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Photophysical properties of square-planar Pt(II) complexes
from monomers to oligomers

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Isabel Eder BSc

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Univ.-Prof. Dr. Dr. h.c. Leticia Gonzalez Herrero

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Abstract

Platinum(II) complexes can form aggregates such as dimers, trimers or generally called oligomers due to their typical square-planar structure. In the excited state, these are referred to as excimers and usually have altered emissive properties. Currently, excimer emission is linked to at least three types of orbital interaction: d-d orbital interaction based on the platinum centers leading to the so-called metal metal-to-ligand charge transfer (MMLCT), π - π interaction between two ligands and d- π interaction between a platinum center and a ligand. In this thesis, a set of twelve different complexes including bidentate, tridentate, tetradentate ones and a bincuclear pincer complex are studied by the means of density functional theory (DFT) and time-dependent density functional theory (TDDFT).

By analysing geometrical features of the respective optimised monomers, dimers and trimers for both the S_0 and T_1 state, UV-vis absorption spectra, spin density difference plots, natural transition orbitals (NTOs), the one-electron transition density matrix (1TDM) and by comparing phosphorescent rate constants, these complexes are assigned to the three possible interaction schemes. Especially, d-d interaction leading to $^3\text{MMLCT}$ is characterised by close Pt...Pt distances of $\leq 3.0 \text{ \AA}$, overlapping d_{z^2} orbitals building $d\sigma^*$ orbitals visualised in both spin density difference plots and NTOs. Furthermore, the phosphorescent rate constants increase by at least a factor of 10 when comparing dimers to monomers. The $^3\text{MMLCT}$ character can also be attested by analysing the 1TDM. The other two possible interactions are distinguishable with a combined analysis of NTOs and the 1TDM to capture both qualitative and quantitative information of the excitation character.

The results presented in this thesis agree well with experimentally data and allow in principle, to investigate the excimer emission properties of any square-planar platinum(II) complex. This can be used to screen for suitable candidates for applications such as chemosensors, stimuli-responsive or optoelectronic materials.

Zusammenfassung

Platin(II)-Komplexe können aufgrund ihrer typischen quadratisch-planaren Struktur Aggregate wie Dimere, Trimere oder, allgemein gesprochen, Oligomere bilden. Im angeregten Zustand werden diese als Excimere bezeichnet und besitzen normalerweise veränderte Emissionseigenschaften. Zurzeit wird die Emission von Excimeren auf zumindest drei Arten der Orbitalinteraktion zurückgeführt: d-d Orbitalinteraktion, die auf den Platin-Zentralatomen lokalisiert ist und zum sogenannten metal metal-to-ligand charge transfer (MMLCT) führt, d- π Orbitalinteraktion zwischen einem zentralen Platinatom und einem Liganden und π - π Orbitalinteraktion zwischen zwei Liganden. In dieser Arbeit werden insgesamt zwölf verschiedene Komplexe, inklusive zweizähligen, dreizähligen, vierzähligen und einem binuklearen Pincerkomplex mithilfe von Dichtefunktionaltheorie (DFT) und ihrer zeitabhängigen Form (TDDFT) untersucht.

Durch die Analyse der geometrischen Besonderheiten der jeweiligen optimierten S_0 - und T_1 -Strukturen der Monomere, Dimere und Trimere, der UV-vis Absorptionsspektren, Spindichtedifferenzplots, natürlicher Übergangorbitale (NTOs), der Einелеtronübergangsdichtematrix (1TDM) und den Vergleich der Phosphoreszenzgeschwindigkeitskonstanten werden diese Komplexe einer der drei Orbitalinteraktionen zugeordnet. Besonders d-d Orbitalinteraktion, die zu $^3\text{MMLCT}$ führt, wird durch kurze Pt...Pt Distanzen von weniger als 3.0 Å sowie überlappende d_{z^2} -Orbitale, die $d\sigma^*$ -Orbitale bilden und in den Spindichtedifferenzplots sowie den NTOs dargestellt werden können, charakterisiert. Außerdem erhöhen sich die Phosphoreszenzgeschwindigkeitskonstanten der Dimere um zumindest einen Faktor 10 im Vergleich zu Monomeren. Der $^3\text{MMLCT}$ Charakter kann auch über die Analyse der 1TDM nachgewiesen werden. Um die beiden anderen Orbitalinteraktionen zuzuordnen, ist eine kombinierte Analyse der NTOs und der 1TDM nötig, um qualitative und quantitative Information über den Charakter des angeregten Zustandes zu erhalten.

Die Ergebnisse dieser Arbeit stimmen gut mit den experimentellen Daten überein und erlauben es prinzipiell, sämtliche Platin(II)-Komplexe auf ihre Eigenschaften zur Excimeremission zu untersuchen und so geeignete Kandidaten für Chemosensoren, auf Reize reagierende oder optoelektronische Materialien zu finden.

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Abbreviations

1TDM	one-electron transition density matrix
CT	charge transfer
DFT	density functional theory
ECP	effective core potential
GGA	generalised gradient approximation
HOMO	highest occupied molecular orbital
ISC	intersystem crossing
LC	ligand centered
LDA	local density approximation
LLCT	ligand-to-ligand charge transfer
LMCT	ligand-to-metal charge transfer
LSDA	local spin density approximation
LUMO	lowest unoccupied molecular orbital
MC	metal centered
MLCT	metal-to-ligand charge transfer
MMCT	metal-to-metal charge transfer
MMLCT	metal metal-to-ligand charge transfer
NHC	N-heterocyclic carbene
NTO	Natural Transition Orbital
PES	potential energy surface
SOC	spin-orbit coupling
TDA	Tamm-Dancoff approximation
TDDFT	time-dependent density functional theory

1 Introduction

Molecular building blocks are frequently encountered in chemistry: Desoxyribonucleic acid (DNA) consists of four canonical nucleobases, proteins are expressed using 20 different amino acids, membranes can be made up of various phospholipids. Also polymers are synthesised with so-called monomers forming branched or linear chains. Besides the mostly organic building blocks mentioned, also metal complexes can serve as those although they have been much less studied due to their complex electronic structure. Nevertheless, metal complexes are frequently used in photocatalysis,^[1] optoelectronic materials,^[2] bio-imaging,^[3] cancer-therapy^[4] or sensors^[5] making them an interesting compound class for diverse applications. While DNA or proteins in biological systems are synthesised with the help of complex enzymes as DNA-polymerases or transferases, supramolecular assemblies are ordered structures that arrange spontaneously by organising randomly dispersed molecules or building blocks.

The formation of aggregates (ground state) and excimers (excited state) has been reported for various transition metals, e.g. Nickel(II)^[6], Palladium(II)^[7], Gold(I)^[8] and notably Platinum(II)^[9–15]. Nickel, palladium and platinum are located in the tenth group in the periodic table of elements and typically form square-planar metal complexes due to their d^8 electronic structure in their +2 oxidation state. This almost predestines them to build stacking structures in contrary to other commonly used metals used as phosphorescent emitters, namely Iridium(III) or Ruthenium(II) which usually form octahedral complexes due to their d^6 electronic structure.^[16] The stacking can be directed by at least three different intermolecular interactions schematically visualised in Figure 1: (a) d-d orbital interaction based on the metal centers (Figure 1a), (b) π - π orbital interaction based on the ligands (Figure 1b), (c) d- π orbital interaction coming from one metal center and a ligand (Figure 1c). Technically, there is a fourth option of combinations of (a)-(c),^[11] however, this option is not displayed in Figure 1 and also not considered in this investigation.

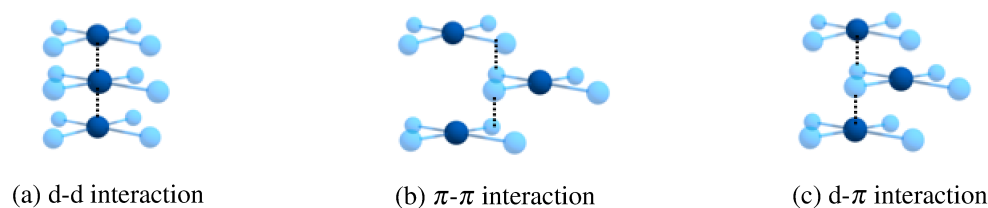


Figure 1: Three different stacking patterns directed by three different interactions. Platinum atoms are depicted in dark blue, the square-planar complex geometry is indicated by the four light blue atoms.

The different stacking patterns are based on different orbital interactions that are further analysed in Figure 2. The characters of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are most important as they typically play the major role in the phosphorescent process going from the T_1 to the S_0 depicted in Figure 3.

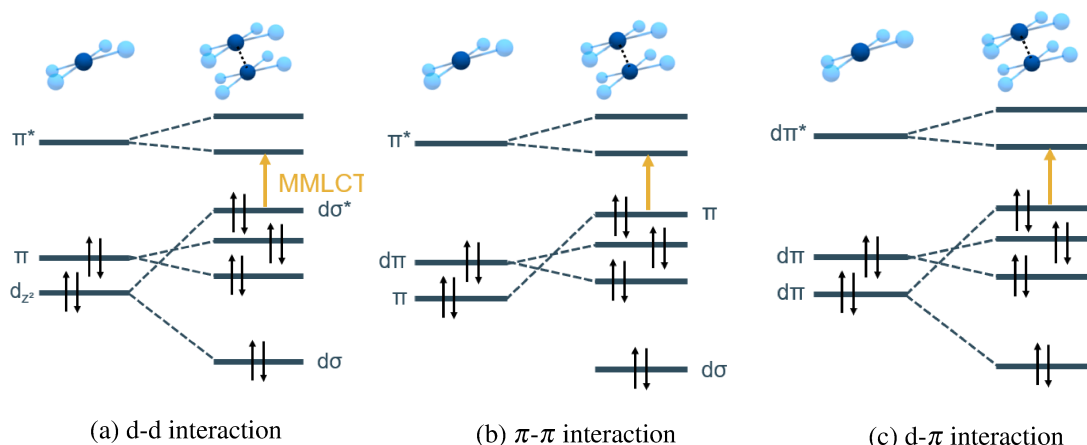


Figure 2: Three possible intermolecular interactions in the formation of aggregates (ground state) and excimers (excited state). The left part of the three subfigures displays the orbital characters of the monomers, whereas the right part depicts the orbital characters for dimers. Note that the number of electrons doubles in the orbital representation for dimers. (a) The overlap of two d_{z^2} orbitals leads to building an occupied $d\sigma$ and $d\sigma^*$ orbital. Excitation of an electron from the HOMO delocalised at the metal centers to the LUMO at the ligand is called MMLCT (metal metal-to-ligand charge transfer). (b) Both HOMO and LUMO are π orbitals located at the ligand. (c) HOMO and LUMO are overlapping $d\pi$ orbitals spread over the metal center and ligands.

