	-0.335968	0.747882
1	-5.425146	-0.994175	-0.903624
1	1.982082	1.955933	-0.554430

P(9-Pt^{II})Oen (14i)

78	-0.547450	0.030395	-0.065680
17	-0.201273	-2.304658	0.268367
17	-0.900407	2.335468	-0.428689
8	3.615092	0.641849	-0.017694
7	1.464363	0.228255	-0.230874
7	3.527164	-0.682660	-0.644267
6	2.346767	0.969029	0.340350
7	2.172572	-0.608311	-1.172705
6	2.172258	2.100332	1.282665
6	3.661161	-1.664778	0.454191
1	1.117415	2.355511	1.376966
1	2.720134	2.969556	0.902911
1	2.595298	1.835775	2.258205
1	2.881043	-1.578911	1.220463
1	4.651681	-1.526655	0.892262
1	3.614022	-2.655166	-0.007431
7	-2.494837	-0.219476	0.091617
6	-3.634605	-0.367751	0.176467
6	-5.074599	-0.554861	0.281038
1	-5.291771	-1.533219	0.720487
1	-5.529950	-0.500015	-0.712700
1	-5.505978	0.226866	0.913813
1	1.746284	-1.539564	-1.089585

P(9-Pt^{II})Mex (15i)

Pt	-0.781102	-0.017611	-0.171458
Cl	-0.815969	0.714025	2.080437

Cl	-0.720436	-0.824239	-2.399066
O	1.796561	1.412589	-0.199947
N	1.222677	0.107408	-0.167614
N	3.157256	1.233159	0.284111
C	2.172716	-0.758386	-0.142577
N	3.432982	-0.136416	-0.021024
C	2.015846	-2.234314	-0.207460
C	3.106799	1.404101	1.747833
H	0.998182	-2.495810	-0.498823
H	2.254434	-2.677087	0.766031
H	2.717273	-2.646564	-0.942344
H	2.389543	0.731170	2.232259
H	2.824117	2.439604	1.942223
H	4.117164	1.219401	2.120683
N	-2.748762	-0.132575	-0.170074
C	-3.899742	-0.187343	-0.167620
C	-5.354040	-0.252817	-0.166406
H	-5.760618	0.541096	0.467587
H	-5.683448	-1.222059	0.220643
H	-5.732367	-0.128057	-1.185650
H	3.983414	-0.200233	-0.880531

P(9-Pt^{II})Men (15i)

78	-0.538857	-0.013563	-0.087167
17	-0.653431	-0.400843	-2.421217
17	-0.401229	0.281951	2.261403
8	1.991551	1.571524	0.031200
7	1.446178	0.245220	-0.218159
7	3.345873	1.364032	0.428330
6	2.452913	-0.519920	-0.468235
7	3.638361	0.186901	-0.367542
6	2.381251	-1.949880	-0.876437
6	3.368526	1.053825	1.876564
1	1.370531	-2.190365	-1.208947
1	2.654810	-2.602007	-0.038580
1	3.081196	-2.128663	-1.699244
1	2.713893	0.218532	2.151699
1	3.041944	1.955580	2.396404
1	4.409122	0.844526	2.145975
7	-2.487719	-0.263150	0.055113
6	-3.629340	-0.396124	0.139274
6	-5.072325	-0.558189	0.243656
1	-5.526413	-0.492825	-0.749848
1	-5.488698	0.228189	0.880787
1	-5.308349	-1.533009	0.681573
1	4.474616	-0.302330	-0.066675

P(9-Pt^{IV})Oex (13i)

78	-0.447292	-0.020355	-0.082562
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17	-0.510733	1.601990	-1.845028
17	-0.526596	1.704468	1.563501
8	3.752480	-0.283021	0.026376
7	1.581548	0.079891	-0.089498
7	3.512976	1.226236	0.173054
6	2.530293	-0.807656	0.013382
7	2.210954	1.368364	-0.283637
6	2.445094	-2.287138	0.122513
6	3.596100	1.454775	1.624806
1	1.503087	-2.657268	-0.276177
1	3.291657	-2.715582	-0.421934
1	2.530129	-2.571983	1.176136
1	2.831994	0.911982	2.192603
1	4.599143	1.169903	1.945921
1	3.455184	2.528566	1.765053
17	-0.449042	-1.750197	-1.748334
17	-0.446397	-1.637344	1.680747
7	-2.448080	-0.064832	-0.086899
6	-3.596327	-0.080588	-0.092571
6	-5.050492	-0.098845	-0.101775
1	-5.431519	0.773174	0.438192
1	-5.409662	-1.011138	0.383823
1	-5.411116	-0.071782	-1.134439
1	2.217280	1.523502	-1.294693

P(9-Pt^{IV})Oen (4i)

Pt	-0.604529	0.142798	0.051793
Cl	-0.405507	-0.438551	-2.273433
Cl	-0.866224	0.747497	2.342010
O	3.559520	-0.167666	0.479015
N	1.427456	0.211115	0.155389
N	3.426932	0.216713	-0.933468
C	2.299027	-0.323740	0.944356
N	2.180247	0.938546	-0.849442
C	2.153909	-1.018348	2.245158
C	3.338441	-1.048349	-1.697555
H	1.148794	-0.899638	2.643025
H	2.887410	-0.595354	2.940426
H	2.378490	-2.081729	2.114453
H	2.490467	-1.681017	-1.409671
H	4.283196	-1.576208	-1.553390
H	3.248320	-0.765970	-2.750101
N	-2.596653	0.069408	-0.108960
C	-3.740919	0.034786	-0.200213
C	-5.190021	-0.006701	-0.315181
H	-5.473203	-0.622118	-1.174366
H	-5.575473	1.008027	-0.452981
H	-5.618031	-0.436473	0.595465

H	1.674900	0.830680	-1.736252
Cl	-0.588460	-2.189482	0.611025
Cl	-0.684985	2.451972	-0.543428

P(9-Pt^{IV})Mex (15i)

Pt	-0.589410	-0.073235	-0.167687
Cl	-0.766309	1.897230	1.168964
Cl	-0.498728	-2.055172	-1.518756
O	2.004323	1.316196	-0.437849
N	1.437232	0.043719	-0.099403
N	3.281375	1.333058	0.223436
C	2.398368	-0.754788	0.233236
N	3.608135	-0.056523	0.318554
C	2.346497	-2.210653	0.524557
C	3.076248	1.878157	1.578531
H	1.441456	-2.663644	0.125348
H	2.386972	-2.364202	1.607525
H	3.230574	-2.685126	0.081993
H	2.339881	1.311965	2.160510
H	2.739641	2.908901	1.462848
H	4.049680	1.856917	2.074444
N	-2.580384	-0.164834	-0.233399
C	-3.726818	-0.207406	-0.278826
C	-5.178791	-0.258854	-0.339523
H	-5.587837	0.741905	-0.171146
H	-5.555385	-0.938812	0.430472
H	-5.491845	-0.617180	-1.324810
H	4.298727	-0.329736	-0.382487
Cl	-0.640945	1.236879	-2.160510
Cl	-0.623111	-1.384760	1.844671

P(9-Pt^{IV})Men (no)

78	0.538099	0.181193	-0.259241
17	0.338260	-1.889176	-1.454866
17	0.645651	2.246876	0.936757
8	3.233205	1.340731	-0.824771
7	2.558767	0.127933	-0.382530
7	4.510622	1.305220	-0.208889
6	3.493702	-0.720252	-0.078718
7	4.719699	-0.123272	-0.228398
6	3.358316	-2.147220	0.325097
6	4.401498	1.814802	1.177535
1	2.417815	-2.561448	-0.035912
1	3.380449	-2.228045	1.416447
1	4.197665	-2.711224	-0.094950
1	3.669030	1.268048	1.782581
1	4.107567	2.862388	1.103982
1	5.399740	1.750720	1.622347
7	-1.452296	0.257102	-0.136054

6	-2.597632	0.308003	-0.073126
6	-4.048324	0.374554	0.003430
1	-4.486150	-0.276105	-0.759533
1	-4.376874	1.404241	-0.166938
1	-4.380171	0.047307	0.993298
1	5.523651	-0.452764	0.292032
17	0.406541	1.354912	-2.328548
17	0.601033	-0.985133	1.843930

P(10-L)O_{acyc} (no)

8	1.752246	0.978811	-0.217226
7	-0.160216	0.396251	-1.345839
8	-1.634209	0.502957	0.389843
6	0.919713	0.128692	-0.410229
7	-1.297322	0.539359	-0.809713
6	0.960446	-1.281667	0.123576
1	0.030903	-1.506174	0.656307
1	1.056434	-1.989936	-0.707948
1	1.813198	-1.387649	0.796634
1	-2.045921	0.729777	-1.496494

P(10-L)M_{acyc} (no)

8	-1.271483	1.374616	0.163225
7	-1.294741	0.144632	0.209945
8	1.373232	1.303234	-0.273222
6	-0.064647	-0.521533	0.028863
7	1.102600	0.087463	-0.185968
6	-0.103739	-2.019127	0.087289
1	-0.769751	-2.421766	-0.683721
1	0.889693	-2.456678	-0.061544
1	-0.482484	-2.361309	1.056598
1	1.903853	-0.563756	-0.296103

P(10-Pt^{II})O (no)

Pt	-0.580470	0.019443	-0.049550
Cl	-0.572445	-1.740150	-1.624439
Cl	-0.585918	1.807765	1.520165
N	-2.537527	-0.128131	0.082511
C	-3.684982	-0.204964	0.154607
C	-5.134903	-0.299957	0.242876
H	-5.416725	-0.911229	1.105822
H	-5.532386	-0.760201	-0.666900
H	-5.565407	0.699560	0.357775
O	3.632160	0.036705	-0.034427
N	1.437715	0.222205	-0.153883
O	3.313860	1.457151	0.122899
C	2.428748	-0.577098	0.007867
N	1.950835	1.533551	-0.436030
C	2.439136	-2.047326	0.208354
H	1.449412	-2.454933	0.003491

H	3.167442	-2.499548	-0.472693
H	2.746107	-2.271417	1.235822
H	1.478857	2.130197	0.263032

P(10-Pt^{II})O_{acyc} (7i)

78	-0.365750	0.073569	0.014367
17	-0.637213	1.607437	1.830069
17	-0.134826	-1.484179	-1.736619
8	3.043133	0.163739	-1.509552
7	1.647191	0.028561	0.337787
8	3.361009	0.552876	1.691428
6	2.675127	-0.538508	-0.616798
7	2.163713	0.547759	1.391946
6	3.086282	-1.941598	-0.297540
1	3.485732	-1.985105	0.721613
1	3.846069	-2.262911	-1.012180
1	2.209406	-2.593712	-0.360905
7	-2.308394	0.109668	-0.308157
6	-3.443940	0.134755	-0.503080
6	-4.877754	0.166511	-0.751822
1	-5.397242	0.568499	0.123370
1	-5.241789	-0.845710	-0.953016
1	-5.090499	0.801218	-1.617695
1	1.452503	1.022134	1.998910

P(10-Pt^{II})M (no)

78	-0.385516	0.015467	-0.150082
17	-0.357875	0.013181	-2.511947
17	-0.400918	-0.059408	2.219367
7	-2.347244	-0.126713	-0.177698
6	-3.496884	-0.197370	-0.200864
6	-4.949635	-0.283232	-0.230783
1	-5.283664	-1.144745	0.355580
1	-5.293388	-0.396113	-1.263495
1	-5.384063	0.626901	0.194349
8	2.151847	1.417905	-0.513888
7	1.621398	0.165651	-0.125573
8	3.561495	1.129707	-0.796318
6	2.585632	-0.594436	0.249858
7	3.824196	0.048112	0.138762
6	2.454270	-1.964020	0.813699
1	1.403609	-2.183454	1.005557
1	2.864512	-2.704687	0.117064
1	3.010603	-2.023313	1.754805
1	4.516828	-0.526949	-0.346061

P(10-Pt^{IV})O (12i)

78	0.995782	0.225330	-0.023016
17	0.941146	-1.493555	-1.676134
17	1.022193	1.973778	1.622543

7	-0.994542	0.275272	-0.053686
6	-2.142368	0.305369	-0.067568
6	-3.595811	0.344385	-0.085012
1	-3.989426	-0.300990	0.706064
1	-3.960268	-0.006648	-1.055149
1	-3.936689	1.370819	0.080751
8	5.161815	-0.184979	0.383692
7	3.034122	0.226302	0.043609
8	4.924857	1.220343	0.711044
6	3.920337	-0.690738	0.224727
7	3.730065	1.488820	-0.086517
6	3.820613	-2.169738	0.238079
1	2.877609	-2.493174	-0.198279
1	4.663250	-2.576587	-0.331075
1	3.893752	-2.523399	1.271239
1	3.210876	2.130906	0.534018
17	0.888878	-1.399518	1.735551
17	1.027910	1.865860	-1.756601

P(10-Pt^{IV})O_{acvc} (13i)

78	-0.299648	0.076449	0.005285
17	-0.187077	1.544526	-1.867141
17	-0.460007	1.990272	1.469868
8	3.149181	-0.640509	-1.564383
7	1.741635	0.087954	0.149877
8	3.543612	1.107016	0.989861
6	2.687382	-0.926569	-0.506107
7	2.333120	1.017585	0.805413
6	2.904541	-2.137674	0.340044
1	1.943709	-2.566349	0.638866
1	3.500693	-2.861004	-0.219019
1	3.437944	-1.839250	1.251216
17	-0.189264	-1.806265	-1.436027
17	-0.402953	-1.375769	1.909937
7	-2.291774	0.042541	-0.143995
6	-3.436686	0.026692	-0.235483
6	-4.885801	0.006110	-0.353734
1	-5.316946	0.780821	0.287514
1	-5.265132	-0.972797	-0.045370
1	-5.170821	0.195321	-1.393101
1	1.671378	1.723294	1.213602

P(10-Pt^{IV})M (no)

78	-0.317282	0.027145	-0.008266
17	-0.166574	-1.635876	-1.738294
17	-0.545853	1.681599	1.693469
7	-2.295057	-0.092726	-0.109943
6	-3.440176	-0.149961	-0.166630
6	-4.890702	-0.219695	-0.237520

1	-5.259405	-0.945543	0.493482
1	-5.194690	-0.529037	-1.242033
1	-5.314804	0.764591	-0.017085
8	2.217413	1.497080	0.247062
7	1.710304	0.172942	0.098640
8	3.584764	1.370925	-0.216720
6	2.705562	-0.647655	0.158718
7	3.904231	0.048030	0.282726
6	2.680997	-2.133910	0.208998
1	1.750069	-2.512963	-0.210297
1	3.533216	-2.540322	-0.344640
1	2.751270	-2.450488	1.254961
1	4.639830	-0.293642	-0.336948
17	-0.332600	-1.675103	1.684431
17	-0.375288	1.715007	-1.691180

P(11-L) (no)

8	0.885716	-0.395092	0.380343
7	-1.317885	-0.048804	0.140651
7	0.708603	1.049768	0.412267
6	-0.356162	-0.885049	0.070937
8	-0.723443	1.165702	0.606651
6	-0.460118	-2.327519	-0.272317
6	1.005776	1.530800	-0.949937
1	-1.506776	-2.592193	-0.430659
1	-0.053418	-2.933766	0.544589
1	0.116586	-2.552844	-1.175705
1	0.396107	1.038993	-1.716626
1	2.068311	1.353761	-1.132512
1	0.808996	2.605023	-0.947571

P(11-Pt^H) (15i)

Pt	-0.800685	-0.005929	-0.043961
Cl	-1.359936	-1.512694	1.693868
Cl	-0.208715	1.436811	-1.828270
O	3.256444	-0.389357	0.936353
N	1.117375	-0.016575	0.554872
N	3.083051	1.076299	0.915538
C	2.061779	-0.888042	0.559426
O	1.679513	1.190605	1.109583
C	1.965661	-2.327388	0.213630
C	3.419606	1.514285	-0.453342
H	0.918654	-2.625491	0.153693
H	2.469888	-2.911360	0.990277
H	2.470410	-2.517112	-0.739907
H	2.788832	1.054038	-1.220846
H	4.475393	1.281365	-0.607792
H	3.275213	2.596451	-0.463024
N	-2.675402	0.012929	-0.642470