For the monomer in Figure 2a, the HOMO is a π -orbital belonging to the ligand, as well as the LUMO being a π^* orbital. However, square-planar platinum(II) complexes have one sterically unhindered axes, the z-axis, where the d_{z^2} is located. In this case, this is the HOMO-1. If two monomers stack to form a dimer, the two d_{z^2} will overlap and build a $d\sigma$ orbital that is the new HOMO delocalised between the two metal centers. The new π^* orbital being the LUMO is energetically lower than the one in the monomer leading to a reduced HOMO-LUMO gap and therefore to a redshift in emissive spectra. The HOMO-LUMO excitation is called metal metal-to-ligand charge transfer (MMLCT), because an electron moves from an $d\sigma$ orbital that as is spread over at least two metal centers to a ligand. This form of interaction is often dominant in linearly stacking complexes with short Pt...Pt contacts. The energy gap between $d\sigma$ and π^* indicated by the orange arrow in Figure 2a is connected to interlayer distance of excimers: Usually, smaller distances reduce the gap and vice versa.^[10,17] For complexes with shifted platinum centers, e.g. due to sterically more demanding ligands, two other kinds of interactions are favoured. One of them is π - π interaction, where both HOMO and LUMO are located on the ligands as π and π^* orbitals (see Figure 2b). If a d-orbital based on a metal center and a π -orbital based on a ligand overlap, the system will be stabilised by $d\pi$ interaction. Here, both HOMO and LUMO are $d\pi$ orbitals (see Figure 2c).

The HOMO-LUMO transition being mostly responsible for the excimer emission is embedded in a photophysical pathway platinum complexes undergo after being excited by light. A very simplified scheme is depicted in Figure 3. After excitation, the complex undergoes ultrafast

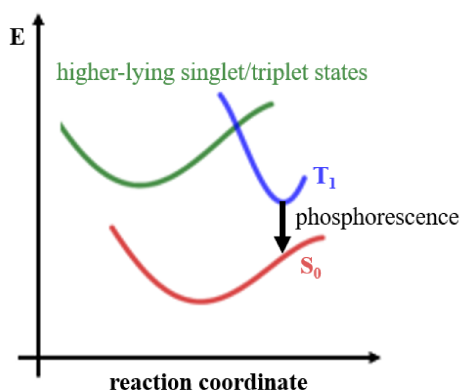


Figure 3: Jablonski scheme. Normally, after excitation the complex proceeds from the ground state S_0 (red) to higher-lying singlet/triplet states (green) until the complex goes to the lowest lying triplet state T_1 (blue). Until here, all processes are ultrafast. The final decay is the radiative phosphorescent decay to S_0 signalled by the black arrow.

intersystem crossing (ISC) processes between the manifold of singlet and triplet excited states (green curve) until it reaches the lowest lying triplet state (T_1 , blue curve). The radiative decay from T_1 to S_0 is called phosphorescence and modulated by the gap visualised by the black arrow.

This thesis investigates different stacking patterns and orbital interactions in a set of twelve different complexes depicted in Figure 4 to shed light on the factors leading to excimer emission and how to computationally analyse them. This is achieved by optimising the S_0 and T_1 state in the monomer, dimer and trimer structures and analysing their geometries, UV-vis absorption spectra and determining phosphorescence rate constants. The choice of complexes was motivated by a variety of factors: the availability of experimental data confirming the formation of excimers as well as experimentally obtained emissive spectra, especially concentration-dependent ones, reasonable atom numbers to ensure feasibility of a computational study, availability of crystal structures and/or previously optimised structures to facilitate optimisation of dimers/trimers. Additionally, a large scope of complexes should be investigated. Besides including similar complexes to determine how little changes influence the complexes' behaviour, we decided on different bidentate and tridentate, one tetradentate and one binuclear complex. The structures of all complexes can be found in Figure 4 with their corresponding numbering.

All complexes from **Pt-1** to **Pt-11** are neutrally charged to avoid considering potential effects of counterions^[12] and possess a square-planar scaffold. Most complexes contain a cyano-ligand because it was found to rise the d_{z^2} orbitals in crystal structures and to support stacking.^[18]

The photophysical properties of the first four bidentate complexes, **Pt-1** to **Pt-4** have already been experimentally investigated with respect to the increasing sterical hindrance of the rest R by Saito et al.^[10] The complexes consist of the platinum(II) metal center, two cyano groups and a 1-alkyl-3-(2-pyridyl)-1H-imidazolium ligand with four different alkyl groups: methyl, ethyl, isopropyl and tertbutyl. This kind of N-heterocyclic carbene ligand acts as strong π -acceptor facilitating

³MMLCT also at shorter wavelengths.^[19] All four complexes show ³MMLCT excimer emission caused by stacking of the complexes. The strength of the typical redshift is modulated by the bulkiness of the ligand as well as the interplanar distances.

Pt(II)(2-(4',6'-difluorophenyl)pyridinato-N,C2')(acetylacetonate), **Pt-5**, showed excimer emission in the experimental study conducted by Cho et al. The bands of the monomeric species can be assigned to ligand centered (LC) and singlet metal-to-ligand charge transfer (MLCT) states.^[11,20] A redshifted peak in concentrated solutions indicates excimer emission that was also observed in the crystal sample. Nevertheless, ³MMLCT was excluded due to shifted Pt metal centers in the crystal structures preventing overlapping d-orbitals. **Pt-6** is a isoquinolinyl pyrazolate complex that has already been studied computationally by Sukpattanacharoen et al.^[14] The spectrum of the monomer is characterised by singlet LC and ¹MLCT states, as well as the T₁ of the dimeric structure being a mixture of ³LC and ³MLCT. For the trimer, ³MMLCT is observed together with ³LC directed by short interlayer distances of approximately 3.3 Å based on Pt...Pt and π - π interaction.^[21]

Four different tridentate complexes studied by Sivchik et al.^[12] were also included in this investigation. All of them possess a cyano ligand and a ⁻C[^]N[^]N ligand, being pyridinyl- for **Pt-7**, benzyltriazolyl- for **Pt-8**, indazolyl- for **Pt-9** and pyrazolyl-phenylpyridine for **Pt-10**. All four complexes display redshifts in the spectra pointing towards excimer emission. However, only the crystal structures of **Pt-7** and **Pt-9** show metallophilic interaction with Pt-Pt distances < 3.3 Å suggesting ³MMLCT. **Pt-10** shows stacking directed by the ligands implying π - π interaction and some mixture of ³MLCT and ligand-to-ligand charge transfer (LLCT). The experimental interpretation of **Pt-8**'s spectrum is complex due to the polycrystalline structure, however, ³MMLCT cannot be excluded.

Pt-11 is the only tetradentate complex in this investigation and was already experimentally studied by Vezzu et al.^[13] This complex consists of a C[^]N^{*}N[^]C ligand (N,N-di(2-phenylpyrid-6-yl)aniline). It also shows excimer emission that has not been experimentally characterised for aggregates, but for the monomer showing mostly ¹MLCT transitions. Diplatinum tetrapyrrophosphate (**Pt-12**) is the only anionic and only binuclear pincer complex in this study with the formula [Pt₂(P₂O₅H₂)₄]⁴⁻. It is experimentally reported to have shortened Pt-Pt bonds in the excited triplet state compared to the ground state by approximately 0.3 Å.^[22]

The goal of this master thesis is to present a computational protocol reliably reproducing experimentally obtained photophysical characteristics of the previously introduced complexes. Close attention is paid to the different causes of excimer emission based on geometrical characteristics of the S₀ and T₁ geometries with respect to the three different possible interactions, the redshift in computed UV-vis absorption spectra, the one-electron transition density matrices to determine the excited-state character and the spin-density plots as well as the natural transition orbitals to confirm the orbitals involved. A second, minor focus is laid on the phosphorescent rate constants of excimer and monomer emission using Einstein's formula^[23,24] and Marcus' theory.^[25,26]