C	-3.773717	0.034325	-0.990197
C	-5.162049	0.064349	-1.426868
H	-5.823765	0.124492	-0.557313
H	-5.395227	-0.844523	-1.990163
H	-5.330501	0.935157	-2.067763

P(11-Pt^{IV}) (15i)

78	-0.450288	-0.024153	-0.034670
17	-0.904548	1.462680	-1.840621
17	-0.223601	1.823691	1.463239
8	3.717490	-0.192650	-0.541355
7	1.539432	0.047230	-0.433494
7	3.454677	1.250430	-0.357711
6	2.522568	-0.791105	-0.406391
8	2.106143	1.328175	-0.768598
6	2.513663	-2.267748	-0.270009
6	3.558575	1.510407	1.091287
1	1.516258	-2.666643	-0.443519
1	3.221015	-2.676130	-0.999426
1	2.852946	-2.540397	0.734135
1	2.880746	0.895386	1.691819
1	4.601117	1.335727	1.365386
1	3.311962	2.565785	1.220739
17	-0.752601	-1.879064	-1.522237
17	-0.049986	-1.512250	1.809754
7	-2.397946	-0.072399	0.366899
6	-3.523665	-0.092516	0.591562
6	-4.949921	-0.116034	0.873490
1	-5.232167	0.794720	1.410200
1	-5.188587	-0.988612	1.488927
1	-5.507860	-0.170935	-0.066145

P(12-L) (no)

8	3.620886	-0.398275	-0.157876
7	1.452360	0.039212	0.195754
8	3.539861	1.037059	-0.002914
6	2.335722	-0.850889	-0.019979
8	2.027774	1.267164	0.237585
6	2.127196	-2.317429	-0.138704
1	1.067723	-2.540218	-0.003486
1	2.711376	-2.847238	0.620905
1	2.450752	-2.668930	-1.124034

P(12-Pt^{II}) (2i)

Pt	-0.566243	0.127881	0.017339
Cl	-0.646386	-1.254470	1.943877
Cl	-0.485652	1.457064	-1.930327
O	3.605072	-0.412711	0.083637
N	1.444961	0.062502	0.060299
O	3.445951	1.025829	-0.180902

C	2.333082	-0.862869	-0.008582
O	2.128622	1.281523	0.345407
C	2.124093	-2.323878	-0.150407
H	1.079442	-2.564571	0.047910
H	2.762404	-2.846112	0.569563
H	2.410024	-2.639255	-1.159673
N	-2.530285	0.195753	-0.028137
C	-3.680528	0.249980	-0.058714
C	-5.133689	0.322752	-0.097124
H	-5.524442	0.483434	0.912369
H	-5.542574	-0.611709	-0.493747
H	-5.445488	1.151428	-0.740175

P(12-Pt^{IV}) (8i)

78	-0.314205	0.063800	-0.020654
17	-0.303546	1.797672	-1.659042
17	-0.223430	1.684407	1.724374
8	3.875081	-0.445768	0.038644
7	1.719967	-0.008061	-0.062040
8	3.648228	0.963470	0.421177
6	2.620131	-0.931369	-0.008890
8	2.407111	1.234945	-0.225652
6	2.480676	-2.407319	-0.018952
1	1.502695	-2.693838	-0.402313
1	3.276669	-2.819713	-0.647721
1	2.607900	-2.783123	1.001247
17	-0.457092	-1.564961	-1.779961
17	-0.381670	-1.671501	1.635109
7	-2.291618	0.156380	0.030302
6	-3.437149	0.220172	0.068978
6	-4.887717	0.303588	0.119366
1	-5.182973	1.166547	0.723890
1	-5.292098	-0.608971	0.567621
1	-5.284063	0.417330	-0.894104

TS(1-L) (272i)

6	1.201155	0.211175	-0.293520
7	-1.572439	-0.474964	-0.629114
7	0.472771	1.124511	0.424610
6	-0.581657	-1.125734	-0.680238
6	-0.544971	1.790728	-0.093285
6	0.070744	-2.434658	-0.923263
6	0.497792	0.969166	1.887116
1	-0.673201	-3.189577	-1.204034
1	0.811100	-2.351910	-1.725696
1	0.598356	-2.772946	-0.025743
1	-0.129330	0.117916	2.168045
1	1.525119	0.798925	2.214333
1	0.118444	1.878548	2.355639

1	2.075317	-0.182171	0.215997
1	1.333788	0.453059	-1.342987
1	-1.202581	2.344812	0.559879
1	-0.617702	1.892451	-1.164772

TS(1-Pt^{II})₁ (26i; 15i)

C	3.777007	1.363191	-0.188599
N	1.319678	-0.983959	-0.286241
N	2.681227	1.935723	0.373094
C	2.428152	-1.296517	-0.380151
C	1.596720	2.379572	-0.245816
C	3.723637	-1.951503	-0.524207
C	2.630327	1.947171	1.854450
H	3.585251	-3.039268	-0.510094
H	4.183575	-1.657895	-1.471423
H	4.384758	-1.650641	0.290754
H	1.965426	1.148696	2.193368
H	3.634569	1.801778	2.251382
H	2.242118	2.912327	2.184902
H	4.680369	1.370381	0.407218
H	3.861256	1.452877	-1.265921
H	0.742606	2.674505	0.343713
H	1.553763	2.349124	-1.325652
Pt	-0.539216	-0.370544	-0.102421
Cl	-0.748807	-0.281424	-2.460700
Cl	-0.343678	-0.469482	2.268046
N	-2.407158	0.199566	0.077191
C	-3.510554	0.517133	0.178418
C	-4.906484	0.910243	0.306155
H	-5.003081	1.994601	0.193335
H	-5.285522	0.618622	1.290498
H	-5.503035	0.417649	-0.467953

TS(1-Pt^{II})₂ (232i)

Pt	-0.461540	-0.346992	-0.016931
Cl	-0.578098	-0.852653	-2.337720
C	3.413723	1.051722	-0.377445
N	1.498715	-0.482576	-0.069657
N	2.402267	2.061924	-0.237883
C	2.725429	-0.352014	-0.039413
C	1.292302	1.824262	-0.918197
H	1.343161	1.309833	-1.868822
C	3.730475	-1.448416	0.260487
C	2.303932	2.738246	1.064890
H	0.403345	2.395261	-0.681918
H	3.222036	-2.410287	0.339428
H	4.491158	-1.504619	-0.529524
H	4.252315	-1.239989	1.203408
H	1.953423	2.031198	1.825811

H	3.282807	3.141336	1.332467
H	1.588686	3.558757	0.987324
Cl	-0.353205	0.265346	2.283415
N	-2.424013	-0.298790	0.069088
C	-3.577103	-0.290247	0.122046
C	-5.031864	-0.289162	0.190926
H	-5.366132	0.354195	1.010852
H	-5.402077	-1.304835	0.363905
H	-5.450656	0.084965	-0.748559
H	4.266190	1.264414	0.271660
H	3.767853	0.999103	-1.412813

TS(1-Pt^{IV}) (28i; 7i)

78	-0.566520	-0.336545	-0.099988
17	-0.945288	-2.665859	0.305302
17	-0.792825	-0.709880	-2.449150
17	-0.354118	0.036370	2.259356
17	-0.211908	2.001242	-0.508329
7	-2.515522	-0.000248	0.025756
6	-3.647513	0.180343	0.088935
6	-5.081260	0.409409	0.167512
1	-5.287117	1.480736	0.083508
1	-5.459912	0.041140	1.125705
1	-5.581959	-0.120956	-0.648104
6	4.357050	1.179237	0.427319
7	1.371933	-0.707409	-0.237191
7	3.536664	2.257150	0.563530
6	2.459865	-1.069926	-0.349680
6	3.271633	3.184868	-0.341132
6	3.709825	-1.783060	-0.578114
6	2.779335	2.333452	1.835154
1	3.474158	-2.806295	-0.894827
1	4.287383	-1.276886	-1.354169
1	4.297297	-1.801939	0.341742
1	1.878947	1.721580	1.760543
1	3.414101	1.969343	2.644350
1	2.508456	3.372085	2.025083
1	4.759421	0.775937	1.348200
1	4.990536	1.182173	-0.453824
1	2.461009	3.874672	-0.166306
1	3.771497	3.134745	-1.299558

TS(2-L) (190i)

C	1.411259	0.288293	0.210906
N	-1.514400	-0.091801	-0.437711
O	0.668026	1.159542	0.900244
C	-0.712215	-0.948047	-0.453713
C	-0.217557	1.960861	0.414732
C	-0.094183	-2.272863	-0.615244

H	-0.840002	-2.993924	-0.971425
H	0.727936	-2.228478	-1.334855
H	0.312035	-2.621867	0.337777
H	2.194468	-0.142651	0.822645
H	1.619981	0.544440	-0.825654
H	-0.827127	2.476496	1.141902
H	-0.254526	2.162788	-0.648447

TS(2-Pt^{II})₂ (305i)

78	-0.351940	0.144819	-0.148322
17	-0.431758	2.401837	0.602952
6	3.495477	-0.376905	0.855897
7	1.584881	0.299147	-0.497535
8	2.478367	-0.962551	1.635829
6	2.816714	0.140404	-0.442427
6	1.395818	-0.206977	1.740872
1	1.509967	0.859026	1.927482
6	3.762484	0.454911	-1.582379
1	0.580700	-0.731562	2.224735
1	3.221584	0.937534	-2.397260
1	4.571693	1.114373	-1.242823
1	4.222192	-0.469720	-1.953193
17	-0.311307	-2.117227	-0.855326
7	-2.308144	0.014560	0.069407
6	-3.454463	-0.061139	0.173363
6	-4.902658	-0.154233	0.293307
1	-5.276665	-0.952058	-0.355875
1	-5.361786	0.793362	-0.005275
1	-5.184012	-0.375581	1.327658
1	4.250125	-1.143734	0.670376
1	3.957118	0.472640	1.379608

TS(2-Pt^{IV}) (9i)

Pt	-0.460557	-0.189278	-0.036314
Cl	-1.096073	-2.175484	1.129565
Cl	-0.706432	-1.334245	-2.121927
Cl	-0.235330	0.961553	2.053048
Cl	0.153879	1.809581	-1.213634
N	-2.359535	0.361839	-0.123369
C	-3.463837	0.670797	-0.176853
C	-4.862762	1.061049	-0.245265
H	-4.976624	1.897474	-0.941400
H	-5.207675	1.365399	0.747490
H	-5.462181	0.214670	-0.593942
C	4.110893	1.148889	-0.695210
N	1.426466	-0.774727	0.045103
O	4.102575	1.675800	0.529647
C	2.493869	-1.205523	0.064427
C	3.161777	2.310937	1.149539

C	3.746247	-1.942375	0.161121
H	3.528165	-2.968321	0.479978
H	4.241584	-1.950663	-0.812168
H	4.402922	-1.456878	0.886349
H	5.116117	0.947862	-1.041806
H	3.319038	1.455522	-1.372033
H	3.368856	2.533022	2.186264
H	2.214267	2.502902	0.657960

TS(3-L)Oex (416i)

N	1.170955	0.137490	-0.254603
N	-1.522336	-0.186823	-0.565637
N	0.532516	0.955362	0.617029
C	-0.549975	-0.834167	-0.828737
C	-0.548626	1.626665	0.240307
C	-0.028783	-2.093923	-1.410384
H	-0.844462	-2.704737	-1.810886
H	0.683905	-1.878258	-2.213671
H	0.512540	-2.660843	-0.647250
H	-1.150138	2.111096	1.000737
C	0.624075	0.478148	1.999772
H	1.673638	0.289660	2.225555
H	0.053299	-0.451447	2.100252
H	0.223395	1.233735	2.677937
H	1.184465	0.640532	-1.148983
H	-0.584722	2.017715	-0.766963

TS(3-L)Oen (373i)

7	0.916864	0.495858	-0.496361
7	-1.127242	-1.201690	-0.201489
7	-0.106073	1.249283	-0.033098
6	0.065258	-1.290175	-0.212371
6	-1.270022	1.033108	-0.620546
6	1.230570	-2.207035	-0.176440
1	0.901788	-3.250708	-0.197941
1	1.880262	-2.013797	-1.036155
1	1.824801	-2.046822	0.730662
1	-2.165012	1.438238	-0.169633
6	-0.094457	1.680974	1.370617
1	0.839900	2.212431	1.569258
1	-0.170207	0.801300	2.019637
1	-0.931174	2.356448	1.559813
1	1.710309	0.654666	0.132545
1	-1.263604	0.742855	-1.659111

TS(3-L)Mex (361i)

7	-0.696242	1.421731	0.989421
7	-0.223170	-0.958249	0.610278
7	0.353712	1.690106	0.275410
6	0.932528	-0.811579	0.318442

6	1.550216	1.053730	0.474748
6	2.133966	-1.608658	-0.082830
1	1.902978	-2.677389	-0.064929
1	2.459619	-1.332953	-1.092301
1	2.972585	-1.414615	0.596088
1	2.341692	1.333798	-0.216242
6	0.035880	2.180031	-1.073286
1	-0.801757	2.871145	-0.987901
1	-0.255596	1.329946	-1.698705
1	0.905790	2.685426	-1.495989
1	1.864814	0.997491	1.514663
1	-0.376944	0.984151	1.857443

TS(3-L)Men (376i)

7	0.571861	-0.963446	1.420959
7	1.583598	0.518193	-0.164520
7	-0.510414	-0.941499	0.693468
6	0.570201	1.075745	-0.474765
6	-1.047507	0.291333	0.476461
6	0.044105	2.196763	-1.308101
1	0.866325	2.740953	-1.782422
1	-0.624902	1.816477	-2.088295
1	-0.534650	2.895566	-0.693381
1	-1.969420	0.309766	-0.096897
6	-0.728353	-1.974175	-0.332959
1	-0.632220	-2.957406	0.133694
1	0.032186	-1.854534	-1.112586
1	-1.727719	-1.875932	-0.760012
1	1.039347	-1.861178	1.254325
1	-0.994949	0.955555	1.332409

TS(3-Pt^{II})Oex (186i)

Pt	-0.621385	-0.069728	-0.176377
Cl	-0.693282	-1.213060	-2.247407
Cl	-0.558527	1.074286	1.915352
N	-2.586250	0.051350	-0.176727
C	-3.738434	0.097989	-0.184162
C	-5.193381	0.155952	-0.193441
H	-5.607930	-0.856804	-0.171775
H	-5.540998	0.661739	-1.099658
H	-5.550210	0.706665	0.682317
N	3.974047	0.242175	0.136652
N	1.358770	-0.226834	-0.188350
N	3.399207	1.056643	1.050122
C	2.366752	-0.811522	-0.414278
C	2.512012	1.971129	0.770751
C	2.985287	-2.042350	-0.957951
H	2.204353	-2.660197	-1.410102
H	3.738642	-1.790901	-1.710795

H	3.491316	-2.589866	-0.157354
H	1.999238	2.486290	1.569949
C	3.550949	0.566497	2.428174
H	4.610766	0.391281	2.612475
H	2.994373	-0.369908	2.518088
H	3.146429	1.298673	3.126068
H	3.981568	0.769116	-0.743646
H	2.361710	2.262351	-0.259652

TS(3-Pt^{II})Oex₁ (185i)

Pt	0.643910	-1.164313	-0.398931
Cl	0.669204	-0.205611	-2.575879
Cl	0.606300	-2.059311	1.803865
N	-1.333689	-1.062716	-0.380589
C	-2.486843	-1.034200	-0.384963
C	-3.943068	-1.013706	-0.396092
H	-4.325051	-1.933857	-0.849600
H	-4.301354	-0.157314	-0.975643
H	-4.323462	-0.938160	0.627255
N	3.760002	1.063259	0.179367
N	2.603199	-1.399758	-0.477310
N	2.654712	1.245621	0.921975
C	3.695676	-0.958634	-0.365186
C	1.454305	1.538223	0.482610
C	5.145191	-1.216715	-0.473898
H	5.307919	-2.241297	-0.821897
H	5.600175	-0.512248	-1.175962
H	5.622347	-1.070190	0.498318
H	0.657062	1.677528	1.198672
C	2.837655	0.863057	2.333379
H	3.859431	1.115238	2.613130
H	2.653756	-0.211714	2.423066
H	2.122549	1.404502	2.953310
H	1.313451	1.763981	-0.566216
H	3.515434	1.385429	-0.764519

TS(3-Pt^{II})Oex₂ (238i)

78	0.511800	-0.018426	-0.283059
17	0.818140	-2.349506	0.078938
7	-3.515259	-0.118544	0.451805
7	-1.392257	-0.323371	-0.696281
7	-2.716563	0.273445	1.526690
6	-2.619825	-0.360275	-0.763996
6	-1.587694	-0.399480	1.690917
1	-1.554885	-1.461172	1.486015
6	-3.480674	-0.584876	-1.984405
6	-2.759193	1.720960	1.783866
1	-0.825872	0.027625	2.332311
1	-2.861032	-0.927438	-2.813508

1	-4.259764	-1.331415	-1.782821
1	-3.984194	0.347306	-2.262282
1	-2.291892	2.253842	0.948188
1	-3.802735	2.016212	1.893018
1	-2.211612	1.933940	2.703919
17	0.202984	2.324219	-0.553549
7	2.426740	0.282336	0.046251
6	3.554789	0.456797	0.215994
6	4.980489	0.674803	0.418033
1	5.539467	-0.213994	0.108972
1	5.188794	0.875712	1.473736
1	5.313752	1.529892	-0.178423
1	-4.002674	-0.985538	0.680639

TS(3-Pt^{II})Oen₁ (174i)

78	0.475552	-0.009889	-0.460300
17	0.883255	-2.268532	0.137937
17	0.071784	2.274241	-1.011819
7	2.349288	0.422180	-0.033665
6	3.455998	0.656929	0.191070
6	4.857061	0.947161	0.462250
1	5.480023	0.576390	-0.357951
1	5.167852	0.459209	1.391308
1	5.002868	2.027402	0.559095
7	-3.379069	0.097494	0.893675
7	-1.373579	-0.461487	-0.975236
7	-2.380797	0.633246	1.617035
6	-2.547901	-0.531163	-0.912721
6	-1.384771	-0.099773	2.036880
6	-3.797967	-0.949119	-1.579126
1	-3.557918	-1.443426	-2.524886
1	-4.349748	-1.630350	-0.926978
1	-4.431426	-0.079446	-1.781686
1	-0.580499	0.369497	2.581759
6	-2.316881	2.101249	1.772570
1	-3.314610	2.464232	2.029835
1	-1.968446	2.528381	0.827240
1	-1.618510	2.357794	2.569378
1	-4.001280	0.871612	0.649523
1	-1.413095	-1.167039	1.871798

TS(3-Pt^{II})Oen₂ (198i)

Pt	0.703829	-0.568893	-0.341240
Cl	0.842551	-1.203821	-2.623462
N	4.534565	0.931227	-0.370911
N	2.667539	-0.586077	-0.196894
N	3.575271	1.921281	-0.352625
C	3.867717	-0.430972	-0.032798
C	2.576915	1.684092	-1.177255

H	2.760919	1.122507	-2.081815
C	4.926493	-1.412522	0.408334
C	3.334391	2.631251	0.915526
H	1.658182	2.240648	-1.052470
H	4.497662	-2.414152	0.445868
H	5.770350	-1.402869	-0.291424
H	5.307979	-1.155388	1.404745
H	2.878853	1.941151	1.634928
H	4.285559	3.019422	1.287948
H	2.658698	3.467522	0.729856
Cl	0.564804	0.183366	1.919221
N	-1.255921	-0.611452	-0.450659
C	-2.407133	-0.660435	-0.516263
C	-3.859237	-0.734652	-0.599619
H	-4.151288	-1.243395	-1.523626
H	-4.291797	0.270891	-0.595768
H	-4.254905	-1.293812	0.254173
H	5.284476	1.168641	0.277189

TS(3-Pt^{II})Mex₁ (251i)

78	-0.453112	-0.385184	0.146466
17	-0.368549	-1.105710	-2.116224
17	-0.500201	0.389128	2.399491
7	-2.304709	0.254153	-0.124584
6	-3.377784	0.643230	-0.285907
6	-4.735444	1.129125	-0.487643
1	-5.284786	1.100546	0.458444
1	-5.250997	0.499645	-1.219514
1	-4.714169	2.159480	-0.856180
7	0.984633	2.127898	-0.213043
7	1.361096	-1.077997	0.432165
7	2.161174	1.738244	-0.577491
6	2.530838	-0.942506	0.493041
6	3.142640	1.228970	0.205994
6	3.844821	-1.573327	0.736144
1	3.695117	-2.624451	1.003702
1	4.466575	-1.515096	-0.162033
1	4.367905	-1.064258	1.550913
1	4.127536	1.177906	-0.240115
6	2.310674	1.644658	-2.045746
1	1.881773	2.546769	-2.480688
1	1.743391	0.770680	-2.380741
1	3.365737	1.552537	-2.304116
1	0.937028	2.084314	0.813248
1	3.066583	1.461157	1.262582

TS(3-Pt^{II})Mex₂ (135i; 15i)

Pt	0.367692	-1.074655	-0.213353
Cl	0.436815	-0.304128	-2.479634

C	4.247647	0.435362	-0.424291
N	2.321017	-1.163296	-0.244705
N	3.377136	1.343666	0.221758
C	3.533471	-1.060035	-0.324453
N	2.165357	1.475534	-0.168247
H	2.059620	1.126448	-1.131381
C	4.571617	-2.159522	-0.431462
C	3.622168	1.672314	1.634712
H	4.074657	-3.127257	-0.511093
H	5.207042	-2.003316	-1.312391
H	5.222209	-2.158781	0.451609
H	3.394273	0.791143	2.245026
H	4.664061	1.970098	1.764406
H	2.950334	2.484649	1.906777
Cl	0.335084	-1.755775	2.055294
N	-1.596320	-1.032579	-0.223781
C	-2.749677	-1.005137	-0.228915
C	-4.205468	-0.974015	-0.235126
H	-4.602469	-1.960359	-0.495588
H	-4.560254	-0.243063	-0.968396
H	-4.575506	-0.693120	0.755857
H	5.243325	0.446840	0.019867
H	4.305239	0.636283	-1.497440

TS(3-Pt^{II})Men (212i)

78	0.622437	0.111380	-0.056945
17	0.021821	-2.166420	-0.496588
17	1.249581	2.352455	0.340795
7	2.513889	-0.417573	0.009942
6	3.629317	-0.707245	0.044368
6	5.038416	-1.071114	0.088238
1	5.646644	-0.253375	-0.310647
1	5.209787	-1.970389	-0.511391
1	5.341791	-1.268758	1.121152
7	-2.367693	-0.953977	1.608870
7	-1.263416	0.686038	-0.152069
7	-3.357224	-0.852685	0.792016
6	-2.267465	1.240189	-0.428096
6	-3.939756	0.358401	0.624008
6	-2.891521	2.344216	-1.198780
1	-2.108805	2.923587	-1.698248
1	-3.584488	1.943027	-1.945045
1	-3.456878	3.000949	-0.530407
1	-4.850595	0.379481	0.038338
6	-3.618118	-1.915301	-0.206669
1	-3.799491	-2.849623	0.328978
1	-2.722897	-2.015791	-0.828188
1	-4.489527	-1.657773	-0.808255

1	-1.880508	-1.835065	1.411251
1	-3.853045	1.025992	1.472915

TS(3-Pt^{II})Men₁ (246i)

78	0.879123	-0.919230	-0.049909
17	0.784992	-0.238045	-2.344992
17	0.927325	-1.605550	2.211650
7	-1.087458	-1.049719	-0.019636
6	-2.236649	-1.137346	0.021532
6	-3.686492	-1.260831	0.077630
1	-3.977823	-1.770419	1.001324
1	-4.045597	-1.840761	-0.778306
1	-4.151319	-0.270167	0.056040
7	1.737064	1.970511	0.419797
7	2.844293	-0.885684	-0.066896
7	2.888323	2.102126	-0.147395
6	3.936615	-0.439312	0.023766
6	4.008941	1.653472	0.471646
6	5.374894	-0.808396	-0.015654
1	5.467172	-1.891575	-0.139178
1	5.875844	-0.304672	-0.848189
1	5.869519	-0.506743	0.912786
1	4.944852	2.028547	0.076326
6	2.981083	2.507775	-1.570645
1	2.442799	3.450811	-1.690729
1	2.507786	1.724233	-2.170921
1	4.025395	2.638621	-1.853091
1	3.910132	1.531598	1.544062
1	1.020266	2.172926	-0.284688

TS(3-Pt^{II})Men₂ (134i)

Pt	0.378657	-0.794138	-0.571493
Cl	0.297795	-0.206673	-2.858875
C	4.162393	0.770184	0.092233
N	2.334959	-0.800198	-0.636740
N	3.177668	1.265524	0.970895
C	3.539720	-0.631349	-0.544879
N	2.084340	1.594423	0.376211
C	4.651222	-1.557913	-0.997364
C	3.201117	0.833998	2.381911
H	1.331389	1.631805	1.075463
H	4.230004	-2.403939	-1.541921
H	5.353714	-1.021470	-1.647336
H	5.215158	-1.927485	-0.132094
H	2.689945	-0.132916	2.460883
H	4.235050	0.767620	2.722639
H	2.667542	1.577338	2.978129
Cl	0.409829	-1.348474	1.761990
N	-1.587153	-0.871824	-0.551262

C	-2.739818	-0.921704	-0.558863
C	-4.194291	-0.990776	-0.575692
H	-4.590386	-0.291059	-1.318239
H	-4.593871	-0.729831	0.409231
H	-4.519774	-2.003535	-0.834075
H	5.112110	0.597383	0.597752
H	4.278190	1.429819	-0.769297

TS(3-Pt^{IV})Oex (41i; 4i)

78	0.762758	0.539550	0.128856
17	1.367730	1.790822	2.075639
17	1.607298	2.290494	-1.259999
17	-0.063457	-1.223709	1.530361
17	0.177636	-0.719172	-1.824788
7	2.551410	-0.312207	0.129428
6	3.592422	-0.796045	0.125104
6	4.911031	-1.408773	0.118815
1	5.427077	-1.178963	1.055854
1	5.492913	-1.016547	-0.721342
1	4.811577	-2.493001	0.015632
7	-3.878073	-0.101702	-0.709802
7	-1.010128	1.405191	0.132843
7	-3.646539	-1.328025	-0.267886
6	-2.042946	1.910518	0.135147
6	-3.223049	-2.386919	-0.921039
6	-3.264624	2.696982	0.192912
1	-3.013830	3.726212	0.470503
1	-3.758329	2.673664	-0.780557
1	-3.944842	2.254984	0.922852
1	-3.061637	-3.309903	-0.386102
6	-3.885413	-1.453319	1.184916
1	-4.774591	-0.869745	1.422344
1	-3.012438	-1.056714	1.707420
1	-4.034178	-2.500616	1.447694
1	-3.613974	-0.113751	-1.702717
1	-2.959816	-2.283931	-1.965101

TS(3-Pt^{IV})Oen (41i; 13i)

78	-0.520051	-0.215398	-0.198465
17	-0.706231	-1.362391	-2.285292
17	-0.388479	0.932741	1.906266
7	-2.491307	0.008741	-0.157123
6	-3.633636	0.122323	-0.143299
6	-5.080634	0.265124	-0.126140
1	-5.362451	1.072771	0.556048
1	-5.537067	-0.670302	0.211251
1	-5.437755	0.499977	-1.133344
7	4.091251	0.628874	0.862556
7	1.439836	-0.498799	-0.269158

7	3.298719	1.632149	1.239717
6	2.513775	-0.900466	-0.414142
6	2.726148	2.439014	0.384436
6	3.692734	-1.651759	-0.830936
1	3.391869	-2.383077	-1.589391
1	4.441333	-0.961891	-1.222250
1	4.118401	-2.170043	0.032175
1	2.029540	3.181861	0.736914
6	3.001803	1.797943	2.680030
1	3.952374	1.815321	3.219056
1	2.390351	0.952450	3.000890
1	2.458567	2.726356	2.850864
1	4.407042	0.181452	1.726762
1	2.922779	2.292959	-0.667511
17	-0.334219	1.868071	-1.365912
17	-0.741758	-2.295281	0.964182

TS(3-Pt^{IV})Mex (80i)

78	-0.601868	0.071249	0.021002
17	-0.998064	1.509810	1.888939
17	-0.212220	-1.352027	-1.872765
7	-2.526325	-0.419663	-0.016725
6	-3.640712	-0.695343	-0.036321
6	-5.051570	-1.046860	-0.061383
1	-5.581937	-0.491884	0.718278
1	-5.165184	-2.120390	0.116857
1	-5.475439	-0.794533	-1.038006
7	2.903047	-1.860258	-0.311007
7	1.310183	0.624910	0.037638
7	3.870719	-1.014210	-0.227804
6	2.189244	1.386789	0.041345
6	4.094245	0.087269	-0.967489
6	2.900731	2.658557	0.201894
1	2.183160	3.406661	0.558338
1	3.714400	2.554762	0.923576
1	3.317435	2.975800	-0.757386
1	5.044154	0.588304	-0.843531
6	4.729011	-1.248411	0.957662
1	4.946566	-2.314874	0.997804
1	4.165587	-0.962496	1.847977
1	5.647946	-0.668063	0.875467
1	2.315159	-1.611527	-1.116246
1	3.560787	0.164102	-1.906587
17	-0.213052	-1.748041	1.514819
17	-1.042128	1.902545	-1.470135

TS(3-Pt^{IV})Men (64i)

Pt	-0.508752	-0.183605	0.126798
Cl	-0.535948	1.710186	-1.357911

Cl	-0.558056	-2.080303	1.574778
N	-2.496488	-0.211806	0.031513
C	-3.643758	-0.238077	-0.007288
C	-5.096927	-0.267745	-0.054247
H	-5.430643	-1.190767	-0.537698
H	-5.463372	0.592395	-0.622603
H	-5.496787	-0.226308	0.963406
N	2.499189	2.402221	0.127216
N	1.485527	-0.243773	0.231471
N	3.308251	1.799257	-0.680573
C	2.496786	-0.809323	0.327055
C	4.294713	1.020666	-0.222361
C	3.469491	-1.878455	0.559307
H	2.918636	-2.779786	0.853460
H	4.037188	-2.074255	-0.353594
H	4.163577	-1.596245	1.354476
H	5.030019	0.662614	-0.927906
C	3.061908	1.836094	-2.145083
H	3.082204	2.880591	-2.463375
H	2.071047	1.414459	-2.329906
H	3.827801	1.268279	-2.672184
H	1.729059	2.788484	-0.425816
H	4.518739	1.106547	0.832252
Cl	-0.659638	1.266127	2.014829
Cl	-0.385972	-1.644546	-1.777133

TS(4-L)O (265i)

N	0.855377	1.035449	-0.268361
N	-1.087649	-1.019539	0.147937
O	-0.214459	1.508029	0.469355
C	0.070081	-1.134467	-0.041135
C	-1.374160	1.253727	-0.007100
C	1.360068	-1.801286	-0.267403
H	1.219004	-2.885303	-0.343961
H	1.813450	-1.425536	-1.188320
H	2.046777	-1.591828	0.558290
H	-2.202578	1.540898	0.627375
H	1.617651	1.253021	0.387355
H	-1.488660	1.025304	-1.058779

TS(4-L)M (336i)

N	-1.328994	1.583135	0.305508
N	-0.648407	-0.724246	0.171844
O	-0.225481	1.901487	-0.375856
C	0.528084	-0.602286	0.116885
C	0.909818	1.601864	0.205262
C	1.896317	-1.163285	0.035303
H	1.857910	-2.256792	0.075695
H	2.378347	-0.861355	-0.899906

H	2.514449	-0.802174	0.863578
H	1.773740	1.935225	-0.358118
H	-2.042583	1.670022	-0.431562
H	0.923930	1.563055	1.290328

TS(4-Pt^{II})O₁ (152i)

Pt	0.941572	0.122636	0.262066
Cl	0.887028	-0.883848	-1.891509
Cl	0.967469	1.148385	2.397015
N	-1.023851	0.050974	0.336128
C	-2.173427	-0.012317	0.393639
C	-3.624635	-0.100924	0.470736
H	-3.917334	-1.082213	0.857346
H	-4.060124	0.033636	-0.524172
H	-4.009995	0.674748	1.139607
N	4.182452	2.550094	-0.777306
N	2.911068	0.144590	0.218747
O	2.892270	3.004675	-0.597623
C	4.032803	0.446724	0.106902
C	1.939217	2.457969	-1.244137
C	5.483135	0.233112	0.166800
H	5.686908	-0.809145	0.433006
H	5.925861	0.466656	-0.804150
H	5.927279	0.890477	0.919966
H	0.965553	2.895932	-1.072918
H	2.147392	1.719310	-2.010943
H	4.656168	3.127667	-0.071790