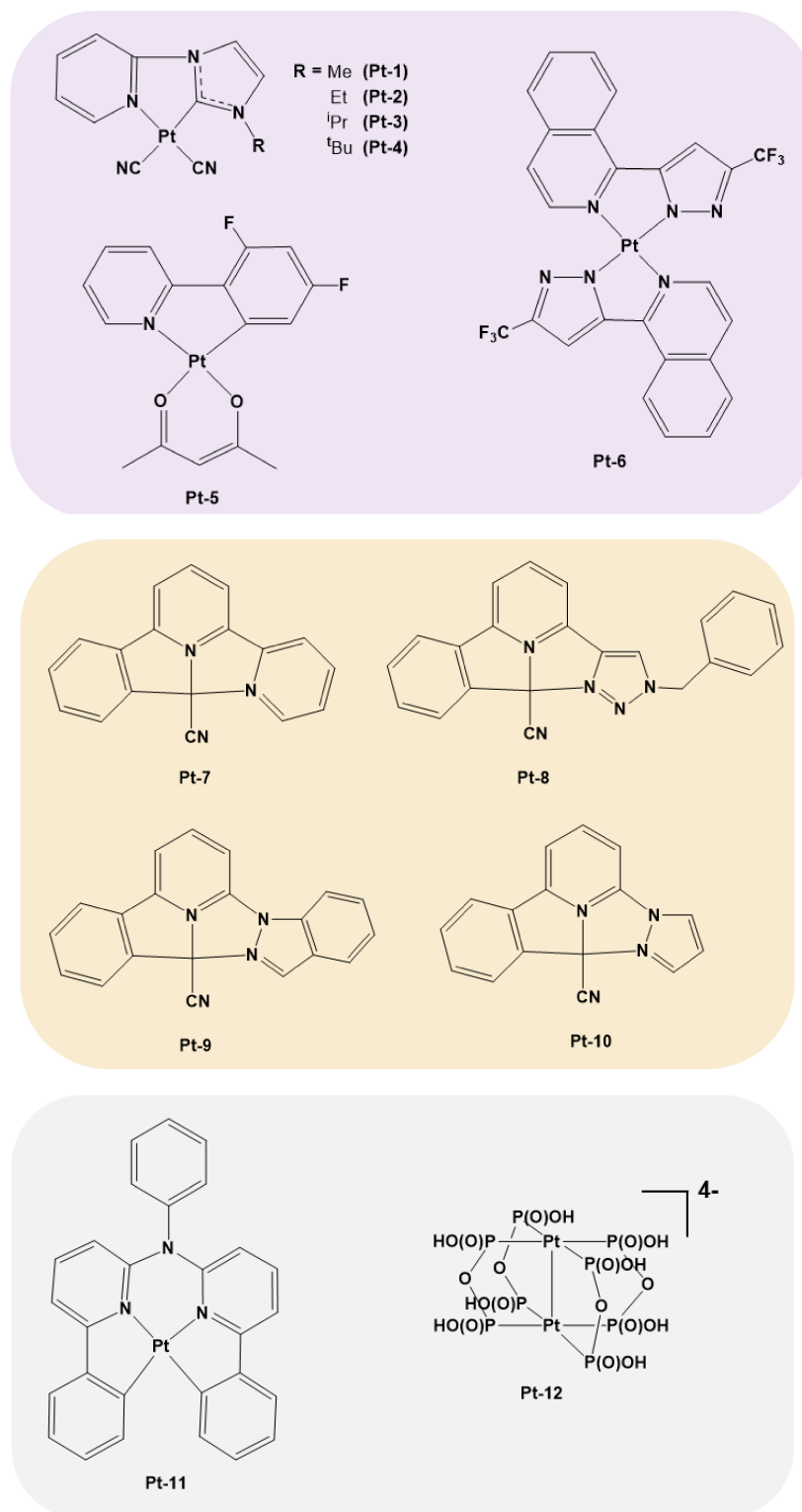


Figure 4: Structure of all twelve studied complexes. Violet background: bidentate complexes, **Pt-1** to **Pt-6**. Orange background: tridentate complexes, **Pt-7** to **Pt-10**. Grey background: tetradentate complex, **Pt-11** and a binuclear pincer complex, **Pt-12**.

2 Theoretical background

The following section will present the basic theoretical concepts used for the performed calculations together with some explanations important for the result analysis. It includes the basic principles of quantum chemistry, density function theory and its time-dependent version as well as information on the one-electron transition density matrix and effective core potentials including relativistic corrections. Additionally, different concepts to calculate phosphorescent rates are discussed.

2.1 Introduction to quantum chemistry

Quantum chemistry is based on the description of a chemical system by a wave function Ψ . Applying different operators on Ψ yields the system's properties. In the famous Schrödinger equation^[27] (eq. 1), an operator called Hamiltonian $\hat{H}$ yields the energy of a system, i.e. E , described by Ψ as eigenvalues.

$$\hat{H}\Psi = E\Psi \quad (1)$$

The Hamiltonian $\hat{H}$ is dependent on the nuclei's positions R and the electron's positions r and consists itself of five different operators describing the kinetic energy of the nuclei $\hat{T}_n$, the kinetic energy of the electrons $\hat{T}_e$, the potential energy between the nuclei $\hat{V}_n$, the potential energy of between electrons $\hat{V}_e$ and the potential energy between nuclei and electrons $\hat{V}_{ne}$ as given in eq. 2 in atomic units. Here, M_I is the mass and Z_I the charge of the nucleus I . Due to the attraction of the nuclei and electrons, V_{ne} 's value is negative and due to the repulsion of likely charges, V_n and V_e 's values are positive.

$$\begin{aligned} \hat{H}(R, r) &= \hat{T}_n(R) + \hat{T}_e(r) + \hat{V}_n(R) + \hat{V}_e(r) + \hat{V}_{ne}(R, r) \\ &= -\sum_I \frac{1}{2M_I} \nabla_I^2 - \sum_i \frac{1}{2} \nabla_i^2 + \sum_{I < J} \frac{Z_I Z_J}{|R_I - R_J|} + \sum_{i < j} \frac{1}{|r_i - r_j|} - \sum_{I, i} \frac{Z_I}{|R_I - r_i|} \end{aligned} \quad (2)$$

This equation is often simplified by the usage of the Born-Oppenheimer Approximation.^[28] It is based on the larger mass of the nuclei leading to their slower movement compared to the electrons. Simply speaking, the position of the nuclei is set fixed and the electrons can easily adapt to the nuclear positions resulting in a constant term for $\hat{V}_n$ and in $\hat{T}_n$ being zero. The remaining three terms in the Hamiltonian given in eq. 2 define a new Hamiltonian, the so-called *electronic* Hamiltonian $\hat{H}_{el}$.

$$(\hat{H}_{el} + \hat{V}_n)\Psi_{el} = E_{el}\Psi_{el} \quad (3)$$

To treat many-electron-systems, their wave function can be written as a so-called Slater determinant. It takes into account that each electron has a spin (α or β) and satisfies the exclusion principle of Pauli demanding an anti-symmetric wave-function: Two electrons in an atom cannot share the same quantum numbers. Therefore, interchanging two electrons has to lead to the

inversion of the wave function's sign - a natural characteristic of determinants that are changing their sign whenever two columns or rows are exchanged. The entries of the determinant are products of the spatial orbital $\psi(i)$ and the spin function $\alpha(i)$ or $\beta(i)$ of the specific electron i .^[29]

$$\chi_i = \psi(i)\alpha(i) \quad (4)$$

$$\Psi = \frac{1}{\sqrt{n!}} \begin{vmatrix} \chi_1(1) & \chi_2(1) & \cdots & \chi_n(1) \\ \chi_1(2) & \chi_2(2) & \cdots & \chi_n(2) \\ \vdots & \vdots & \ddots & \vdots \\ \chi_1(n) & \chi_2(n) & \cdots & \chi_n(n) \end{vmatrix} \quad (5)$$

2.2 Density Functional Theory (DFT)

The Slater determinant introduced in the last section quickly becomes more and more complex with the rising number of electrons with each being dependent on three spatial coordinates and one spin coordinate. With n being the number of electrons, $4n$ variables are therefore needed.^[29] To simplify the description of a chemical system, the electron density ρ can be used which needs only three spatial coordinates for description. Additionally, it contains all information needed: the nuclei's position and charges as well as the total number of electrons n given. The last property is easily accessible by integrating over the electron density over the whole space.

$$n = \int \rho(r) dr \quad (6)$$

The nuclei's positions can be found at the local maxima of $\rho(r)$ because the positively charged nuclei and the negatively charged electrons attract each other. The nuclei's charges can be derived from the electron density's gradient close to the maxima. These three properties are needed to set up the Hamiltonian operator for any system and therefore enable us to solve the Schrödinger equation. (However, this does not help in the question *how* to actually solve the resulting Schrödinger equation.)^[30] Nevertheless, density functional theory (DFT) is often considered the "working horse" of quantum chemistry. The usage of this methodology was justified in 1964, when Hohenberg and Kohn published two important theorems.^[31] The first one is the *Theorem of Existence*. It states that "the energy is a unique functional of the electron density $E[\rho]$ ".^[32] The proof is obtained by the method *reductio ad absurdum*. In principle, two Hamiltonians $\hat{H}^a$ and $\hat{H}^b$ only differing by the external potential V_{ext}^a and V_{ext}^b have two different ground state wave functions ψ^a and ψ^b resulting in two different ground state energies E^a and E^b . It is assumed that these two systems still have the same electron density ρ which is mathematically possible because this property is obtained by integrating a squared wave function.

$$\rho(\vec{r}) = n \int \dots \int |\Psi(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_n)|^2 ds_1 d\vec{x}_2 \dots d\vec{x}_n \quad (7)$$

According to the variational principle, applying $\hat{H}^a$ on Ψ^b yields an energy bigger than E_a :

$$E^a < \langle \Psi^b | \hat{H}^a | \Psi^b \rangle = \langle \Psi^b | \hat{H}^b | \Psi^b \rangle + \langle \Psi^b | \hat{H}^b - \hat{H}^a | \Psi^b \rangle \quad (8)$$

The two Hamiltonians only differ in their external potentials, therefore, eq. 8 can be rewritten as follows:

$$E_a < E_b + \int \rho(\vec{r})(V_{ext}^a - V_{ext}^b) d\vec{r} \quad (9)$$

Repeating the same steps with interchanged properties leads subsequently to

$$E_b < E_a + \int \rho(\vec{r})(V_{ext}^b - V_{ext}^a) d\vec{r} \quad (10)$$

The addition of eq. 9 and eq. 10 leads to an obvious contraction - it is impossible for a sum of two numbers to be bigger than their sum.

$$E_a + E_b < E_b + E_a \quad (11)$$

The second Hohenberg-Kohn Theorem is the *Theorem of Variation*. It simply states that only using the true ground state density will lead to the true (lowest) ground state energy E_0 . Any deviation from the correct ground state density yields a higher ground state energy. This facilitates the usage of DFT as it is no longer necessary to solve the Schrödinger equation but to search for the density functional resulting in the lowest energy.^[30]

2.2.1 Exchange Correlation Functional

Although the two Hohenberg-Kohn theorems set the basis for the usage of DFT, the electronic energy of any given chemical system still has to be computed. The remaining bottleneck is the Schrödinger equation that would be considerably easier to solve with non-interacting electrons. Kohn and Sham suggested taking a hypothetical system with non-interacting electrons which has the same ground state density as another real system with interacting electrons. Then, the electron density consists of five different terms: the kinetic energy term of non-interacting electrons $T_{ni}[\rho(r)]$, the kinetic correction term $\Delta T[\rho(r)]$ to take electron interaction into account, the nuclear-electron interaction $V_{ne}[\rho(r)]$, the classical electron-electron interaction $V_{ee}[\rho(r)]$ and a correction term for the non-classical electron-electron interaction $\Delta V_{ee}[\rho(r)]$.^[29]

$$E[\rho(r)] = T_{ni}[\rho(r)] + V_{ne}[\rho(r)] + V_{ee}[\rho(r)] + \Delta T[\rho(r)] + \Delta V_{ee}[\rho(r)] \quad (12)$$

The two correction terms ΔT and ΔV_{ee} can be rewritten as E_{xc} , the exchange-correlation functional. Knowing the exact E_{xc} functional would provide access to the true, minimum ground state energy. However, E_{xc} remains unknown and therefore has to be approximated. One approach is to ignore this term, another one uses hole functions. If electrons did not have charges or spin, one electron's position (or its probability) would be independent from the position of a second electron. However, electrons are all negatively charged and can have different spins leading to a lower probability of finding one electron nearby a second electron since negative charges repel each other. Exchange-correlation functionals try to approximate these holes, nevertheless, the

success of those functionals describing a chemical system correctly is very system-dependent. Therefore, different functionals have emerged to e.g. describe NMR shifts, delocalised electrons etc. well.^[32] A common approach is to separate E_{xc} in an exchange E_x and a correlation part E_c . E_x only considers exchange energy between electrons with parallel spin, whereas E_c includes correlation energy of electrons with parallel and opposite spin.

An approach to compute E_x is the local density approximation (LDA) assuming that the electron density ρ behaves like uniform electron gas, which is, however, often not accurate enough. When the density of α spins is different to the one of β spins, the local spin density approximation (LSDA) is used. Nevertheless, these methods underestimate the exchange energy and overestimate correlation energy. Including the gradient of the local electron density will improve the methodology if certain requirements for computing the holes are included. The generalised gradient approximation (GGA) uses the density's gradient as a variable and satisfies additional mathematical requirements leading to a reduced error for E_x .^[32] One famous exchange functional was published in 1988 by Becke and is usually abbreviated with B or B88.^[33] Similarly, correlation functionals using GGA have been proposed with one of the most popular being LYP, published by Lee, Yang and Parr.^[34]

Hybrid or hyper-GGA usually include the exact Hartree-Fock exchange energy as well as the one obtained by LSDA and add another term for gradient correction. The most popular example for such a functional is B3LYP.^[35,36] The variables a , b and c in eq. 13 are obtained by fitting experimental data. For B3LYP: $a = 0.20$, $b = 0.72$, $c = 0.81$.

$$E_{xc}^{B3LYP} = (1 - a)E_x^{LSDA} + aE_x^{HF} + b\Delta E_x^{B88} + (1 - c)E_c^{LSDA} + cE_c^{LYP} \quad (13)$$

Despite the broad applications of the B3LYP functional, it is known to regularly fail for charge transfer excitations. Therefore, a modification of B3LYP is used in this work: CAM-B3LYP. The reason for the inaccurate behaviour is the way the long-range exchange potential is treated: In reality, this potential decreases with $-r^{-1}$ whereas in B3LYP, it decreases with $-0.2r^{-1}$. The trick here is to separate the potential into a short-range and long-range interaction part. The short-range interaction part takes DFT exchange interaction into account whereas Hartree-Fock exchange interaction is included in the long-range interaction part. The description of the two terms with Hartree-Fock or DFT is modulated by three different parameters. This approach is called the *Coulomb-attenuating method (CAM)* giving the new resulting functional the name CAM-B3LYP.^[37]

2.3 Time-Dependent Density Functional Theory (TDDFT)

DFT as previously presented only allows to access the energy of the ground state. To expand DFT to excited states, its time-dependent version must be employed. The Schrödinger equation can be expanded to the time-dependent dimension which can be used for the dynamics of a system (TDSE), see eq. 14. Here, the Hamilton operator can be expressed as the sum of a time-independent term $\hat{H}_0$ and a time-dependent perturbation of an external electric field $\hat{V}_{ext}$ given

in eq. 15.

$$\hat{H}\Psi(r,t) = i\frac{\partial}{\partial t}\Psi(r,t) \quad (14)$$

$$\hat{H}(r,t) = \hat{H}_0(r) + V_{ext}(r,t) \quad (15)$$

As Hohenberg-Kohn laid the foundations of DFT with the discussed theorems, Runge and Gross^[38] proved that also for time-dependent density functional theory (TDDFT), "two different time-dependent potentials [...] acting on a system with given fixed initial state will always cause different time-dependent densities".^[39] In other terms, each time-dependent potential V is solely linked to one time-dependent density ρ and vice versa. The potential V_{ext} can be written as follows:^[40]

$$V_{ext}(r,t) = V_{ext}[\rho, \Psi_0](r,t) \quad (16)$$

One difficulty arising from switching to TDDFT is that the exchange-correlation function also becomes time-dependent and it is rather challenging to approximate it. Therefore, usually the adiabatic approximation is used, where the exchange-correlation term only depends on its instantaneous density, therefore ignoring any time-memory effects. Another simplification is to assume that the exchange-correlation term at t_0 is also a good descriptor for all other times t . However, also in this approach, the necessary DFT exchange-correlation functional remains unknown and has to be further approximated as previously discussed.^[41]

In this work, excitation energies are computed with TDDFT. Linear response TDDFT (LR-TDDFT) uses a small time-dependent perturbation by employing an external potential leading to changes in the unperturbed density. This response is written as Taylor series truncated after the linear term leading to the method's name. The density-density response function $\chi(r, r', t, t')$ undergoes a Fourier transformation resulting in the Lehmann representation $\chi(r, r', \omega)$ that is depending on the frequency ω . The denominator of the Lehmann representation will become 0 if the energy gap of the n -th excited state E_n and the ground state energy E_0 ($E_n - E_0$) is equal to ω . Therefore, the response function must have a pole at the exact excitation energies.^[40] However, the denominator will also become 0 if the frequency is equal to the energy difference between two eigenvalues. To only compute the true excitation energy, so-called exchange-correlation kernel $f_{H_{xc}}$ is employed that can distinguish between the two cases.^[41]

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{Y} \end{bmatrix} = \omega \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{Y} \end{bmatrix} \quad (17)$$

If the density-density response function χ is derived from single excitations between Kohn-Sham orbitals, this can be described using the Casida equation in eq. 17. It is an pseudo-eigenvalue problem with the matrix elements $\mathbf{A}$ and $\mathbf{B}$ given in eq. 18 and 19. The excitation and de-excitation energies are accessible by ω and $-\omega$, whereas $\mathbf{X}$ and $\mathbf{Y}$ describe the excitation (particle-hole) and de-excitation (hole-particle) amplitudes.^[39,42]

$$A_{ia,jb} = \delta_{ij}\delta_{ab}(\epsilon_a - \epsilon_i) + 2 \int dr \int dr' \phi^*(r) \phi_a(r) f_{H_{xc}}(r, r') \phi_j^* \phi_b \quad (18)$$

$$B_{ia,jb} = 2 \int dr \int dr' \phi_i^*(r) \phi_a(r) f_{H_{xc}}(r, r') \phi_j^* \phi_b \quad (19)$$

In this thesis, the Tamm-Dancoff approximation (TDA) is used instead of the classical TDDFT.^[43] Here, the de-excitations are neglected by setting $\mathbf{B}$ to zero simplifying the eigenvalue problem to:

$$\mathbf{A}\mathbf{X} = \omega\mathbf{X} \quad (20)$$

The TDA is an approximation. However, it is known to yield better qualitative results compared to the classical TDDFT approach since it partially compensates errors deriving from the exchange-correlation functional that is not exactly known. It reduces ground state instabilities, triplet instabilities and saves computation time.^[40,44,45]

2.4 Effective core potential and relativistic corrections

Heavy metal atoms, such as platinum with the atomic number 78, possess many electrons leading to the challenge of large basis sets needed to describe all of them as well as considering the increasing of influence electron-electron correlation. However, most of electrons are core electrons that can be described with analytical functions, so-called effective core potentials (ECPs) reducing the complexity of describing this heavy atoms. Typically, "large-core" ECPs describe electrons belonging to the inner shells with analytical functions and the electrons belonging to the valence shell with a basis set. Contrarily, "small-core" ECPs describe the valence shell and the next inner lying shell with a basis set and the remaining electrons with analytical functions. Additionally, these ECPs also consider relativistic effects that occur due the highly positively charged nuclei accelerating the core electrons close(r) to the speed of light.^[29]

In this study, the Stuttgart/Dresden ECP MWB60 was employed for platinum.^[46] "60" means that 60 out of the 78 electrons of a platinum (or 76 electrons for platinum(II)) are described by the pseudopotential. "M" signifies that a neutral atom was used for developing the pseudopotential and "WB" denotes that the quasirelativistic Wood-Boring method^[47] was used to derive the parameters. It is called quasirelativistic as it considers not all relativistic correction terms, but only the two major ones: the mass-velocity term and the Darwin spin-orbit term.