TS(4-Pt^{II})O₂ (295i; 6i)

Pt	0.769040	-0.035679	-0.278398
Cl	0.741883	1.155971	-2.334084
N	4.348135	1.364992	0.742591
N	2.747973	-0.061302	-0.283410
O	3.212524	1.822346	1.455103
C	3.931443	0.147774	0.013578
C	2.193310	1.953018	0.623107
H	2.369836	2.378565	-0.359912
C	5.118634	-0.704413	-0.369975
H	1.283715	2.193424	1.159888
H	4.808253	-1.444974	-1.107026
H	5.916128	-0.081563	-0.791102
H	5.516351	-1.225509	0.509659
Cl	0.752323	-1.186480	1.795896
N	-1.200879	-0.124007	-0.314667
C	-2.351474	-0.199030	-0.341599
C	-3.803540	-0.301440	-0.377676
H	-4.249851	0.696692	-0.426830
H	-4.160973	-0.808654	0.523793
H	-4.115964	-0.873964	-1.256693

H	5.012473	1.143203	1.486958
TS(4-Pt^{II})M (229i)			
Pt	0.968940	-0.003755	-0.002937
Cl	0.467376	1.606525	-1.688958
Cl	1.441141	-1.630385	1.649690
N	-0.946207	-0.382520	0.185211
C	-2.067930	-0.619431	0.302570
C	-3.484138	-0.920798	0.453536
H	-4.046942	0.003080	0.619112
H	-3.631473	-1.588223	1.308174
H	-3.860178	-1.409392	-0.450743
N	2.769402	2.792138	0.438678
N	2.908897	0.308513	-0.195608
O	3.846711	2.908452	-0.321469
C	4.065091	0.215177	-0.355141
C	4.941866	2.323512	0.084075
C	5.285462	-0.545294	-0.687066
H	5.020673	-1.596848	-0.839023
H	5.741874	-0.148832	-1.598603
H	6.014016	-0.472129	0.125373
H	5.800496	2.543378	-0.537408
H	5.025080	2.081554	1.139443
H	2.030584	3.108998	-0.204526
TS(4-Pt^{II})M₁ (276i)			
Pt	0.592265	-0.689229	0.585993
Cl	0.665533	-2.678088	-0.710585
Cl	0.488742	1.276405	1.927661
N	-1.390801	-0.731555	0.514314
C	-2.540971	-0.764392	0.447198
C	-3.994062	-0.816609	0.370426
H	-4.429323	-0.459701	1.308923
H	-4.317877	-1.846991	0.194160
H	-4.349710	-0.186225	-0.450496
C	3.178516	0.601758	-1.795642
N	2.546901	-0.748943	0.718739
O	2.219215	1.400605	-1.409817
C	3.614824	-0.545458	0.278183
N	0.948402	0.973049	-1.436833
C	5.083259	-0.615545	0.292589
H	5.407100	-1.180962	1.173158
H	5.449182	-1.116299	-0.608354
H	5.510866	0.390273	0.333966
H	0.486928	1.747970	-0.943081
H	4.122424	1.113499	-1.931298
H	2.902603	-0.300195	-2.333954
TS(4-Pt^{II})M₂ (221i)			
Pt	0.543221	-0.373381	-0.088161

Cl	0.541211	-1.038207	-2.360669
C	4.248418	1.130483	-0.097514
N	2.485810	-0.578067	-0.012205
O	3.211393	1.988526	0.256097
C	3.691534	-0.339788	0.079718
N	2.166883	1.774794	-0.551757
C	4.763416	-1.382333	0.330454
H	1.407878	2.240925	-0.030426
H	4.331160	-2.382748	0.298645
H	5.551435	-1.301670	-0.428342
H	5.221287	-1.213793	1.312307
Cl	0.496894	0.327025	2.185342
N	-1.430943	-0.287198	-0.143652
C	-2.582171	-0.242287	-0.188821
C	-4.036189	-0.196101	-0.249472
H	-4.362215	-0.199601	-1.294171
H	-4.403429	0.712759	0.237129
H	-4.459658	-1.068081	0.258803
H	4.523735	1.241970	-1.152475
H	5.089620	1.341455	0.563812

TS(4-Pt^{IV})O (35i)

Pt	1.122976	0.023192	0.150631
Cl	1.053437	-1.254393	2.167368
Cl	1.207841	-1.997764	-1.125552
Cl	0.993050	2.042734	1.434514
Cl	1.160316	1.298324	-1.882256
N	-0.855206	-0.021137	0.069710
C	-2.001406	-0.069811	0.028157
C	-3.453090	-0.133926	-0.023224
H	-3.868671	0.875602	0.049077
H	-3.822005	-0.738665	0.810737
H	-3.766638	-0.589020	-0.967563
N	5.562171	2.022289	0.443372
N	3.105191	-0.001878	0.236132
O	4.521979	2.915081	0.494085
C	4.225696	-0.268534	0.306742
C	3.730429	3.048278	-0.488530
C	5.544154	-0.886472	0.352677
H	5.437612	-1.955072	0.135291
H	6.195154	-0.402315	-0.376898
H	5.973534	-0.754214	1.349090
H	2.911306	3.736330	-0.337400
H	3.884294	2.468221	-1.392049
H	5.959477	2.184230	1.376555

TS(4-Pt^{IV})M (110i)

Pt	1.151710	0.431254	0.061973
Cl	1.244185	-0.741616	-2.031012

Cl	0.998063	1.571969	2.152369
N	-0.748007	-0.099833	0.268774
C	-1.844342	-0.419126	0.387571
C	-3.233304	-0.821774	0.539540
H	-3.310355	-1.910437	0.461930
H	-3.837684	-0.358515	-0.246132
H	-3.602788	-0.500806	1.518133
N	3.267098	3.398799	0.545882
N	3.083237	0.881431	-0.196729
O	4.041963	3.492249	-0.525163
C	4.159008	0.640521	-0.564116
C	5.241214	2.998741	-0.479899
C	5.333560	-0.081573	-1.057873
H	5.070286	-1.142395	-1.138502
H	5.619687	0.298481	-2.042004
H	6.175440	0.034372	-0.370617
H	5.832325	3.193253	-1.364074
H	5.652856	2.738849	0.490049
Cl	1.829557	-1.559933	1.195609
Cl	0.438764	2.412517	-1.091921
H	2.361589	3.709591	0.170223

TS(5-L)O (450i)

8	1.062733	0.089761	-0.270011
7	-1.519222	-0.145768	-0.493105
7	0.532195	0.921904	0.615282
6	-0.569671	-0.814854	-0.782958
6	-0.557942	1.549655	0.190843
6	-0.023718	-2.042405	-1.393720
1	-0.820129	-2.628017	-1.862826
1	0.725280	-1.774925	-2.145341
1	0.476944	-2.651090	-0.634796
1	-1.177100	2.054834	0.924264
6	0.639525	0.473690	2.005368
1	1.692610	0.280635	2.214768
1	0.063552	-0.449604	2.139091
1	0.266269	1.249686	2.678317
1	-0.546046	1.926172	-0.821720

TS(5-L)M (387i)

8	-1.500639	0.701613	0.541378
7	-0.908460	-1.352024	-0.260717
7	-0.350421	1.180086	0.297031
6	0.267665	-1.203521	-0.036616
6	0.694124	0.431739	0.756462
1	0.582005	0.116874	1.791031
6	1.531021	-2.003294	-0.171048
1	1.686243	0.790424	0.487225
1	1.303823	-3.018299	-0.504695

1	2.206535	-1.533630	-0.895070
1	2.059128	-2.052923	0.788339
6	-0.224522	1.933563	-0.959485
1	-0.994832	2.705579	-0.960541
1	-0.401323	1.244234	-1.793090
1	0.765975	2.387482	-1.034300

TS(5-Pt^{II})O (268i)

Pt	-0.632283	-0.053919	-0.058256
Cl	-0.942790	-2.005005	1.249171
Cl	-0.362906	1.925446	-1.356146
N	-2.588372	0.196812	-0.094938
C	-3.734813	0.320476	-0.108047
C	-5.182837	0.473574	-0.123253
H	-5.661328	-0.502641	0.002340
H	-5.502486	0.909141	-1.074963
H	-5.498265	1.131648	0.692512
O	3.796904	-0.409417	-0.055996
N	1.348663	-0.297494	-0.030657
N	3.639430	0.917103	-0.081036
C	2.248874	-1.066911	0.193211
C	2.774010	1.391733	-0.934089
H	2.555527	0.830684	-1.828494
C	2.553059	-2.461916	0.598210
C	3.988144	1.592085	1.170945
H	2.446760	2.418694	-0.842353
H	1.617274	-3.018822	0.665345
H	3.227654	-2.921232	-0.131687
H	3.054862	-2.470940	1.571016
H	3.302499	1.256004	1.955161
H	5.012203	1.319815	1.429686
H	3.908338	2.671988	1.036491

TS(5-Pt^{II})O₁ (216i)

78	0.580677	-1.663756	-0.307232
17	0.738223	-2.137058	-2.630927
17	0.361629	-1.244950	2.023997
7	-1.408547	-1.800794	-0.450059
6	-2.551920	-1.924605	-0.539763
6	-3.993293	-2.099510	-0.655031
1	-4.244381	-2.442164	-1.663612
1	-4.506624	-1.152600	-0.461218
1	-4.336093	-2.844052	0.070272
8	3.333141	0.748354	-0.500006
7	2.555267	-1.713589	-0.148430
7	2.102550	1.173943	-0.227873
6	3.513883	-0.995528	-0.207957
6	1.096966	0.825170	-0.989271
6	4.994142	-1.073652	-0.142671

1	5.297061	-2.121802	-0.096921
1	5.429306	-0.600589	-1.027742
1	5.362932	-0.543049	0.740027
6	1.944775	1.771942	1.099476
1	1.977166	0.972608	1.845968
1	0.983885	2.285116	1.159375
1	2.765664	2.475687	1.243993
1	1.315048	0.437269	-1.974800
1	0.118295	1.215169	-0.743823

TS(5-Pt^{II})M (288i)

78	0.554415	0.096374	0.162153
17	0.116572	-1.287294	-1.733855
17	0.996163	1.503937	2.010528
7	2.455006	-0.411401	0.100182
6	3.570508	-0.700224	0.063658
6	4.978869	-1.066192	0.018857
1	5.221491	-1.491757	-0.959721
1	5.197093	-1.807469	0.794051
1	5.599785	-0.181096	0.188664
8	-2.483201	-1.309673	1.219995
7	-1.324537	0.626227	0.178089
7	-3.425155	-1.035524	0.441778
6	-2.355216	1.185591	-0.049485
6	-3.893166	0.244109	0.470607
6	-2.801637	2.489139	-0.640892
1	-1.930624	3.126249	-0.809260
1	-3.313507	2.313875	-1.593436
1	-3.500700	2.996966	0.032059
1	-4.715961	0.459031	-0.205991
6	-3.556261	-1.879171	-0.760815
1	-3.618039	-2.915724	-0.427098
1	-2.642901	-1.743144	-1.353757
1	-4.448974	-1.599551	-1.322207
1	-3.977259	0.652413	1.474186

TS(5-Pt^{II})M₁ (342i)

78	0.295923	-0.740911	0.533937
17	0.211914	-1.744143	-1.611019
17	0.366683	0.211523	2.722634
7	-1.699781	-0.675954	0.574243
6	-2.851376	-0.626048	0.575526
6	-4.306504	-0.571519	0.578861
1	-4.655415	0.155256	-0.161272
1	-4.665283	-0.273901	1.568894
1	-4.716235	-1.555653	0.331119
6	2.947775	1.395788	-0.826717
7	2.246678	-0.895981	0.519808
7	1.844525	2.002811	-0.322927

6	3.231485	-0.312154	0.167711
8	0.688384	1.635961	-0.656408
6	4.709823	-0.510853	0.180410
1	4.934034	-1.496876	0.595175
1	5.114562	-0.446196	-0.834951
1	5.194668	0.256886	0.792346
1	3.875401	1.934294	-0.665584
1	2.785086	0.940640	-1.798494
6	1.931224	2.888567	0.853399
1	1.572159	2.310993	1.713410
1	1.265860	3.735043	0.676664
1	2.958642	3.224708	0.999527

TS(5-Pt^{IV})O (143i)

Pt	-0.542833	0.046337	-0.001842
Cl	-0.487857	0.373299	-2.367893
Cl	-1.011771	2.366838	0.307084
Cl	-0.082997	-2.294394	-0.308439
Cl	-0.573288	-0.284310	2.375378
N	-2.517808	-0.334411	-0.093531
C	-3.647962	-0.532540	-0.151242
C	-5.078955	-0.783853	-0.224144
H	-5.452262	-1.074615	0.762359
H	-5.275157	-1.590197	-0.937180
H	-5.595105	0.123069	-0.553068
O	3.860907	0.506195	0.324764
N	1.404339	0.386164	0.106431
N	3.712008	-0.809446	0.415743
C	2.277622	1.171699	-0.104081
C	2.884497	-1.301472	1.280882
H	2.500745	-0.672876	2.070815
C	2.640830	2.524658	-0.575341
C	4.230695	-1.562259	-0.732584
H	2.644857	-2.355824	1.237971
H	1.719963	3.093953	-0.719378
H	3.279837	3.017254	0.163241
H	3.192616	2.457326	-1.517574
H	3.623833	-1.307352	-1.605707
H	5.266513	-1.260674	-0.892267
H	4.168236	-2.631825	-0.529288

TS(5-Pt^{IV})M (259i)

Pt	0.349506	-0.406941	0.294493
Cl	0.075801	0.802834	-1.758932
Cl	0.633082	-1.639445	2.323552
N	-1.631081	-0.661184	0.407345
C	-2.766476	-0.817830	0.479981
C	-4.204718	-1.013329	0.573365
H	-4.416524	-2.035609	0.900731

H	-4.663141	-0.844315	-0.405600
H	-4.624516	-0.307405	1.296276
O	3.218388	2.117339	-0.170794
N	2.319543	-0.190667	0.158252
N	4.070359	1.536997	-0.865959
C	3.360366	-0.753720	0.072835
C	4.834769	0.578547	-0.296631
C	4.031764	-2.078596	0.152020
H	3.282326	-2.815077	0.453598
H	4.441089	-2.352467	-0.825231
H	4.849216	-2.052084	0.879212
H	5.588639	0.118780	-0.925989
C	3.889658	1.618426	-2.331308
H	3.845266	2.675970	-2.593654
H	2.924681	1.149692	-2.555104
H	4.712406	1.120922	-2.845534
H	5.065880	0.750272	0.748855
Cl	0.119922	1.608957	1.543328
Cl	0.534882	-2.452836	-0.961656

TS(6-L)O (277i)

O	-1.317006	-0.257290	-0.043502
N	1.456635	0.089512	-0.070877
O	-0.674069	-1.277961	0.631593
C	0.623155	0.916686	-0.155068
C	0.317932	-1.746767	-0.018696
H	0.332129	-1.675397	-1.098992
C	-0.068977	2.201537	-0.277267
H	0.924971	-2.464509	0.524291
H	0.657597	3.013495	-0.389554
H	-0.730968	2.178996	-1.147045
H	-0.684235	2.374098	0.608900

TS(6-L)M (400i)

8	1.731955	2.020828	-0.712507
7	1.532123	-0.181258	-0.037513
8	2.963205	1.786302	-1.180023
6	2.681889	-0.462092	0.080835
6	3.753121	1.288719	-0.271732
1	3.602916	1.606977	0.756105
6	3.703311	-1.493413	0.402892
1	4.748574	1.062743	-0.645848
1	3.212954	-2.412822	0.734261
1	4.311253	-1.713693	-0.480414
1	4.372264	-1.143001	1.195799

TS(6-Pt^{II})O (167i)

78	-0.476540	0.045513	0.014590
17	-0.709364	2.387451	-0.197301
17	-0.260095	-2.312473	0.239864