Another quantum relativistic effect that has to be taken into account when describing normally spin-forbidden singlet-triplet transitions violating the selection rules, is spin-orbit coupling (SOC). This effects scales with Z^4 , Z being the atomic number. For elements in the sixth shell, this effect is in the order of magnitude of several electron volts.^[48] It is caused by the interaction of two magnetic fields, caused by the spin of the electron and the orbital movement of an electron.^[49] Normally, the term given in eq. 21 is zero due to the orthogonality of the triplet wave function Ψ_T and the singlet wave function Ψ_S . The integrals run over the whole volume element $d\tau$ and the spin coordinate $d\omega$ with $\hat{\mu}$ being the transition dipole moment operator.

$$\int \int \Psi_T^* \hat{\mu} \Psi_S d\tau d\omega \quad (21)$$

According to the selection rules, singlet-triplet transitions are therefore forbidden. However, this integral becomes non-zero when SOC is considered allowing (non-)radiative ISC and phosphorescence. The importance and challenges connected to SOC when computing excited state decay rates are further discussed in the corresponding section 2.6.

2.5 One-electron transition density matrix (1TDM)

2.5.1 On the way to charge-transfer numbers

In a simplified way, one-electron excitations can be described as one electron leaving its initial orbital and occupying another, typically higher lying orbital leaving a hole in the initial orbital. To describe this excitation scheme, the one-electron transition density matrix (1TDM) can be used as it unites the wave functions of the ground state Ψ_0 and the excited state Ψ_1 and the positions of the hole r_h and the electron r_e .^[50,51] It is given as:

$$\gamma_{01}(r_h, r_e) = n \int \dots \int \Psi_0(r_h, r_2, \dots, r_n) \Psi_1(r_e, r_2, \dots, r_n) dr_2 \dots dr_n \quad (22)$$

From this expression, the densities of the electron hole ρ_h and the excited electron ρ_e can be derived:^[50]

$$\rho_e(r_e) = \int |\gamma_{01}(r_h, r_e)|^2 dr_h \quad (23)$$

$$\rho_h(r_h) = \int |\gamma_{01}(r_h, r_e)|^2 dr_e \quad (24)$$

The excitation can be either local or a charge-transfer process. The latter one needs the decomposition of the studied molecule in at least two fragments, chosen by analysing. Eq. 25 reports the computation of the charge transfer numbers Ω_{AB} between two fragments A and B, where the hole is located on A and the electron on B by combining the densities given in eq. 23 and 24.

$$\Omega_{AB} = \int_A \int_B |\gamma_{01}(r_h, r_e)|^2 dr_e dr_h \quad (25)$$

Different values between 0 and 1 are possible for Ω_{AB} . If the charge transfer can be solely described with an electron transition from fragment A to B, Ω_{AB} will be equal to 1. Contrarily, Ω_{AB} will be 0 if there is no contribution. Also local excitations can be described with this scheme: Ω_{AA} will be 1 if both electron and hole are located on fragment A and 0 if both are not.

Having obtained the charge transfer numbers Ω_{AB} gives access to compute the charge transfer (CT) character as given in eq. 26. Note that Ω is a normalisation factor close to 1. For locally excited excitations, the CT character will be equal to 0, as terms where A = B are not considered. Contrarily, the CT character is equal to 1 if all electron-hole pairs are located on different fragments.

$$CT = \frac{1}{\Omega} \sum_A \Omega_{AB} \quad A \neq B \quad (26)$$

Normally, the excited electron is not located on one fragment, but various. To facilitate the description, the *conditional electron density* may be used. Here, the hole remains located on one single fragment, e.g. A. The excited electron, however, can be located on various fragments, e.g. A, B or C and for each of these possibilities, the conditional electron density $\rho_e^{h:A}$ is computed.^[51]

$$\rho_e^{h:A}(r_e) = \int_A |\gamma_I(r_h, r_e)|^2 dr_h \quad (27)$$

2.5.2 Natural Transition Orbitals (NTOs)

Usually, the computation of excited states (e.g. by TDDFT) yields a list of coefficients describing different hole-electron pairs that compose an excited state. Often, these excited states' characters are defined by multiple excitations meaning there is no prevalent hole-electron pair representing it. Natural Transition Orbitals (NTOs) have been developed as a simple approach of visualising orbitals to answer the question: "What got excited to where?"^[52]

To access this orbital representation by using the ITDM, Eq. 22 has to be rewritten and decomposed in three different terms: the transition amplitude λ_t , the NTO of the hole ϕ_t^h and the NTO of the electron ϕ_t^e :^[51,53]

$$\gamma_I(r_h, r_e) = \sum_{tr} \sqrt{\lambda_{tr}} \phi_{tr}^h(r_h) \phi_{tr}^e(r_e) \quad (28)$$

Note that the sum runs over all transitions tr , but λ_t is predominantly very close to zero leading to a reasonably low number of transitions necessary to consider. Nevertheless, excited states are rarely described by just *one* excitation. To determine, how many configurations are necessary to describe the character of an excited state, the participation ratio of the NTOs (PR_{NTO}) is described as follows:^[54,55]

$$PR_{NTO} = \frac{(\sum_{tr} \lambda_{tr})^2}{\sum_{tr} \lambda_{tr}^2} \quad (29)$$

If PR_{NTO} equals 1, the excited state can be described by one single excitation between two NTOs. If $PR_{NTO} > 1$, it is described by multiple excitations.

2.6 Excited state decay rates

Phosphorescence is a luminescent decay involving two states of different multiplicity (in this investigation: from the T_1 to the S_0). As e.g. Saito et al.^[10] have reported, the T_1 - S_0 gap closes when forming excimers leading to $^3\text{MMLCT}$. This influences the kinetics of the photophysical pathway that these complexes undergo. In the following paragraphs, possibilities to calculate phosphorescent rate constants are presented and discussed.

A simple approach to access radiative decay constants for both fluorescence (radiate decay between two states of the same multiplicity) and phosphorescence is the Einstein's formula.^[23,24,56]

It is given in eq. 30 with respect to phosphorescent processes:^[57]

$$k_{Einstein}(i) = \frac{4}{3t_0} \alpha_0^3 (\Delta E_i)^3 \sum_{\alpha \in x,y,z} |M_j^i|^2, \quad t_0 = \frac{(4\pi\epsilon_0)^2 \hbar^3 e^4}{m_e} \quad (30)$$

Here, ΔE_i is the vertical energy difference between the S_0 and the T_1 at the T_1 geometry. M_j^i is the transition dipole moment including SOCs, α_0 is the fine-structure constant and t_0 a term summarising several remaining constants: ϵ_0 as the vacuum permittivity, $\hbar$ as the reduced Planck constant, m_e as the rest mass and e as the charge of an electron. This equation can be simplified as given in eq. 31.^[58]

$$k_{Einstein}(i) = \frac{f(i) \cdot \Delta E_i^2(i)}{1.499} \quad (31)$$

Each triplet state consists of three spin sublevels i (T_x , T_y , T_z) due to the three different M_S quantum numbers with $M_S = -1, 0, +1$. Each spin substate contributes to the phosphorescent rate constants differently, therefore the three states are usually averaged as in eq. 32 to yield k_{phosph} .

$$k_{phosph} = \frac{1}{3} \sum_{i=1}^3 k_{Einstein}(i) \quad (32)$$

Einstein's simplified formula is only dependent on the dimensionless oscillator strength f and the vertical energy in cm^{-1} between T_1 and S_0 . Whereas the vertical energy is easily accessible, the computation of f is more challenging as it is mostly dependent on the electric transition dipole moment M_j^i as included in eq. 30. It can be computed as follows:^[56]

$$M_j^i = \sum_{n,m=0}^{\infty} \frac{\langle S_0 | \hat{\mu}_j | S_m \rangle \langle S_m | \hat{H}_{SO} | T_1^i \rangle}{E(S_m) - E(T_1)} + \frac{\langle S_0 | \hat{H}_{SO} | T_n \rangle \langle T_n | \hat{\mu}_j | T_1^i \rangle}{E(T_n) - E(S_0)} \quad (33)$$

$\hat{H}_{SO}$ is the Hamiltonian including SOCs, $\hat{\mu}$ is the dipole operator and S_m and T_n the intermediate singlet and triplet state, respectively. M_j^i and therefore f are thus dependent on the SOC and the dipole moment itself.

At this point, it shall be noticed that other methods to compute ISC or phosphorescence rate constants exist, e.g. Marcus' theory or Fermi's Golden Rule based approaches. In the studied systems of this thesis, neither of both is practicable as they require closely related singlet and triplet states. Fermi's Golden Rule is derived from perturbation theory, where the transition from one state to another is treated as an external perturbation of the system. For ISC, the SOC-operator is perturbed. To reduce the computational cost coming from characterising the potential energy surface (PES), usually the harmonic approximation is applied.^[59] It assumes that the potential around the Franck-Condon-region can be described by an harmonic oscillator and anharmonicities are neglected. As it will be discussed in Section 4.1, the geometries of the T_1 and S_0 are rather different, especially for the aggregates/excimers, leading to shifted minima on the respective PESs, and therefore to a breakdown of the harmonic approximation.

Marcus' theory^[25,26] has also been used to predict ISC rate constants when using the spin-orbit coupling matrix elements H_{SOC} . The formula to compute k_{ISC} is given in eq. 34, where $\hbar$ is the reduced Planck constant, λ the reorganisation energy, k_B the Boltzmann constant, T the temperature and ΔE the adiabatic energy gap between the two respective states.

$$k_{ISC} = \frac{2\pi}{\hbar} |H_{SOC}|^2 (4\pi\lambda k_B T)^{-\frac{1}{2}} \exp\left(-\frac{(\Delta E + \lambda)^2}{4\lambda k_B T}\right) \quad (34)$$

The limitation of Marcus' theory is based on the coupling elements: This formula is only reliable for weak couplings elements.^[60–62] High SOC's as can be expected for transition metal complexes yield unphysical, high k_{ISC} rate constants as H_{SOC} scales quadratically. Successful reproduction of ISC using Marcus' theory is reported for SOC's $< 5 \text{ cm}^{-1}$.^[60]

3 Computational details

3.1 Geometry optimisations

For the ground state (S_0) optimisations of **Pt-1** to **Pt-12** the atomic basis set 6-31G(d)^[63,64] was used for all non-metal atoms while Pt was treated with the ECP MWB60 pseudopotential^[46] to include relativistic effects. The Becke's three-parameter hybrid exchange functional combined with the Lee-Yang-Parr correlation functional^[34,35], which was improved for long-range-interaction by the Coloumb-attenuating method^[37], was applied including Grimme's D3 dispersion correction (CAM-B3LYP-D3).^[65] No symmetry constraints were set and all minima were confirmed by only positive frequencies. The T_1 state was optimised with unrestricted DFT using the same basis set and settings. All calculations were carried out with the Gaussian 16 A.03 package.^[66] The geometry guesses for both S_0 and T_1 optimisations of all complexes were based on the crystal structure or previous optimised geometries reported by literature.

3.2 Analysis

The UV-vis absorption spectra were obtained using TDDFT including TDA at the same level of theory for 30 singlet and 30 triplet states. Data was visualised using GaussSum.^[67] For the 1TDM analysis, the TDA^[43] was employed since it was previously shown to be more accurate for metal complexes and assumed to be more reliable for excited state characterisation.^[68,69] The number of states was reduced to five singlet and five triplet states.

To compute the phosphorescent rate constants based on Einstein's formula, the SOCs were computed with the ORCA 5.0.4 package.^[70] Due to technical difficulties, the basis set was changed to "ZORA-def2-TZVP" for all non-metal atoms and "SARC-ZORA-TZVP" for platinum. The Zeroth-Order Regular Approximation (ZORA) uses a scalar relativistic Hamiltonian, whereas the segmented all-electron relativistically contracted basis sets can be used to replace effective core potentials.^[71–73] To speed up the calculation, the keywords RIJCOSX and RI-SOMF(1X)^[74] were included as well as TDA and SOCs. The number of roots was set to 10.

4 Results and Discussion

4.1 Geometrical characteristics of oligomers and excimers

As indicated by Figure 1, the different kinds of excimer emission are highly dependent on the geometry and the arrangement of the complex layers in both their S_0 and T_1 state. Thus, it is a good start to analyse the stacking of the complex layers and especially of the platinum centers. In this section, the optimised S_0 and T_1 geometries of all twelve complexes in their monomeric, dimeric and trimeric form will be discussed and analysed. Similar complexes will be discussed together. Aggregation was created based on experimentally determined crystal structures. The coordinates of all structures can be found in section 5.2.

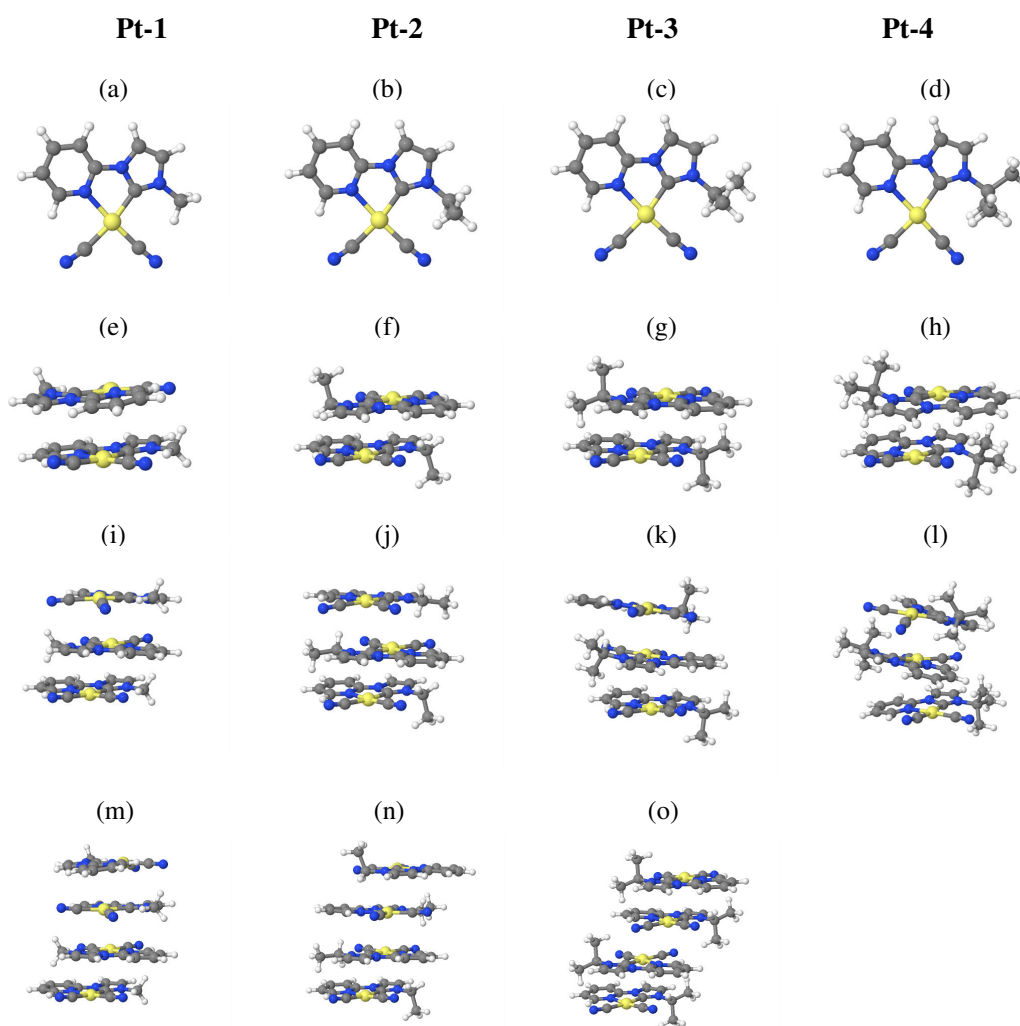


Figure 5: Optimised S_0 geometries for **Pt-1**, **Pt-2**, **Pt-3** and **Pt-4**. First row: monomers, second row: dimers, third row: trimers, fourth rows: tetramers. Carbon atoms are depicted in grey, hydrogen in white, nitrogen in blue and platinum in yellow.

Figure 5 displays the optimised S_0 geometries for the monomers, dimers, trimers and tetramers for the four bidentate complexes **Pt-1** to **Pt-4** that only differ by an alkyl group (see Figure 4). For the monomers, the complexes are nearly perfectly square planar, apart from the different alkyl chains. For the dimers, the platinum centers stack in an anti-parallel way to minimise steric interaction arising from the alkyl groups. This also leads to shift in the alignment of the platinum centers, except for **Pt-1** in Figure 5e. In the trimers, the complexes also stack anti-parallelly and the shift of the metal centers is even more distinct. For **Pt-4** (Figure 5l), the increased sterical influence of the tert-butyl group prevents the formation of parallel planes. Also for **Pt-3**, the upper layer is not parallel anymore, whereas for **Pt-1** and **Pt-2** the planes align as expected due to the smaller alkyl chains. The tetramers were only optimised for **Pt-1**, **Pt-2** and **Pt-3** as **Pt-4** showed its inability to stack already in the trimer structure. Here, **Pt-1** still aligns linearly with only limited deviation due to the methyl-group. For **Pt-2**, the upper layer misaligns visibly and **Pt-3** resembles two dimers shifted from each other.

Figure 7 displays the optimised T_1 geometries for the monomers, dimers and trimers for all four complexes. The T_1 monomers' geometries are comparable to those in the S_0 . In the dimers, the complexes align parallelly and stack closer together as can be seen by the visualised "Pt-Pt" bond. The implied Pt...Pt interaction leads to a nearly perfect alignment of the layers regardless of the alkylrests. In the trimers, stacking and formation of two "Pt-Pt" bonds can be also observed for all complexes except **Pt-4**. Here, the upper layer is shifted due to the sterical demand of the tert-butyl group of the complex in the middle layer. This behaviour already implies that the maximum number of layers forming an excimer is 2. It is notable for **Pt-3**, that for the T_1 geometry the shift in alignment completely vanishes despite the bigger sterical demand of the iso-propyl group compared to ethyl or methyl. For the tetramers, three of the four layers in **Pt-1** and **Pt-2** stack similarly as the dimers and trimers, whereas for **Pt-3** all four layers stack. This is rather surprising since the iso-propyl group is the sterical most demanding group. For **Pt-1**, the single platinum(II) complexes are not perfectly square-planar, but slightly bent and the methyl-groups are rather close to the metal center compared to the other centers. If the last, most detached layer moved closer, this would lead to a sterical conflict of the cyano-groups and the N-heterocyclic carbene (NHC)-ligands or the methyl-group and the cyano groups. Also in **Pt-2**, one layer is shifted. The two layers at the top and at the bottom have their ethyl groups pointing up- and downwards, respectively. The potential sterical conflict arising from the slightly bent complex layer and the upwards pointing hydrogen atoms of the CH_2 -group prevents further stacking. For **Pt-3**, the linear stacking pattern is maintained due to the distance between the iso-propyl group and the metal center, preventing sterical hindrance within the layers.