7	-2.432270	-0.137789	-0.025141
6	-3.581724	-0.220660	-0.047926
6	-5.033752	-0.322541	-0.076763
1	-5.471320	0.405977	0.613104
1	-5.342917	-1.329265	0.221038
1	-5.401334	-0.119990	-1.087811
8	4.130745	-0.173824	0.032949
7	1.502586	0.294880	0.058368
8	3.652773	-1.294319	-0.613824
6	2.472091	0.958533	0.126306
6	2.790850	-1.960338	0.032982
1	2.618915	-1.763658	1.083484
6	3.188163	2.235875	0.250269
1	2.354224	-2.794264	-0.502921
1	2.448689	3.026000	0.409088
1	3.887740	2.192760	1.089803
1	3.758131	2.430533	-0.661786

TS(6-Pt^{II})O₁ (148I; 14i)

78	0.390215	-1.153454	-0.306132
17	0.351295	0.150582	-2.290816
17	0.368328	-2.474019	1.656496
7	-1.580677	-1.002201	-0.192898
6	-2.730842	-0.945164	-0.145657
6	-4.184427	-0.882698	-0.093143
1	-4.512944	-0.674908	0.929821
1	-4.607382	-1.839419	-0.415231
1	-4.546331	-0.090720	-0.755911
8	3.451501	0.882903	0.881167
7	2.349071	-1.350911	-0.456173
8	2.283246	0.765866	1.610884
6	3.454733	-1.024868	-0.283286
6	1.199945	1.034254	0.994017
6	4.915060	-1.042940	-0.325408
1	5.253544	-1.903523	-0.911149
1	5.275593	-0.117170	-0.781098
1	5.305054	-1.099649	0.693076
1	0.316842	1.019514	1.622530
1	1.247849	1.509806	0.019292

TS(6-Pt^{II})O₂ (304i)

78	-0.349646	0.037454	-0.184934
17	-0.466079	2.406942	-0.042550
8	3.468538	-0.109790	0.890162
7	1.597803	0.133834	-0.528397
8	2.461769	-0.556637	1.801219
6	2.818697	0.043193	-0.399836
6	1.394879	0.220382	1.690327
1	1.523071	1.296738	1.626817

6	3.901149	0.094874	-1.441346
1	0.588339	-0.187497	2.292232
1	3.471517	0.416663	-2.390066
1	4.687669	0.792846	-1.135757
1	4.351387	-0.896516	-1.555724
17	-0.274867	-2.325930	-0.287463
7	-2.307915	-0.061421	0.054753
6	-3.453662	-0.124431	0.167123
6	-4.900918	-0.203888	0.304269
1	-5.369335	-0.218958	-0.685257
1	-5.269983	0.663895	0.859949
1	-5.174381	-1.117395	0.841823

TS(6-Pt^{II})M (349i)

78	0.426193	-0.005340	-0.125943
17	0.424361	2.367849	-0.185669
17	0.455774	-2.375467	-0.139106
7	2.381562	0.006542	0.092707
6	3.526054	0.011536	0.224500
6	4.971641	0.017517	0.392728
1	5.454150	0.325855	-0.540295
1	5.317866	-0.985586	0.660886
1	5.250142	0.717973	1.186401
8	-2.016791	0.083291	2.009082
7	-1.494779	-0.013417	-0.413327
8	-3.224106	-0.393854	1.704748
6	-2.611168	0.004764	-0.794665
6	-3.861158	0.334019	0.835798
1	-3.642664	1.398614	0.813951
6	-3.503323	-0.074401	-1.980898
1	-4.847510	-0.051682	0.593610
1	-2.891546	-0.109323	-2.886303
1	-4.120035	-0.976506	-1.923679
1	-4.164094	0.796826	-2.021616

TS(6-Pt^{II})M₁ (351i)

Pt	0.638611	-1.126898	0.035686
Cl	0.557518	-1.425124	-2.324528
Cl	0.704025	-0.950505	2.401869
N	-1.360314	-1.011733	0.101971
C	-2.505935	-0.902818	0.149562
C	-3.954527	-0.774687	0.215034
H	-4.426697	-1.635464	-0.268365
H	-4.270849	0.139980	-0.295606
H	-4.274147	-0.730001	1.260628
C	3.102235	1.335559	-0.621620
N	2.570081	-1.352084	-0.017143
O	2.098705	1.656153	0.141786
C	3.603180	-0.793282	-0.162245

O	0.873743	1.291774	-0.292482
C	5.077000	-0.867416	-0.216927
H	5.386685	-1.912735	-0.120043
H	5.446467	-0.471057	-1.167583
H	5.514672	-0.285760	0.600081
H	4.033501	1.781218	-0.287915
H	2.893131	1.110277	-1.663831

TS(6-Pt^{II})M₂ (189i)

78	0.479618	-0.451769	0.036539
17	0.532242	-0.394695	-2.333434
6	4.023940	1.213065	0.456063
7	2.398500	-0.600136	0.110534
8	2.933813	1.928584	0.897417
6	3.573754	-0.316576	0.321468
8	1.941441	1.774798	0.005264
6	4.710859	-1.311990	0.429841
1	4.367813	-2.310320	0.157827
1	5.531087	-1.010988	-0.231927
1	5.085927	-1.321643	1.459290
17	0.381922	-0.549186	2.406190
7	-1.504849	-0.379657	-0.026318
6	-2.653787	-0.302495	-0.065187
6	-4.105432	-0.210773	-0.117606
1	-4.551744	-1.099493	0.339228
1	-4.433414	-0.139698	-1.159182
1	-4.442395	0.677329	0.425929
1	4.826464	1.326411	1.188210
1	4.332901	1.505181	-0.553996

TS(6-Pt^{IV})O (102i)

78	-0.388944	-0.110862	-0.016821
17	-0.498124	-1.817336	1.644250
17	-0.456302	-1.771203	-1.726190
17	-0.349992	1.566200	1.703050
17	-0.277458	1.613636	-1.688732
7	-2.377014	-0.021507	-0.042352
6	-3.524909	0.002563	-0.064043
6	-4.978590	0.030418	-0.091541
1	-5.322123	0.258341	-1.105056
1	-5.345100	0.797704	0.596960
1	-5.368876	-0.945597	0.212380
8	4.120593	0.746501	0.016503
7	1.593440	-0.230223	-0.022890
8	3.532526	1.641970	0.885169
6	2.643921	-0.705370	-0.211436
6	2.529608	2.271677	0.449387
1	2.218517	2.184835	-0.587198
6	3.613028	-1.755383	-0.537333

1	2.054017	2.926631	1.170048
1	3.060995	-2.647375	-0.848534
1	4.267252	-1.414519	-1.343708
1	4.226574	-1.973931	0.339878

TS(6-Pt^{IV})M (280i)

78	0.378763	0.017221	0.006969
17	0.463323	1.407958	1.964234
17	0.471927	1.988576	-1.373266
17	0.346614	-1.918967	1.392885
17	0.314830	-1.344878	-1.949365
7	2.356594	-0.089596	-0.009986
6	3.502894	-0.149962	-0.021622
6	4.954637	-0.230092	-0.035560
1	5.374312	0.606637	0.531319
1	5.314554	-0.186062	-1.068118
1	5.273352	-1.172931	0.419680
8	-2.582473	-1.878576	0.124195
7	-1.606286	0.237330	0.010528
8	-3.698041	-1.378805	-0.392710
6	-2.540781	0.948072	-0.006819
6	-4.228774	-0.429361	0.309750
1	-4.019431	-0.401181	1.375092
6	-3.145371	2.293270	-0.099031
1	-5.130257	-0.011681	-0.127171
1	-2.327609	3.014678	-0.190520
1	-3.793476	2.357601	-0.977501
1	-3.735556	2.509405	0.796326

TS(7-L)exex (485i)

7	3.849275	-0.295029	0.582967
7	1.372896	0.215735	0.090118
7	3.616820	-0.791153	-0.657727
6	2.272188	0.576564	0.818343
7	2.468127	-1.336929	-0.943606
6	2.508431	1.565722	1.910619
1	1.576155	2.067854	2.179393
1	2.918875	1.068970	2.797180
1	3.245469	2.308112	1.588598
1	2.153068	-1.856644	-0.120697
6	4.162390	0.051102	-1.728902
1	5.212967	0.244472	-1.514620
1	3.602498	0.992466	-1.764601
1	4.046724	-0.480930	-2.672356
1	3.645516	-1.051990	1.245581

TS(7-L)exen (467i)

7	3.032455	2.558517	-0.259366
7	1.154262	0.775948	-0.328666
7	1.941528	3.113205	0.305803

6	2.361995	0.833074	-0.391040
7	0.827593	2.854608	-0.334399
6	3.540820	-0.066271	-0.529047
1	3.223154	-1.100368	-0.684852
1	4.163352	0.249449	-1.374037
1	4.164453	-0.005393	0.368461
1	0.042058	3.011240	0.310822
6	1.982435	3.103530	1.775379
1	2.969296	3.436421	2.095145
1	1.788212	2.085253	2.132971
1	1.218465	3.785091	2.156012
1	2.923554	2.736619	-1.264490

TS(7-L)enen (425i)

7	3.906038	0.258583	-0.373385
7	1.401173	-0.200728	-0.293346
7	3.369091	1.490691	-0.305886
6	2.449182	-0.750488	-0.049401
7	2.366161	1.595047	-1.128317
6	2.959543	-2.080040	0.397217
1	2.143720	-2.805294	0.436688
1	3.726406	-2.434999	-0.300046
1	3.416974	-2.014962	1.392049
1	1.781553	2.374447	-0.804713
6	3.326554	2.167162	1.007144
1	4.314742	2.125648	1.470937
1	2.583047	1.662636	1.636144
1	3.051105	3.213676	0.859265
1	4.581504	0.172488	0.391967

TS(7-Pt^{II})exex (271i; 13i)

78	-0.638298	0.049091	0.025226
17	-0.806563	2.339140	-0.532430
17	-0.399464	-2.252112	0.637306
7	-2.595180	-0.145832	-0.136377
6	-3.740580	-0.248996	-0.223204
6	-5.186704	-0.377289	-0.335141
1	-5.438531	-1.194490	-1.018249
1	-5.612941	0.554295	-0.720004
1	-5.620888	-0.588896	0.647034
7	3.743911	-0.240878	0.569767
7	1.318287	0.181841	0.218364
7	3.564789	-0.748539	-0.681682
6	2.256198	0.581631	0.867975
7	2.576616	-1.475030	-1.015888
6	2.520982	1.589287	1.937441
1	1.582994	2.076915	2.209719
1	2.959795	1.106550	2.818211
1	3.237461	2.334551	1.578881

1	2.130749	-1.897757	-0.191542
6	4.186616	0.052357	-1.747068
1	5.240951	0.187237	-1.508111
1	3.680135	1.022430	-1.784665
1	4.049655	-0.476800	-2.688104
1	3.602260	-1.015474	1.226990

TS(7-Pt^{II})_{exen} (325i)

78	0.604865	0.072971	-0.038316
17	1.072505	2.376630	-0.271194
17	0.126540	-2.257475	0.229647
7	2.540494	-0.305470	0.054554
6	3.674639	-0.504568	0.115127
6	5.107166	-0.754206	0.190495
1	5.335898	-1.351259	1.078485
1	5.647101	0.196106	0.249545
1	5.439421	-1.298829	-0.698914
7	-3.845904	0.409406	-0.251281
7	-1.333092	0.451697	-0.106803
7	-3.478602	-0.882090	-0.412908
6	-2.283203	1.124446	0.207358
7	-2.572633	-1.097536	-1.292221
6	-2.580413	2.407110	0.904857
1	-1.646376	2.946929	1.073584
1	-3.259399	3.019348	0.301563
1	-3.082294	2.203274	1.856423
1	-2.136491	-2.013633	-1.112227
6	-3.623939	-1.718050	0.792765
1	-4.509406	-1.386367	1.331858
1	-2.718504	-1.606461	1.399642
1	-3.729791	-2.759280	0.484125
1	-3.861989	0.800039	-1.200936

TS(7-Pt^{II})_{enen} (248i)

78	-0.596166	-0.179890	-0.046871
17	-0.797650	-2.444204	-0.683807
17	-0.388707	2.107745	0.648028
7	-2.557937	-0.052023	0.101498
6	-3.706987	0.000389	0.184299
6	-5.158094	0.066086	0.285180
1	-5.504864	1.074783	0.040160
1	-5.474627	-0.181584	1.303255
1	-5.611016	-0.646779	-0.410817
7	3.807478	0.236679	-0.305664
7	1.367027	-0.310865	-0.178969
7	3.286808	1.469508	-0.259658
6	2.433255	-0.831115	-0.008423
7	2.389613	1.672775	-1.140828
6	3.009530	-2.156828	0.361296

1	2.204684	-2.894581	0.375016
1	3.769428	-2.448372	-0.371010
1	3.482533	-2.118936	1.350035
1	1.816346	2.471549	-0.840207
6	3.331862	2.245480	1.002845
1	4.284244	2.067601	1.504985
1	2.484612	1.924295	1.619354
1	3.236006	3.305254	0.763404
1	4.473367	0.141423	0.464141

TS(7-Pt^{II})₁

78	0.582047	-1.321007	-0.269642
17	0.723429	-0.700100	-2.558496
17	0.450805	-1.901194	2.037996
7	-1.400982	-1.161669	-0.347110
6	-2.549061	-1.068590	-0.402018
6	-3.999394	-0.958976	-0.475806
1	-4.349638	-1.315012	-1.449647
1	-4.305143	0.084097	-0.347851
1	-4.458756	-1.564306	0.311726
7	3.574545	0.719904	0.568641
7	2.536724	-1.590566	-0.233231
7	2.365179	1.195615	0.894125
6	3.568641	-1.029674	0.014203
7	1.421677	1.321691	0.054550
6	5.025562	-1.338145	-0.042859
1	5.157681	-2.340287	-0.455574
1	5.537789	-0.606838	-0.675124
1	5.476024	-1.306163	0.955868
6	1.992070	1.362433	2.313591
1	2.852533	1.741045	2.868670
1	1.675615	0.378128	2.679599
1	1.162347	2.064985	2.358975
1	4.143931	0.731373	1.416775
1	1.789876	1.119346	-0.885331

TS(7-Pt^{IV})_{exex} (172i; 2i)

Pt	-0.542356	-0.072626	-0.101190
Cl	-0.705150	-2.008027	1.290866
Cl	-0.347022	-1.479584	-2.033279
Cl	-0.743340	1.327416	1.825696
Cl	-0.334753	1.867795	-1.502899
N	-2.548081	-0.050004	-0.316276
C	-3.690646	-0.054486	-0.437051
C	-5.137391	-0.059397	-0.589485
H	-5.476390	-1.066300	-0.850901
H	-5.426407	0.636659	-1.382605
H	-5.607002	0.247729	0.349791
N	3.913289	0.134300	-0.036173

N	1.433382	-0.038460	0.076842
N	3.650617	1.247329	0.688092
C	2.367411	-0.794014	0.022058
N	2.869193	2.185400	0.380938
C	2.748868	-2.224702	-0.080272
H	1.834283	-2.815687	-0.162699
H	3.382611	-2.384635	-0.958478
H	3.317459	-2.523321	0.805542
H	2.493643	2.037669	-0.565506
C	4.104027	1.179356	2.089071
H	5.161203	0.916447	2.098060
H	3.515730	0.402820	2.586590
H	3.913168	2.146817	2.548042
H	3.827525	0.406941	-1.021394

TS(7-Pt^{IV})_{exen} (231i)

78	-0.352171	-0.361411	-0.110732
17	0.680951	-1.256256	1.864640
17	0.659406	-2.070113	-1.426837
17	-1.391638	1.352579	1.235403
17	-1.382039	0.538777	-2.065657
7	-1.960440	-1.547254	0.170664
6	-2.865951	-2.239613	0.314559
6	-4.013742	-3.115070	0.494413
1	-4.355526	-3.066505	1.532615
1	-3.731817	-4.144630	0.254314
1	-4.824506	-2.798462	-0.168589
7	3.050956	2.503528	-0.207121
7	1.213382	0.830424	-0.341490
7	2.008852	3.114763	0.400326
6	2.417559	0.847685	-0.371400
7	0.945298	3.254126	-0.274629
6	3.599039	-0.050408	-0.463600
1	3.251590	-1.067343	-0.654584
1	4.264708	0.279867	-1.268086
1	4.161049	-0.009150	0.474252
1	0.164794	3.481881	0.356979
6	2.034882	3.050723	1.875592
1	3.065032	3.178130	2.202634
1	1.640126	2.072737	2.173824
1	1.398811	3.843577	2.270408
1	2.964433	2.766194	-1.196607