In the following, the Pt...Pt distances are compared to the experimentally obtained values in the crystal structures.^[10] The experimental values given in Table 1 are measured between the Pt atoms in the layers themselves. This method of measurement is indicated in the following with "Pt...Pt" and visualised in Figure 6. In dimers, trimers and tetramers less geometric constraint can be found compared to the crystal structure leading to a shift of the complexes' alignment which explains the increasing Pt...Pt distances found for the ground state. To compare the computational

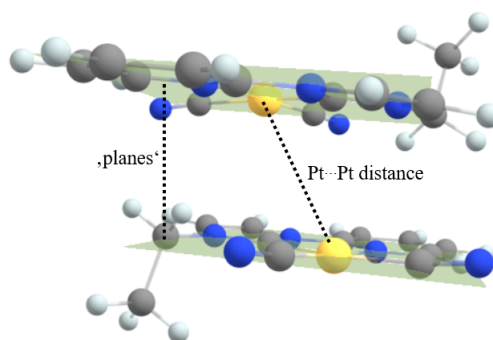


Figure 6: Illustration of the two distance measurement methods explained in the main text with the example of the **Pt-2** dimer: The interplatinum distance Pt··Pt is measured directly between the metal atoms, whereas the interplanar distance, abbreviated with 'planes', is measured between two planes containing the square-planar scaffold atoms. Platinum atoms are coloured in yellow, carbon in grey, hydrogen in white and nitrogen in blue.

protocol to the experimental data, a different method of measuring was chosen: A plane including the Pt center, the NHC and the two cyano ligands was set up and the distance between the different layers approximated, in the following referred to as "planes", also visualised in Figure 6. The crystal structures obtained for **Pt-1**, **Pt-2**, **Pt-3** and **Pt-4** show that the interlayer distance decreases with rising sterical hindrance based on the alkyl groups. The distances obtained with the latter method agree well with the experimental data and also captures the trend of increasing distances with increasing the bulkyness of the alkyl group.

In the T_1 -state, this pattern changes. As visualised in Figure 7, the shift in complex layers does no longer occur in the dimers and the Pt centers stack closer together leading to distance reduction from approximately 3.9 Å ("Pt··Pt") and 3.3 Å ("planes") to 2.8 Å ("Pt··Pt") and 2.9 Å ("planes"). This serves as a hint that shortening Pt··Pt bonds do indeed play a role for the formation of excimers. For the trimers, two Pt··Pt distances can be measured. In the S_0 state, one shorter distance of approximately 3.6 Å and one longer of 3.8 Å is measured for **Pt-1** and **Pt-3**, whereas **Pt-2** and **Pt-4** exhibit similar distances of 3.8 Å and 4.1 Å, respectively. The increase in distance for **Pt-4** can be explained with the steric demand of the tert-butyl group, whereas the other distances are within the same range. When comparing the S_0 planes distances given in Figure 5, the distance decrease from 3.2 Å to 3.5 Å can be clearly linked to the sterical hindrance of the alkyl chains. In the T_1 state, typically one shorter (2.8 to 2.9 Å) and one longer (3.0 to 3.2 Å) Pt··Pt distance exists for **Pt-1**, **Pt-2** and **Pt-3**. The pattern also occurs for **Pt-4**, but with a maximum Pt··Pt distance of more than 3.7 Å. This already signals the stacking limit for this complex. This is confirmed by analysing the T_1 planes distance. **Pt-4** shows a maximum distance of 3.3 Å, whereas the other complexes display one of approximately 3.1 Å. The shorter distances range for all four complexes between 2.9 and 3.0 Å.

In the tetramers, three Pt··Pt distances can be measured. In **Pt-1**, **Pt-2** and **Pt-3** S_0 Pt··Pt distances

between 3.7 and 3.9 Å are measured, whereas the interplane distances range between 3.2 and 3.3 Å and thus significantly lower as previously reported. In the T_1 state, typically three of the four layers stack together signified by Pt...Pt distances between 2.8 and 3.0 Å, whereas one layer is further shifted by > 3.6 Å. **Pt-3** is an exception here; although keeping this pattern the largest distance is < 3.4 Å and all four complex layers contribute to the stacking. However, all three investigated complexes show similar values when analysing the interplane distances: The two shorter distance between 2.9 and 3.1 Å, whereas the larger one oscillates between 3.2 and 3.3 Å.

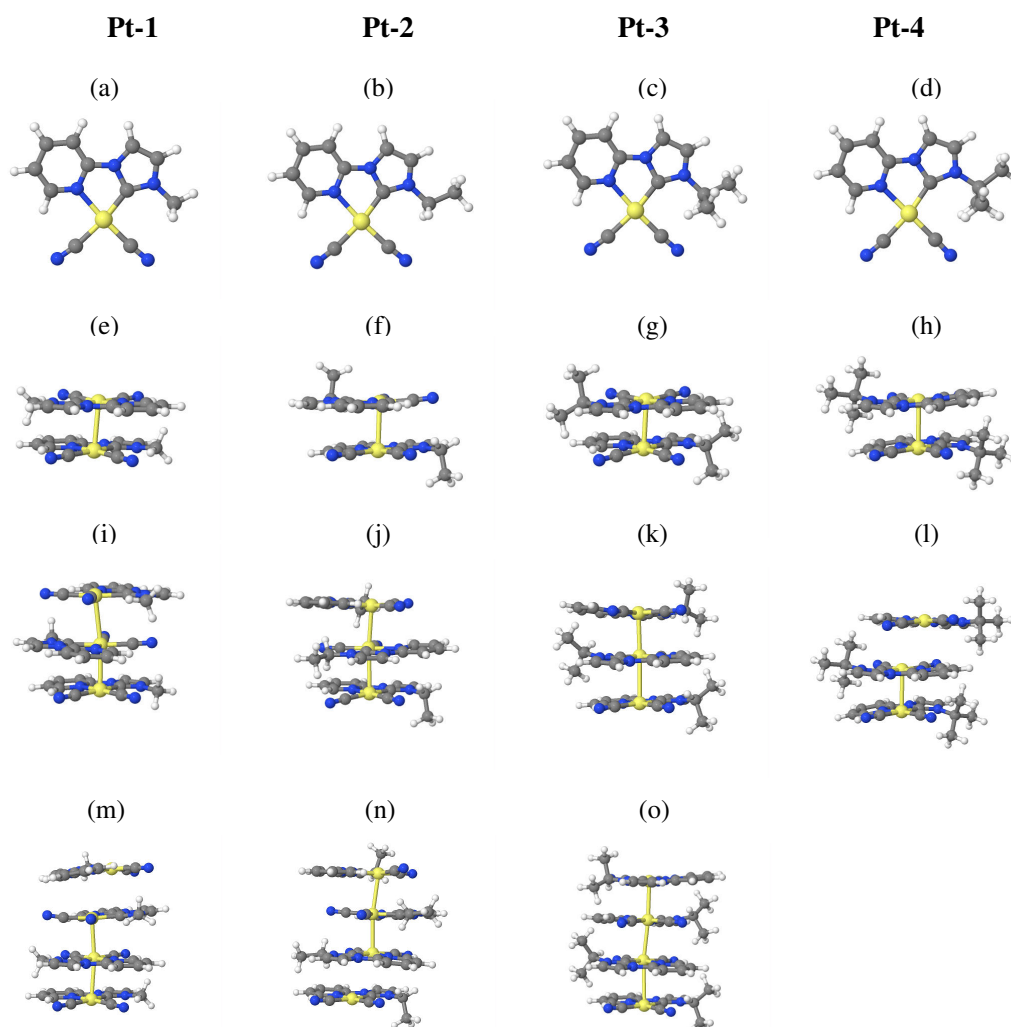


Figure 7: Optimised T_1 geometries for **Pt-1**, **Pt-2**, **Pt-3** and **Pt-4**. First row: monomers, second row: dimers, third row: trimers, fourth row: tetramers. Carbon atoms are depicted in grey, hydrogen in white, nitrogen in blue and platinum in yellow.

This initial analysis already reveals that the stacking pattern in the S_0 is not directly linked to the stacking pattern in the T_1 . Due to less constraint in oligomers compared to crystal structures, interplanar distances are also more reliable than interplatinum distances. For these four complexes, $^3\text{MMLCT}$ was experimentally determined^[10] that is linked to close Pt...Pt contacts, often even below $< 3.0 \text{ \AA}$. Visualising T_1 geometries also hints the maximum number of closely stacking complex layers possible, which is 2 in case of **Pt-4**, 3 for **Pt-1** and **Pt-2** and at least 4 for **Pt-3**.

Table 1: Distances in Å between the different complex layers for the dimers, trimers and tetramers of **Pt-1**, **Pt-2**, **Pt-3** and **Pt-4**. Pt...Pt indicates that the distances were measured directly between the Pt atoms, whereas "planes" indicates that planes covering the backbone of the complex were used to approximate the distance.