TS(7-Pt^{IV})_{enen} (189i)

78	-0.521651	0.073465	0.050307
17	-1.063841	2.390679	0.176084
17	-0.005397	-2.281378	-0.103300
7	-2.467064	-0.362254	-0.193944
6	-3.585154	-0.590289	-0.325924

6	-5.000987	-0.880383	-0.490587
1	-5.395456	-0.318319	-1.342380
1	-5.542160	-0.591234	0.415339
1	-5.139350	-1.951111	-0.668069
7	3.944102	0.345497	0.200094
7	1.400787	0.489579	0.253966
7	3.605686	-0.941945	0.218659
6	2.306520	1.235788	0.063801
7	2.923916	-1.308566	1.219807
6	2.684435	2.636258	-0.245075
1	1.772892	3.238170	-0.262334
1	3.374588	3.008384	0.517678
1	3.176985	2.697846	-1.221627
1	2.506196	-2.223539	1.015594
6	3.671665	-1.739775	-1.033574
1	4.572159	-1.467244	-1.586212
1	2.767612	-1.514599	-1.609473
1	3.701616	-2.798240	-0.774366
1	4.451157	0.520256	-0.670729
17	-0.246542	0.260101	-2.331725
17	-0.794122	-0.125664	2.409573

TS(8-L)ex (403i)

7	1.248490	-0.316683	0.111646
7	-1.402117	0.193291	0.079509
8	0.599905	-1.346587	-0.434132
6	-0.438268	0.895092	0.035801
7	-0.440195	-1.744304	0.275358
6	0.155332	2.245241	-0.071804
1	-0.630392	3.006397	-0.071867
1	0.836124	2.430360	0.765024
1	0.739267	2.317889	-0.993476
1	-0.939909	-2.344300	-0.400565
1	1.050041	-0.405779	1.124369

TS(8-L)en (366i)

7	0.852388	0.899123	-0.174374
7	-1.088475	-0.952655	-0.017188
8	-0.289312	1.523689	0.174143
6	0.094809	-0.996016	0.106600
7	-1.270091	1.155227	-0.614794
6	1.330242	-1.778774	0.323601
1	1.104128	-2.848960	0.322869
1	2.049970	-1.558635	-0.470685
1	1.790779	-1.517700	1.282440
1	-2.085598	1.510433	-0.089794
1	1.448152	1.162216	0.625307

TS(8-Pt^{II})ex (307i)

78	0.447540	0.048950	0.004404
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17	0.639975	2.398817	-0.185615
17	0.288134	-2.317163	0.225309
7	2.406924	-0.103641	-0.007895
6	3.557189	-0.173917	-0.009522
6	5.010317	-0.260565	-0.012997
1	5.367280	-0.573416	0.973164
1	5.438965	0.716724	-0.255254
1	5.338364	-0.991242	-0.758767
7	-4.118716	-0.227235	-0.371116
7	-1.523812	0.281571	0.058363
8	-3.492475	-1.400201	-0.298437
6	-2.522182	0.850191	0.342037
7	-2.488601	-1.535847	-1.116580
6	-3.192715	1.991266	0.996608
1	-2.430333	2.702091	1.327175
1	-3.877539	2.480591	0.298003
1	-3.779263	1.632022	1.846743
1	-2.000579	-2.372174	-0.753258
1	-3.878189	0.123091	-1.316991

TS(8-Pt^{II})ex₁ (263i)

78	0.603046	-1.459187	-0.307519
17	0.572177	0.158132	-2.054859
17	0.607468	-3.133585	1.368257
7	-1.378271	-1.323393	-0.141087
6	-2.519478	-1.232040	-0.014543
6	-3.962142	-1.120946	0.145309
1	-4.278413	-0.090884	-0.045348
1	-4.243606	-1.400106	1.165259
1	-4.468095	-1.786871	-0.560531
7	3.400445	0.295275	1.360595
7	2.553885	-1.649554	-0.517598
8	2.155866	0.149177	1.885880
6	3.610674	-1.273125	-0.160309
7	1.134111	0.478225	1.158808
6	5.078299	-1.272341	-0.247015
1	5.387280	-1.884275	-1.100074
1	5.437898	-0.248330	-0.376726
1	5.514204	-1.687118	0.667009
1	3.958875	-0.074033	2.142209
1	1.515037	0.960350	0.322044

TS(8-Pt^{II})ex₂ (228i)

78	0.547687	-0.990890	0.189460
17	0.405498	-1.980899	-1.956185
7	4.267415	0.444990	-0.249753
7	2.497397	-1.166287	0.143703
8	3.242748	1.326453	0.055216
6	3.705930	-0.945214	0.098227

7	2.161928	1.037939	-0.675552
6	4.831053	-1.908787	0.368159
1	1.436902	1.586572	-0.182301
1	4.442001	-2.921606	0.473697
1	5.556187	-1.876242	-0.453589
1	5.350897	-1.605937	1.282855
17	0.643715	0.037273	2.329207
7	-1.426453	-0.913569	0.254756
6	-2.578226	-0.879464	0.286309
6	-4.033229	-0.848021	0.327292
1	-4.437854	-1.664956	-0.278195
1	-4.400366	0.104341	-0.067714
1	-4.377715	-0.962550	1.359694
1	4.314395	0.429927	-1.279486

TS(8-Pt^{II})_{en} (264i)

78	-0.437785	-0.108649	0.077389
17	-0.391984	-2.470854	-0.050878
17	-0.521841	2.267172	0.252002
7	-2.387908	-0.171265	0.304392
6	-3.531069	-0.231045	0.437766
6	-4.975122	-0.309440	0.604421
1	-5.310133	-1.339686	0.449745
1	-5.470427	0.341613	-0.122559
1	-5.251986	0.008972	1.614247
7	3.968528	0.823626	-0.762976
7	1.536029	-0.128033	-0.125363
8	3.183239	1.906397	-0.693178
6	2.632289	-0.549988	-0.025029
7	2.133975	1.802661	-1.442977
6	3.540351	-1.653567	0.343987
1	2.934924	-2.532237	0.583197
1	4.209022	-1.873796	-0.492761
1	4.146765	-1.378904	1.213331
1	1.551419	2.587463	-1.106632
1	4.653695	1.047953	-0.026982

TS(8-Pt^{IV})_{ex} (257i)

Pt	-0.375276	0.035536	0.024446
Cl	-0.401904	1.442341	-1.915832
Cl	-0.588171	1.963694	1.414047
Cl	-0.182118	-1.901755	-1.386045
Cl	-0.378607	-1.367689	1.957502
N	-2.356363	-0.119224	-0.065481
C	-3.500873	-0.195361	-0.118054
C	-4.950222	-0.292899	-0.184590
H	-5.313471	-0.921788	0.633772
H	-5.244552	-0.736013	-1.140738
H	-5.389350	0.705457	-0.097271

N	4.218659	-0.327459	0.119854
N	1.607522	0.250672	0.096717
O	3.581742	-1.341850	-0.455246
C	2.554127	0.950547	0.038585
N	2.648743	-1.889642	0.261720
C	3.203054	2.266159	-0.084645
H	2.424491	3.034264	-0.072242
H	3.902034	2.424356	0.741232
H	3.763660	2.304850	-1.022180
H	2.153194	-2.489361	-0.419690
H	4.018749	-0.451890	1.130422

TS(8-Pt^{IV})_{en} (219i)

78	-0.380327	0.044618	0.020938
17	-0.380104	1.148380	-2.108389
17	-0.654840	2.152286	1.107033
17	-0.140408	-2.076150	-1.088573
17	-0.408503	-1.061732	2.136504
7	-2.356525	-0.150249	-0.084782
6	-3.499940	-0.239778	-0.139457
6	-4.948199	-0.351669	-0.207615
1	-5.238005	-1.406075	-0.168391
1	-5.306630	0.088609	-1.143027
1	-5.396426	0.179051	0.637892
7	4.200390	-0.348132	-0.023435
7	1.590533	0.307352	0.110726
8	3.537138	-1.459302	-0.356548
6	2.559524	0.966954	0.053328
7	2.681530	-1.821607	0.538684
6	3.262116	2.259503	0.040171
1	2.526326	3.046367	0.230168
1	4.035445	2.265456	0.812535
1	3.730435	2.425660	-0.934779
1	2.152630	-2.557896	0.042741
1	4.722893	-0.181047	-0.895409

TS(9-L)_{Oex} (527i)

8	3.739824	0.175393	0.775532
7	1.358472	0.062348	0.137325
7	3.519891	1.347696	0.165933
6	2.294830	-0.649941	0.441739
7	2.336921	1.846668	0.357745
6	2.618918	-2.082885	0.670350
1	1.708441	-2.684785	0.639340
1	3.318332	-2.441651	-0.091522
1	3.103522	-2.200477	1.645004
1	2.108685	1.699588	1.343204
6	4.011672	1.399523	-1.215258
1	3.442184	0.690438	-1.826961

1	5.068528	1.132132	-1.208381
1	3.873837	2.413522	-1.590663

TS(9-L)Oen (505i)

8	-0.987508	0.337069	-0.233855
7	1.493153	0.256605	-0.257324
7	-0.692125	-0.944792	-0.400953
6	0.588322	0.984577	0.091536
7	0.332318	-1.065244	-1.207128
6	0.325627	2.305109	0.713740
1	1.256282	2.866377	0.822666
1	-0.371627	2.870941	0.087101
1	-0.140697	2.179063	1.696091
1	0.774786	-1.975885	-1.018859
6	-0.773627	-1.727021	0.846455
1	-1.747065	-1.538428	1.299450
1	0.030517	-1.411132	1.522105
1	-0.677488	-2.789460	0.609740

TS(9-L)Mex (463i)

8	-2.550897	-0.407605	-1.537749
7	-1.353236	0.419935	-0.097278
7	-3.562443	-0.570666	-0.776065
6	-2.274061	0.882245	0.555170
7	-3.856990	0.506689	-0.013506
6	-2.398351	1.731397	1.779567
1	-1.416398	2.074802	2.110215
1	-3.035624	2.598998	1.573927
1	-2.878393	1.159445	2.579811
1	-3.915111	1.290191	-0.674035
6	-3.632802	-1.854566	-0.065342
1	-2.785413	-1.922634	0.627438
1	-3.560325	-2.648521	-0.808773
1	-4.579074	-1.911641	0.472775

TS(9-L)Men (384i)

8	2.592663	1.583495	1.050816
7	1.400393	-0.046987	0.355341
7	3.471000	1.463732	0.152886
6	2.370566	-0.611649	-0.122308
7	3.825712	0.168676	-0.008182
6	2.593974	-1.948495	-0.768343
1	1.699520	-2.564879	-0.668785
1	2.827501	-1.839395	-1.834335
1	3.438619	-2.453152	-0.286175
1	4.354910	0.076380	-0.881746
6	3.283864	2.309135	-1.045584
1	3.151350	3.335641	-0.704627
1	2.380375	1.968229	-1.566447
1	4.161310	2.239174	-1.693167

TS(9-Pt^{II})Oex (330i)

78	0.623237	0.013583	0.012514
17	0.630497	2.338701	-0.432497
17	0.551212	-2.316391	0.504230
7	2.590732	-0.042089	-0.141979
6	3.740638	-0.073698	-0.221999
6	5.192567	-0.114660	-0.323508
1	5.564883	-1.071980	0.054080
1	5.631290	0.697300	0.264819
1	5.497436	-0.000779	-1.368566
8	-3.675362	-0.154106	0.578135
7	-1.342288	0.020627	0.190115
7	-3.598299	-0.673334	-0.668823
6	-2.250682	0.433227	0.891600
7	-2.598631	-1.408852	-0.935582
6	-2.413429	1.349082	2.055364
1	-1.428078	1.678855	2.386808
1	-3.012740	2.219562	1.771142
1	-2.931698	0.828756	2.867597
1	-2.296508	-1.921528	-0.101951
6	-4.104600	0.220718	-1.717472
1	-3.448958	1.096617	-1.774219
1	-5.118800	0.516990	-1.449985
1	-4.090585	-0.326577	-2.658893

TS(9-Pt^{II})Oen (349i, 14i)

78	0.597919	0.063737	-0.054798
17	1.036208	2.378555	-0.221123
17	0.155595	-2.281105	0.139301
7	2.536547	-0.282753	0.078617
6	3.671745	-0.467592	0.159307
6	5.105256	-0.702073	0.259084
1	5.310907	-1.776053	0.216250
1	5.484332	-0.302945	1.205077
1	5.621821	-0.205487	-0.568177
8	-3.737317	0.439839	-0.177314
7	-1.349942	0.391487	-0.173027
7	-3.491238	-0.864810	-0.357757
6	-2.298200	1.089042	0.131124
7	-2.559430	-1.043727	-1.216962
6	-2.562910	2.424350	0.729851
1	-1.621062	2.970752	0.800830
1	-3.269442	2.973187	0.098571
1	-3.013353	2.313541	1.721827
1	-2.110903	-1.957803	-1.041432
6	-3.638728	-1.672773	0.867164
1	-4.590398	-1.411627	1.329144
1	-2.799330	-1.449450	1.535453

1	-3.626920	-2.728101	0.590963
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TS(9-Pt^{II})Mex (276i)

78	0.594381	0.062312	-0.026534
17	0.994471	2.338657	-0.535001
17	0.180484	-2.208849	0.550534
7	2.542912	-0.277355	-0.006003
6	3.680028	-0.465084	0.018155
6	5.115977	-0.702471	0.045131
1	5.517030	-0.455290	1.033833
1	5.609898	-0.077631	-0.705716
1	5.323474	-1.755288	-0.171016
8	-2.591333	-0.458576	-1.600202
7	-1.328747	0.399249	0.006022
7	-3.514694	-0.582230	-0.765270
6	-2.283258	0.886364	0.584917
7	-3.767189	0.524007	-0.011293
6	-2.429395	1.766732	1.787376
1	-1.451957	2.159471	2.070894
1	-3.113116	2.593854	1.567909
1	-2.859968	1.190103	2.612555
1	-3.866362	1.295281	-0.681629
6	-3.638725	-1.872672	-0.071525
1	-2.712834	-2.035350	0.498435
1	-3.727727	-2.647507	-0.833168
1	-4.516274	-1.843845	0.572729

TS(9-Pt^{II})Men (82i)

78	-0.604242	0.075580	-0.065422
17	-1.142164	2.333552	-0.515166
17	-0.051252	-2.178531	0.496781
7	-2.533426	-0.362179	0.028208
6	-3.658996	-0.603395	0.095929
6	-5.080177	-0.908778	0.178190
1	-5.575476	-0.633933	-0.758304
1	-5.536405	-0.346931	0.999253
1	-5.220849	-1.979287	0.356381
8	2.776756	-0.402086	-1.578335
7	1.307564	0.484512	-0.128412
7	3.604442	-0.523250	-0.661080
6	2.222012	0.950518	0.540652
7	3.672084	0.587626	0.114569
6	2.226991	1.855811	1.742187
1	1.258119	2.352493	1.810022
1	2.397837	1.280127	2.659831
1	3.018980	2.606146	1.643860
1	4.263308	0.419082	0.929994
6	3.754318	-1.861225	-0.046649
1	3.931821	-2.570822	-0.853953

1	2.799883	-2.091180	0.450761
1	4.591714	-1.856984	0.654068

TS(9-Pt^{IV})Oex (275i)

78	0.510818	0.000168	0.023423
17	0.495083	1.332690	-1.965348
17	0.520263	-1.331720	2.014147
7	2.509685	-0.211378	-0.138932
6	3.649243	-0.324027	-0.231130
6	5.092060	-0.468517	-0.346901
1	5.399818	-1.432193	0.070571
1	5.587682	0.338309	0.201875
1	5.383194	-0.421191	-1.400827
8	-3.738505	0.572988	0.345834
7	-1.459692	0.149007	0.210419
7	-3.739243	-0.793638	0.244508
6	-2.313324	1.029792	0.096128
7	-2.826822	-1.409331	0.866448
6	-2.355361	2.488189	-0.208653
1	-1.344947	2.892135	-0.163683
1	-2.772787	2.642100	-1.208773
1	-3.002305	2.990543	0.517673
1	-2.585562	-0.917053	1.730194
6	-4.145101	-1.285716	-1.078604
1	-3.371810	-1.005947	-1.802521
1	-5.101791	-0.828827	-1.330228
1	-4.228286	-2.369675	-1.015695
17	0.205778	-1.959375	-1.312160
17	0.841618	1.964256	1.357612

TS(9-Pt^{IV})Oen (266i)

78	-0.456135	-0.094865	-0.198850
17	-0.349589	-1.569929	1.693771
17	-0.262107	-1.952694	-1.676083
17	-0.674784	1.786810	1.298979
17	-0.563348	1.384758	-2.066991
7	-2.461541	-0.288974	-0.254831
6	-3.601496	-0.423956	-0.301837
6	-5.044741	-0.594924	-0.363147
1	-5.474793	-0.458968	0.633664
1	-5.279873	-1.600626	-0.724368
1	-5.473692	0.144075	-1.046510
8	3.769782	0.356500	0.521373
7	1.508775	0.140384	-0.093236
7	3.249592	1.497357	1.007848
6	2.534452	-0.504274	0.050403
7	2.494684	2.063799	0.158480
6	3.012754	-1.907168	-0.063024
1	2.231702	-2.508451	-0.528800

1	3.926007	-1.932085	-0.666522
1	3.245039	-2.301586	0.930934
1	1.836006	2.686862	0.652895
6	3.009104	1.466718	2.463846
1	3.915042	1.099291	2.944787
1	2.159208	0.800915	2.655205
1	2.781715	2.479669	2.798306

TS(9-Pt^{IV})Mex (230i)

78	-0.500579	0.014866	0.051278
17	-0.885619	2.006701	1.320975
17	-0.115226	-1.967670	-1.237428
7	-2.484615	-0.231223	-0.162477
6	-3.619309	-0.359472	-0.286388
6	-5.055988	-0.524183	-0.442032
1	-5.309681	-1.588597	-0.410681
1	-5.372565	-0.104503	-1.402208
1	-5.575475	-0.004249	0.369289
8	2.815026	-1.300625	0.977890
7	1.457719	0.238898	0.243199
7	3.681862	-0.839615	0.220109
6	2.340811	1.066798	0.063461
7	3.845114	0.519537	0.273802
6	2.384424	2.511452	-0.326936
1	1.386915	2.939916	-0.234149
1	3.096838	3.045780	0.310954
1	2.730357	2.590454	-1.362179
1	3.989269	0.747830	1.264404
6	3.847816	-1.458972	-1.104007
1	2.910990	-1.303915	-1.656414
1	3.998792	-2.527151	-0.949243
1	4.697097	-0.997866	-1.605034
17	-0.587295	-1.277582	2.054063
17	-0.463313	1.301724	-1.978315

TS(9-Pt^{IV})Men (155i)

78	0.485326	0.022188	0.066357
17	0.931451	2.093509	1.180766
17	0.073895	-2.043383	-1.075148
7	2.459783	-0.222069	-0.237459
6	3.588265	-0.354129	-0.406181
6	5.017118	-0.525019	-0.617535
1	5.215239	-0.687256	-1.681635
1	5.371624	-1.389286	-0.047212
1	5.548116	0.371619	-0.282922
8	-2.695154	-1.197623	0.989901
7	-1.465823	0.226477	0.369233
7	-3.662938	-0.849865	0.263560
6	-2.373560	1.040065	0.101705

7	-3.744974	0.532707	0.300499
6	-2.316402	2.470521	-0.355173
1	-1.346816	2.895443	-0.097774
1	-2.442945	2.520645	-1.441286
1	-3.117915	3.035121	0.133571
1	-4.419927	0.899689	-0.368501
6	-3.783859	-1.519054	-1.051894
1	-3.829100	-2.590883	-0.862151
1	-2.889335	-1.285585	-1.643635
1	-4.697925	-1.181536	-1.545444
17	0.325575	1.163402	-2.047344
17	0.698108	-1.133832	2.139638

TS(10-L)O (384i)

O	1.132942	0.491915	-0.030947
N	-1.346557	-0.392746	-0.098655
O	0.314873	1.424543	0.484900
C	-0.286902	-0.936561	-0.081940
N	-0.721937	1.557468	-0.293721
C	0.589670	-2.118239	-0.079080
H	-0.004577	-3.027815	-0.205354
H	1.312902	-2.037406	-0.896090
H	1.145774	-2.169517	0.860963
H	-1.373763	2.078819	0.321611

TS(10-L)M (413i)

O	0.759366	0.053893	1.667249
N	1.357888	0.231780	-0.421845
O	-0.290851	-0.663011	1.394242
C	0.256483	0.198874	-0.887385
N	-1.057498	-0.025337	0.508572
C	-0.561574	0.324438	-2.120402
H	0.064534	0.667462	-2.947273
H	-1.005760	-0.639339	-2.391553
H	-1.370173	1.042915	-1.953310
H	-1.708902	-0.783058	0.239838

TS(10-Pt^{II})O (321i; 10i)

78	-0.437035	-0.116396	-0.009872
17	-0.262965	-2.299313	-0.898821
17	-0.641459	2.072424	0.910321
7	-2.390363	-0.321396	0.074653
6	-3.533324	-0.462056	0.118110
6	-4.977097	-0.640179	0.170932
1	-5.247186	-1.235368	1.048796
1	-5.319858	-1.158322	-0.730019
1	-5.470190	0.334661	0.234314
8	3.944904	0.956008	-0.070205
7	1.542486	0.018166	-0.094576
8	3.194842	1.962541	0.413349

6	2.639829	-0.429890	-0.108716
7	2.206910	2.200313	-0.366131
6	3.538512	-1.596926	-0.143892
1	2.930910	-2.490296	-0.309331
1	4.263622	-1.478055	-0.954319
1	4.085354	-1.676797	0.799850
1	1.582545	2.786507	0.223852

TS(10-Pt^{II})M (349i)

78	0.429864	0.036406	-0.109009
17	0.585147	2.390217	0.080653
17	0.297635	-2.323229	-0.337830
7	2.387552	-0.092046	0.072449
6	3.532490	-0.163100	0.179186
6	4.978799	-0.250765	0.314568
1	5.286213	0.154867	1.283455
1	5.461831	0.324274	-0.481568
1	5.295534	-1.295893	0.245831
8	-2.182159	0.110063	1.982453
7	-1.488859	0.151775	-0.356472
8	-3.188432	-0.618246	1.620371
6	-2.615180	0.160419	-0.730260
7	-3.868042	-0.044849	0.638498
6	-3.452635	0.333056	-1.947065
1	-2.825332	0.703310	-2.760603
1	-3.894671	-0.623871	-2.244356
1	-4.255556	1.046855	-1.740998
1	-4.515368	-0.804366	0.370435

TS(10-Pt^{IV})O (288i; 15i)

78	-0.365183	-0.098778	-0.015285
17	-0.163002	-0.833651	2.256067
17	-0.171248	-2.356142	-0.759757
17	-0.595277	2.172421	0.748546
17	-0.581197	0.636988	-2.278113
7	-2.339433	-0.313312	0.093523
6	-3.476919	-0.458512	0.153153
6	-4.917333	-0.642802	0.228339
1	-5.143261	-1.702193	0.382977
1	-5.379394	-0.305831	-0.704472
1	-5.318965	-0.060870	1.063327
8	4.020944	0.965534	-0.039370
7	1.617609	0.065075	-0.113063
8	3.270597	2.003879	0.363865
6	2.691967	-0.424077	-0.069019
7	2.330892	2.237457	-0.465357
6	3.584949	-1.591065	-0.017862
1	2.973952	-2.486808	-0.157246
1	4.336484	-1.514697	-0.808662

1	4.093367	-1.624372	0.949457
1	1.712638	2.884839	0.062898

TS(10-Pt^{IV})M (315i)

78	0.380420	0.041986	0.029102
17	0.541159	2.441067	-0.113704
17	0.285281	-2.331061	0.157863
7	2.358763	-0.080218	-0.047860
6	3.504359	-0.141661	-0.090127
6	4.955195	-0.222334	-0.141849
1	5.384129	0.363028	0.677033
1	5.311323	0.174656	-1.097208
1	5.267630	-1.266349	-0.043649
8	-2.696816	-1.570813	1.096015
7	-1.595115	0.245488	0.077026
8	-3.687366	-1.389633	0.299272
6	-2.570553	0.871628	-0.155700
7	-4.127963	-0.143615	0.329660
6	-3.135165	2.155258	-0.632221
1	-2.306113	2.862798	-0.713845
1	-3.602522	2.024511	-1.613526
1	-3.881765	2.517828	0.079816
1	-4.790954	-0.145424	-0.462846
17	0.271663	-0.083454	-2.364352
17	0.492263	0.180835	2.410569

TS(11-L) (496i)

O	0.980947	-0.263977	0.014598
N	-1.394744	-0.507502	-0.384034
N	0.646017	0.912030	-0.534772
C	-0.446276	-0.968303	0.235814
O	-0.247551	0.768429	-1.413602
C	-0.216645	-2.091511	1.189553
H	-1.110447	-2.712923	1.260267
H	0.625570	-2.696722	0.838458
H	0.039432	-1.703820	2.180585
C	0.439664	1.983730	0.457066
H	1.318798	2.038344	1.099495
H	-0.459187	1.747302	1.038955
H	0.299289	2.917011	-0.088684

TS(11-Pt^{II}) (234i)

78	0.586056	0.054601	-0.062164
17	1.023923	2.337643	-0.499155
17	0.146568	-2.223999	0.461724
7	2.532833	-0.294177	0.030833
6	3.667567	-0.485283	0.098048
6	5.100607	-0.727320	0.180668
1	5.540584	-0.704960	-0.821226
1	5.286805	-1.706941	0.631396

1	5.573569	0.045806	0.794145
8	-3.664472	0.545979	0.117167
7	-1.335626	0.399384	-0.110746
7	-3.556627	-0.565361	-0.673723
6	-2.266091	0.915305	0.505864
8	-2.654300	-0.440060	-1.514632
6	-2.323837	1.894681	1.633990
1	-1.347956	2.368835	1.743745
1	-3.086551	2.649367	1.418326
1	-2.598751	1.381904	2.561637
6	-3.660557	-1.831716	0.075715
1	-4.516242	-1.768575	0.747089
1	-2.714492	-1.973687	0.618181
1	-3.788531	-2.629609	-0.655677

TS(11-Pt^{IV}) (235i)

78	-0.487543	0.014848	0.063457
17	-0.342076	1.187407	-2.030860
17	-0.900496	2.074952	1.207938
17	-0.096194	-2.039906	-1.104483
17	-0.673308	-1.167000	2.125544
7	-2.460909	-0.211388	-0.214700
6	-3.592545	-0.331172	-0.370156
6	-5.025456	-0.485697	-0.564832
1	-5.562543	0.034358	0.234626
1	-5.286246	-1.548518	-0.544196
1	-5.313591	-0.060412	-1.531283
8	3.749410	0.528539	0.210589
7	1.467595	0.216376	0.330551
7	3.645792	-0.849206	0.263451
6	2.374157	1.025853	0.086133
8	2.719826	-1.183999	1.015744
6	2.397843	2.464757	-0.314422
1	1.413902	2.901112	-0.147935
1	3.157986	2.979851	0.281690
1	2.664380	2.544936	-1.372328
6	3.765022	-1.489428	-1.060949
1	4.643530	-1.083944	-1.561389
1	2.840781	-1.284948	-1.617315
1	3.864412	-2.560886	-0.888691

TS(12-L) (442i)

8	3.999049	0.850047	0.319635
7	1.551874	0.149170	-0.037145
8	3.303319	1.385422	1.321809
6	2.625288	-0.287101	-0.339823
8	2.207629	1.885603	0.873325
6	3.434683	-1.317987	-1.020631
1	2.781532	-1.985755	-1.587468

1	4.143874	-0.834182	-1.698977
1	4.002869	-1.894571	-0.285436

TS(12-Pt^{II}) (364i)

78	0.443204	0.019329	0.027026
17	0.715009	2.354040	-0.338750
17	0.250449	-2.282518	0.385797
7	2.415078	-0.142247	0.027106
6	3.565366	-0.203058	0.024137
6	5.018714	-0.278010	0.020393
1	5.347149	-1.150104	0.594013
1	5.436704	0.627594	0.470728
1	5.383491	-0.367198	-1.007573
8	-3.967328	-0.145053	0.036314
7	-1.482903	0.284207	0.023769
8	-3.574420	-1.335738	0.520864
6	-2.510986	0.882250	0.034939
8	-2.652465	-1.861542	-0.177955
6	-3.127894	2.229516	0.025895
1	-2.335023	2.962600	-0.136580
1	-3.872063	2.285528	-0.774194
1	-3.629252	2.415635	0.979944

TS(12-Pt^{II})₁ (282i)

78	0.510823	-1.336898	0.124833
17	0.442780	-1.999555	-2.148332
17	0.493618	-0.909905	2.459500
7	-1.490393	-1.111378	0.099971
6	-2.629975	-0.948778	0.085097
6	-4.071345	-0.748253	0.069023
1	-4.457827	-0.765673	1.092581
1	-4.549267	-1.543255	-0.511436
1	-4.304906	0.218695	-0.386957
8	3.052287	0.860873	-0.471996
7	2.457941	-1.668871	0.169096
8	1.932269	1.223985	0.145748
6	3.456007	-1.059703	-0.006707
8	0.840140	0.785075	-0.433617
6	4.916795	-0.961591	-0.100020
1	5.349460	-1.961948	-0.006934
1	5.190870	-0.527488	-1.065450
1	5.295704	-0.313371	0.694159

TS(12-Pt^{II})₂ (199i)

78	0.582664	-0.873726	-0.029411
17	0.672013	0.521814	-1.935375
8	4.105864	-0.042834	1.490485
7	2.501416	-0.994428	0.046704
8	2.887189	0.542146	2.151933
6	3.662756	-0.900390	0.478955

8	2.108040	0.967809	1.241763
6	4.833648	-1.704378	-0.038370
1	4.534969	-2.259790	-0.927450
1	5.652205	-1.019430	-0.281517
1	5.168455	-2.394310	0.741748
17	0.444024	-2.257843	1.893135
7	-1.409563	-0.821503	-0.113076
6	-2.560025	-0.766134	-0.137724
6	-4.013402	-0.700893	-0.173920
1	-4.346894	0.305792	0.096509
1	-4.434051	-1.420912	0.534605
1	-4.370077	-0.936441	-1.181383

TS(12-Pt^{IV}) (377i; 14i)

78	-0.368569	-0.063289	-0.031109
17	-0.228516	-1.263715	2.036620
17	-0.161030	-2.130128	-1.242022
17	-0.635703	1.968406	1.167968
17	-0.502393	1.126786	-2.100901
7	-2.340464	-0.297629	-0.041337
6	-3.477627	-0.454043	-0.063612
6	-4.917724	-0.651400	-0.093079
1	-5.372246	0.069238	-0.779620
1	-5.328824	-0.506366	0.910472
1	-5.140659	-1.667187	-0.433371
8	3.986855	0.795733	0.212062
7	1.603235	0.096590	-0.055101
8	3.397219	1.585700	1.118540
6	2.684043	-0.347080	-0.269340
8	2.375582	2.160085	0.647582
6	3.482414	-1.475602	-0.793085
1	2.788882	-2.179169	-1.258791
1	4.205999	-1.102281	-1.523542
1	4.021857	-1.956732	0.027349

I(1-Pt^{II}) (15i)

Pt	-0.279083	-0.355437	-0.014630
Cl	-0.294590	-0.608958	-2.384620
C	2.631155	1.138193	-0.586135
N	1.566020	-1.049794	0.033784
N	1.646933	1.919900	0.128700
C	2.605423	-0.382467	-0.217244
C	0.345870	1.771659	-0.253456
H	0.180322	1.834031	-1.325980
C	3.962069	-1.053775	-0.247598
C	1.956578	2.188664	1.533669
H	-0.365616	2.316398	0.362016
H	3.854832	-2.125940	-0.075417
H	4.447093	-0.895175	-1.220245

H	4.623177	-0.629040	0.519263
H	1.936206	1.269901	2.131276
H	2.946120	2.651894	1.591754
H	1.217372	2.881178	1.940487
Cl	-0.373440	-0.215423	2.355334
N	-2.361446	0.005860	-0.067547
C	-3.507016	0.138450	-0.113061
C	-4.954902	0.291661	-0.171358
H	-5.298397	0.921665	0.654692
H	-5.433811	-0.689324	-0.093303
H	-5.243654	0.753718	-1.120284
H	3.625108	1.549650	-0.386723
H	2.440205	1.213594	-1.662996

I(2-Pt^{II}) (no)

Pt	-0.131819	-0.284545	0.026076
Cl	-0.176045	-0.483760	-2.344884
C	2.434776	1.727283	-0.327545
N	1.796616	-0.659012	0.011891
O	1.304265	2.186666	0.386741
C	2.693220	0.216058	-0.136936
C	0.090371	1.818551	-0.095901
H	-0.044849	2.000331	-1.166387
C	4.150474	-0.185653	-0.195734
H	-0.687394	2.233110	0.542194
H	4.241589	-1.272699	-0.172718
H	4.618121	0.193306	-1.114134
H	4.698469	0.240991	0.653966
Cl	-0.173152	-0.205372	2.388740
N	-2.270517	-0.288048	0.039538
C	-3.422778	-0.346853	0.050469
C	-4.877048	-0.431928	0.066555
H	-5.236686	-0.439138	1.099911
H	-5.198627	-1.351736	-0.431540
H	-5.308124	0.426121	-0.458057
H	3.281190	2.303447	0.052655
H	2.323618	1.927386	-1.404729

I(3-Pt^{II})Oex (15i)

Pt	-1.030505	-0.544167	0.043616
N	-3.133115	-0.590455	0.105502
C	-4.283891	-0.672511	0.129493
C	-5.735840	-0.789890	0.158693
H	-6.035220	-1.767181	-0.232491
H	-6.187906	-0.007148	-0.458002
H	-6.097148	-0.691173	1.186805
N	1.625535	1.514003	-0.060227
N	0.918277	-0.829259	-0.082922
N	0.447916	1.994318	0.513665

C	1.789674	0.071756	-0.215570
C	-0.752369	1.638566	-0.039698
C	3.232358	-0.263022	-0.520596
H	3.324488	-1.328142	-0.734755
H	3.582455	0.303726	-1.393894
H	3.875391	0.004313	0.324956
H	-1.608607	2.045242	0.494327
C	0.578558	2.225371	1.952590
H	-0.340946	2.682362	2.324348
H	1.418349	2.905386	2.111087
H	0.747223	1.286466	2.490613
H	-0.791929	1.743813	-1.121134
Cl	-1.154929	-0.564851	-2.338237
Cl	-1.019268	-0.747789	2.407153
H	1.868918	2.027258	-0.904252

I(3-Pt^{II})Oen (no)

Pt	0.300121	-0.151603	-0.301965
N	2.344811	0.080844	0.139019
C	3.478439	0.172806	0.334112
C	4.912207	0.282247	0.569086
H	5.455432	-0.291038	-0.188553
H	5.160687	-0.113021	1.558741
H	5.221101	1.330408	0.512532
N	-2.665389	-0.143386	1.099936
N	-1.512940	-0.503848	-1.001299
N	-1.781733	0.818306	1.596146
C	-2.568110	-0.481378	-0.312040
C	-0.489605	0.387137	1.694317
C	-3.899919	-0.920561	-0.878312
H	-3.755763	-1.288950	-1.893899
H	-4.326168	-1.724827	-0.265700
H	-4.617755	-0.090147	-0.896938
H	0.196730	1.157330	2.035291
C	-2.090618	2.208361	1.249315
H	-1.380645	2.867421	1.752313
H	-3.099392	2.437837	1.608308
H	-2.022987	2.371953	0.168293
H	-3.613726	0.087669	1.380496
H	-0.393278	-0.588196	2.161072
Cl	0.468263	-2.419861	0.388296
Cl	0.297544	2.067713	-1.162072

I(3-Pt^{II})Mex (15i)

Pt	-0.199019	-0.383439	-0.224210
N	-2.283396	-0.332507	-0.352684
C	-3.434376	-0.296922	-0.416251
C	-4.888458	-0.258743	-0.497313
H	-5.240274	-0.994661	-1.226855

H	-5.219305	0.736889	-0.808193
H	-5.320953	-0.490663	0.480676
C	2.391818	1.676536	0.397900
N	1.748075	-0.689812	-0.217927
N	1.156056	1.909668	1.108428
C	2.638163	0.155437	0.044108
N	0.005214	1.789979	0.490479
C	4.110695	-0.192157	-0.038612
H	4.229717	-1.215828	-0.396481
H	4.632221	0.489307	-0.723880
H	4.587458	-0.096636	0.945536
C	1.133575	1.630717	2.544169
H	0.222385	2.062260	2.957787
H	2.012148	2.087191	3.006052
H	1.124849	0.547012	2.718558
H	0.143704	2.083604	-0.485406
Cl	-0.034268	0.572222	-2.409733
Cl	-0.396003	-1.434977	1.891347
H	3.223598	2.056803	0.996121
H	2.368680	2.224318	-0.551481

I(3-Pt^{II})Men (no)

Pt	-0.201111	-0.424650	-0.026173
N	-2.297102	-0.480677	-0.029504
C	-3.446744	-0.550214	-0.097369
C	-4.897264	-0.649472	-0.191210
H	-5.178847	-1.658323	-0.508510
H	-5.273864	0.070996	-0.923720
H	-5.350898	-0.442604	0.782758
C	2.223056	1.723449	-0.617531
N	1.752298	-0.686833	-0.085000
N	1.197547	2.197389	0.274059
C	2.591909	0.211542	-0.342262
N	-0.025564	1.831422	-0.054176
C	4.067489	-0.095056	-0.481305
H	4.239195	-1.165576	-0.358876
H	4.429931	0.213973	-1.470718
H	4.653229	0.453640	0.267882
H	-0.627197	2.057248	0.747403
C	1.581668	2.423345	1.673829
H	0.809048	3.021576	2.162436
H	2.525541	2.972679	1.693769
H	1.677913	1.465390	2.198455
Cl	-0.239767	-0.537431	-2.400465
Cl	-0.245490	-0.434675	2.359309
H	3.112127	2.347623	-0.502187
H	1.849575	1.793684	-1.642719

I(4-Pt^{II})O (10i)

78	0.888013	-0.409942	-0.049679
17	0.824572	-0.321733	-2.421709
7	3.492046	1.536883	-0.083250
7	2.819504	-0.784039	-0.115662
8	2.377726	1.915006	0.723612
6	3.713042	0.106297	-0.108216
6	1.200045	1.672986	0.086624
1	1.187128	1.990751	-0.956843
6	5.178549	-0.235535	-0.251141
1	0.397976	2.053716	0.715738
1	5.279851	-1.303192	-0.446506
1	5.623797	0.323514	-1.083065
1	5.728990	0.014414	0.664771
17	0.841306	-0.653142	2.305114
7	-1.238100	-0.378553	-0.034925
6	-2.391006	-0.420298	-0.031518
6	-3.846300	-0.483738	-0.027976
1	-4.232963	-0.121298	0.929273
1	-4.170274	-1.518712	-0.174862
1	-4.248425	0.133617	-0.836933
1	4.266324	2.006646	0.383194

I(4-Pt^{II})M (14i)

Pt	-0.125883	-0.293305	0.002553
Cl	-0.169105	-0.200573	-2.370643
C	2.352232	1.751041	-0.181684
N	1.798167	-0.667853	-0.084980
O	1.323616	2.069561	0.732790
C	2.675902	0.231174	-0.167633
N	0.077961	1.798371	0.223190
C	4.139847	-0.116200	-0.310772
H	-0.491294	1.966201	1.065248
H	4.264500	-1.197177	-0.390256
H	4.559749	0.359655	-1.206559
H	4.704491	0.251408	0.555253
Cl	-0.182166	-0.527077	2.359893
N	-2.263244	-0.258908	-0.001556
C	-3.414791	-0.273424	-0.066031
C	-4.868542	-0.299346	-0.153871
H	-5.305986	0.038541	0.790361
H	-5.207566	-1.319222	-0.359995
H	-5.202976	0.358008	-0.962164
H	3.219344	2.325838	0.150318
H	2.063253	2.047375	-1.197521

I(5-Pt^{II})O (no)

78	0.560771	-1.372971	-0.297591
17	0.637609	-1.584831	-2.664568
8	3.227437	0.678686	-0.464979

7	2.517115	-1.643247	-0.220349
7	2.069318	1.176669	0.093244
6	3.409939	-0.786876	-0.337827
6	0.910728	0.830487	-0.512588
6	4.887095	-1.032887	-0.434813
1	5.075001	-2.106279	-0.470671
1	5.283336	-0.562200	-1.341445
1	5.407588	-0.593761	0.423222
17	0.370177	-1.369811	2.071358
7	-1.508537	-1.398619	-0.414212
6	-2.657093	-1.465000	-0.499644
6	-4.106263	-1.562259	-0.611283
1	-4.580646	-1.100179	0.259749
1	-4.402923	-2.614513	-0.662213
1	-4.445277	-1.053039	-1.518595
6	2.201984	1.442912	1.519193
1	2.321069	0.509426	2.079762
1	1.300304	1.951127	1.865444
1	3.069153	2.092012	1.659705
1	0.034920	1.278018	-0.050666
1	0.954014	0.847494	-1.597025

I(5-Pt^{II})M (no)

78	0.299065	-0.690207	0.375387
17	0.369494	-1.349595	-1.905713
6	2.754747	1.352682	-0.539326
7	2.248155	-0.905291	0.481131
7	1.582517	1.955639	0.009630
6	3.101383	-0.066763	0.123247
8	0.461873	1.440963	-0.328499
6	4.590939	-0.328444	0.185370
1	4.774083	-1.345995	0.533337
1	5.043565	-0.201109	-0.806395
1	5.079448	0.380325	0.865816
17	0.183205	-0.226573	2.707647
7	-1.780894	-0.713867	0.300564
6	-2.931379	-0.720563	0.226352
6	-4.384766	-0.736113	0.130641
1	-4.814718	-0.057556	0.873568
1	-4.758697	-1.748252	0.313154
1	-4.694256	-0.416632	-0.869120
1	2.581370	1.156957	-1.600835
1	3.605102	2.024809	-0.407855
6	1.639115	2.629001	1.307209
1	1.545027	1.878622	2.105371
1	0.795445	3.318104	1.367506
1	2.582205	3.172918	1.390444

I(6-Pt^{II})O (no)

78	0.744109	-0.995321	0.025609
17	0.695028	-1.186858	-2.340085
8	3.442012	0.829296	-0.254644
7	2.664641	-1.428690	0.008640
8	2.341794	1.321549	0.531445
6	3.581621	-0.587859	-0.136345
6	1.153244	1.061901	-0.081864
1	1.144865	1.275441	-1.151456
6	5.041173	-0.915365	-0.284402
1	0.385641	1.561730	0.509524
1	5.163420	-1.997163	-0.346074
1	5.440531	-0.452103	-1.193607
1	5.603140	-0.522638	0.569443
17	0.676463	-0.958130	2.387657
7	-1.364892	-0.877096	0.015570
6	-2.518271	-0.874126	0.003984
6	-3.974577	-0.879486	-0.010829
1	-4.357984	-0.324634	0.850777
1	-4.339187	-1.910247	0.037357
1	-4.339084	-0.414550	-0.931819

I(6-Pt^{II})M (no)

78	0.687616	-0.866546	-0.412077
17	0.623859	-0.014657	-2.626738
6	3.161365	1.088405	0.311020
7	2.610475	-1.166465	-0.594423
8	1.999447	1.116580	1.107880
6	3.483642	-0.326556	-0.262492
8	0.869574	1.035779	0.324560
6	4.957202	-0.606421	-0.453081
1	5.096766	-1.558634	-0.966794
1	5.423591	0.192546	-1.043305
1	5.462607	-0.641684	0.519739
17	0.665150	-1.938550	1.696325
7	-1.438455	-0.789665	-0.335803
6	-2.583262	-0.690646	-0.246613
6	-4.029626	-0.567091	-0.131371
1	-4.293537	-0.257050	0.884281
1	-4.503259	-1.529780	-0.346206
1	-4.395670	0.179688	-0.842345
1	3.071678	1.790664	-0.526653
1	3.963407	1.401962	0.985577

I(7-Pt^{II}) (no)

78	0.644381	-0.787109	-0.002676
17	0.896816	-0.908846	-2.364896
7	3.380476	1.024968	-0.332848
7	2.557003	-1.257733	0.164473
7	2.381147	1.589476	0.419719

6	3.528195	-0.502280	-0.026363
7	1.160548	1.474585	-0.032891
6	4.976484	-0.895141	-0.044307
6	2.710950	1.767585	1.839084
1	0.536229	1.865042	0.684166
1	5.072932	-1.972265	0.100943
1	5.428174	-0.615734	-1.004106
1	5.527643	-0.361996	0.738767
1	2.601493	0.811152	2.362924
1	3.733472	2.139826	1.898772
1	2.019695	2.492823	2.271844
17	0.330161	-0.722510	2.358216
7	-1.397396	-0.603361	-0.254842
6	-2.531267	-0.538062	-0.456760
6	-3.962268	-0.468289	-0.720503
1	-4.475316	0.012716	0.117740
1	-4.364374	-1.477660	-0.852072
1	-4.144549	0.108610	-1.632364
1	3.053060	1.069214	-1.303738

I(8-Pt^{II})_{ex} (10i)

78	0.801139	-0.962814	0.293796
17	0.767877	-1.204932	-2.070423
7	3.276827	1.042972	-0.218776
7	2.737360	-1.291049	0.243604
8	2.271736	1.440294	0.661310
6	3.586484	-0.406648	-0.032019
7	1.010312	1.128694	0.193218
6	5.051634	-0.685093	-0.215315
1	0.452307	1.460993	0.995192
1	5.241255	-1.757791	-0.156319
1	5.386077	-0.311111	-1.191112
1	5.627966	-0.157294	0.552304
17	0.744939	-0.855482	2.655829
7	-1.319219	-0.970587	0.289490
6	-2.470881	-1.010098	0.243626
6	-3.924860	-1.067760	0.182175
1	-4.355226	-0.554873	1.047574
1	-4.253113	-2.111706	0.185833
1	-4.276572	-0.585756	-0.735029
1	2.902677	1.177443	-1.166989

I(10-Pt^{II}) (no)

78	0.795070	-1.055591	0.193673
17	0.738927	-1.141027	-2.184318
8	3.329643	1.013813	-0.025401
7	2.746418	-1.307203	0.155554
8	2.038442	1.407293	0.661516
6	3.578954	-0.371995	0.068471

7	0.965107	0.997937	0.025681
1	1.116964	1.114158	-0.989278
6	5.070229	-0.580381	-0.023722
1	5.280851	-1.647584	-0.099677
1	5.468562	-0.064871	-0.903990
1	5.556754	-0.163951	0.864063
17	0.778836	-1.160874	2.547915
7	-1.329688	-1.080937	0.237880
6	-2.480690	-1.061566	0.299387
6	-3.934286	-1.038383	0.382844
1	-4.244710	-0.438637	1.243836
1	-4.314978	-2.057510	0.500536
1	-4.352195	-0.602711	-0.529669

I(12-Pt^{II}) (no)

78	0.727532	-1.030952	0.254569
17	0.666136	-1.467317	-2.071788
8	3.381141	0.771730	-0.099012
7	2.639900	-1.473902	0.275887
8	2.204638	1.275681	0.590262
6	3.550588	-0.630404	0.104586
8	1.095325	0.944704	-0.075729
6	5.016154	-0.947385	0.011260
1	5.155788	-2.028586	0.038478
1	5.421505	-0.550211	-0.925727
1	5.552729	-0.477942	0.841980
17	0.662951	-0.878270	2.613775
7	-1.376262	-0.797591	0.234910
6	-2.515220	-0.622432	0.228654
6	-3.954311	-0.402252	0.222197
1	-4.204560	0.422105	0.896829
1	-4.469080	-1.308024	0.556731
1	-4.285895	-0.153313	-0.790373