	Experiment ^[10] Pt...Pt	Dimer Computations				Trimer Computations			
		S ₀ Pt...Pt	T ₁ Pt...Pt	S ₀ planes	T ₁ planes	S ₀ Pt...Pt	T ₁ Pt...Pt	S ₀ planes	T ₁ planes
Pt-1	3.282	3.873	2.831	3.255	2.906	3.829	3.095	3.253	3.076
Pt-2	3.276	3.819	2.822	3.211	2.892	3.695	2.842	3.220	2.914
	3.430					3.772	2.848	3.238	2.944
Pt-3	3.296	3.889	2.836	3.260	2.915	3.775	3.041	3.241	3.040
	3.495					3.646	2.861	3.313	2.963
Pt-4	3.477	3.993	2.867	3.391	2.940	4.027	3.146	3.335	3.120
	3.669					4.105	3.747	3.436	3.307
						4.101	2.885	3.488	2.973
	Experiment ^[10] Pt...Pt	Tetramer Computations							
		S ₀ Pt...Pt	T ₁ Pt...Pt	S ₀ planes	T ₁ planes				
Pt-1	3.282	3.728	3.833	3.207	3.270				
Pt-2		3.779	2.871	3.256	2.951				
		3.851	2.939	3.256	2.973				
	3.276	3.746	3.648	3.234	3.240				
	3.430	3.733	2.876	3.274	2.978				
Pt-3		3.756	3.972	3.231	2.993				
	3.276	3.767	3.382	3.270	3.252				
	3.296	3.875	3.059	3.241	3.072				
	3.495	3.767	2.884	3.270	2.972				
	3.296								

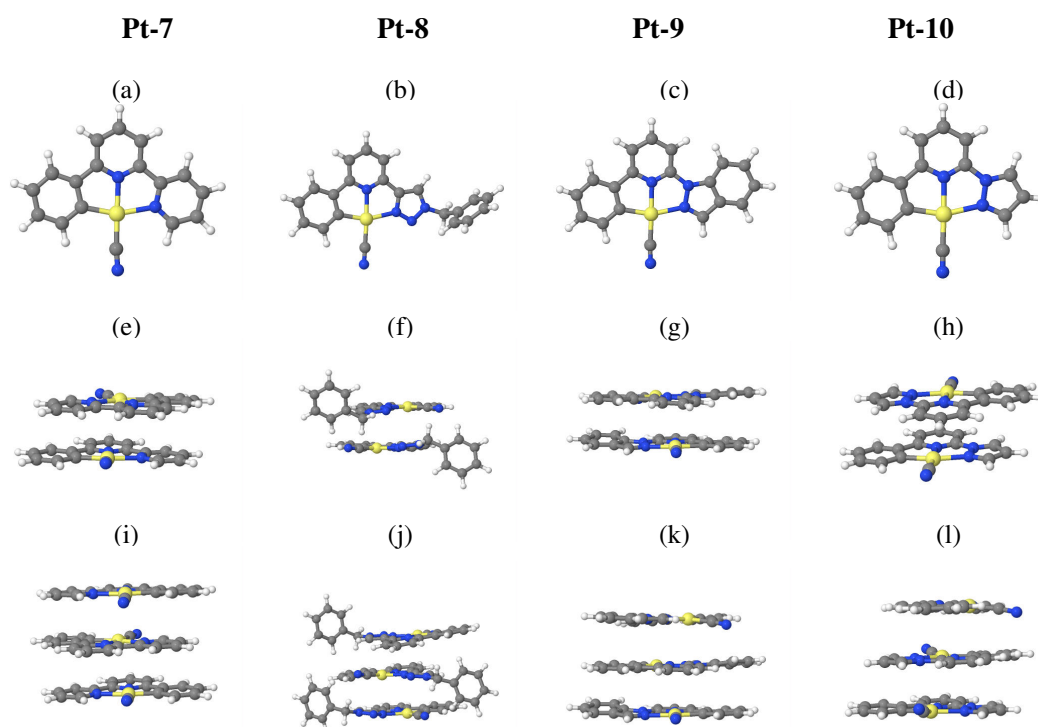


Figure 8: Optimised S_0 geometries for **Pt-7**, **Pt-8**, **Pt-9** and **Pt-10**. First row: monomers, second row: dimers, third row: trimers, fourth rows: tetramers. Carbon atoms are depicted in grey, hydrogen in white, nitrogen in blue and platinum in yellow.

In the previous bidentate complexes, $^3\text{MMLCT}$ has been already observed experimentally^[10] and was linked to close interplatinum distances. The following complexes are analysed to find similar patterns also for other possible excimer emissions. Due to their geometrical similarity, the four tridentate complexes **Pt-7** to **Pt-10** are analysed together. Figure 8 displays the optimised structures of the monomers, dimer and trimers of the named complexes. In the monomers, the core of all four complexes is square-planar, only for **Pt-8** the bent flexible phenylgroup is visible in Figure 8b. The (nearly) anti-parallel stacking is present in all dimer's, for **Pt-9** (Figure 8g), a slightly bent upper movement of the core is visible. In the trimers, the sterical influence of the different ligands increases, leading to shifts in the structures preventing close metallophilic contacts in the ground state. Especially, the curved middle layer of **Pt-8** in figure 8j is noticeable. As for the previously discussed bidentate complexes **Pt-1** to **Pt-4**, no close metallophilic contacts can be observed in the S_0 geometries.

Figure 9 summarises the structures for the optimised T_1 state of the complexes **Pt-7** to **Pt-10**. As observed for the bidentate complexes, the monomers' geometries are not visibly altered. Once again, this changes in the dimers: Whereas the platinum centers remain shifted (similar to the S_0) for **Pt-7** and **Pt-10** (Figure 9e and 9h), **Pt-8** and **Pt-9** (Figure 9f and 9g) show close metallophilic contacts. Surprisingly, **Pt-8** as the complex with the sterically most demanding ligand displays

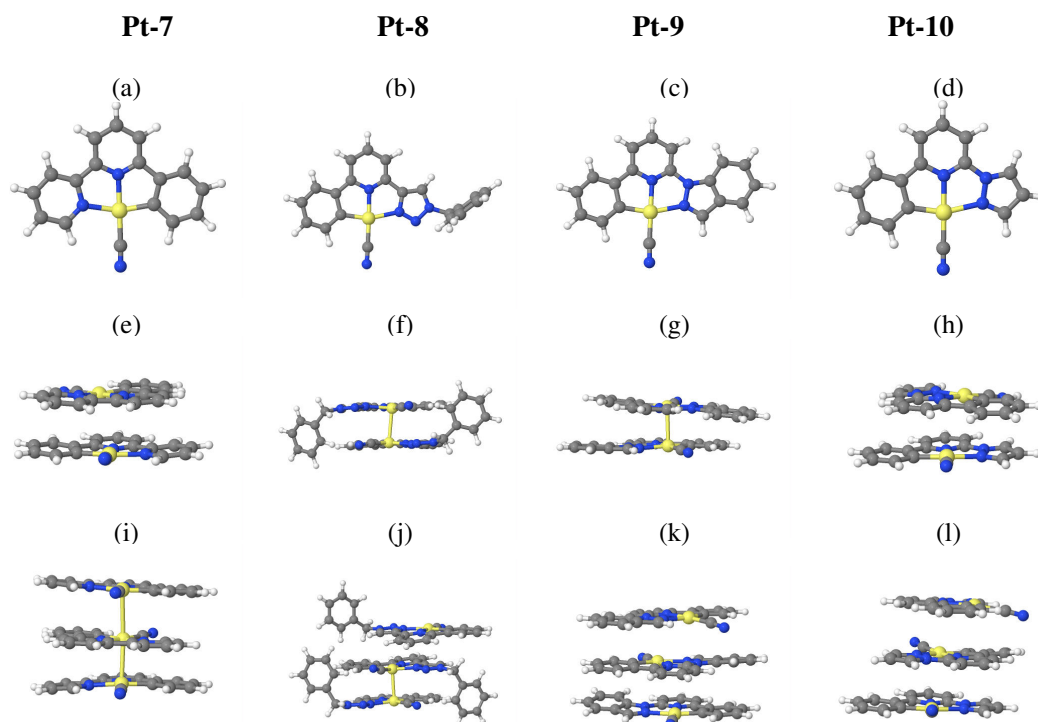


Figure 9: Optimised T_1 geometries for **Pt-7**, **Pt-8**, **Pt-9** and **Pt-10**. First row: monomers, second row: dimers, third row: trimers, fourth rows: tetramers. Carbon atoms are depicted in grey, hydrogen in white, nitrogen in blue, oxygen in red, phosphorus in orange and platinum in yellow.

parallel stacking compared to the crooked alignment of **Pt-9**. For the trimer, the pattern changes again: In **Pt-7** all three platinum centers stack linearly displaying short contacts, whereas in **Pt-8** only two metal centers align, most likely due to the sterical demand of the flexible phenyl group. **Pt-9** displays no close metallophilic contacts anymore, as well as **Pt-10**. The T_1 state of the latter two complexes resembles their S_0 geometry.

Table 2 presents all $Pt \cdots Pt$ and interplanar distances for the remaining complexes **Pt-5** to **Pt-12**. At first, the experimental results for **Pt-7** to **Pt-10** will be linked to the optimised geometries and discussed. The planes used to determine interplanar distances included the platinum center, the cyano ligand and the carbon/nitrogen atoms of the respective tridentate ligand, similar to scheme provided in Figure 6. Note that no crystal structure is available for **Pt-8**.^[12] Similarly to **Pt-1** to **Pt-4**, the $Pt \cdots Pt$ distances for the S_0 dimers are overestimated due to the lack of constraint typically given in a crystal and planes yield the more reliable values. The close $Pt \cdots Pt$ stacking for the dimers of **Pt-8** and **Pt-9** is numerically well reflected with approximately 2.8 Å in the T_1 . The interplane distance is a bit higher with 3.0 and 2.9 Å, respectively. As visualised in Figure 8e, 9e, 8h and 9h, no close stacking occurs for **Pt-7** and **Pt-10** in dimer. In the trimer however, this changes for **Pt-7** displaying close metallophilic contacts (see Figure 9i) of 2.8 Å and 2.9 Å implying that 3MMLCT could be possible for this structure. In **Pt-8**, due to sterical

hindrance only two planes stack close enough to each other with interplatinum distances of 2.8 Å, whereas no interplatinum (approximately 4.0 Å) or interplanar (approximately 3.3 Å) stacking occurs for **Pt-9** and **Pt-10**. Also here, it is confirmed that S_0 structures are not directly related to T_1 structures. Additionally, the characteristic close contacts for complexes showing $^3\text{MMLCT}$ emission experimentally could also be confirmed here. However, no distinct pattern for e.g. π - π stacking or d- π stacking is observed.

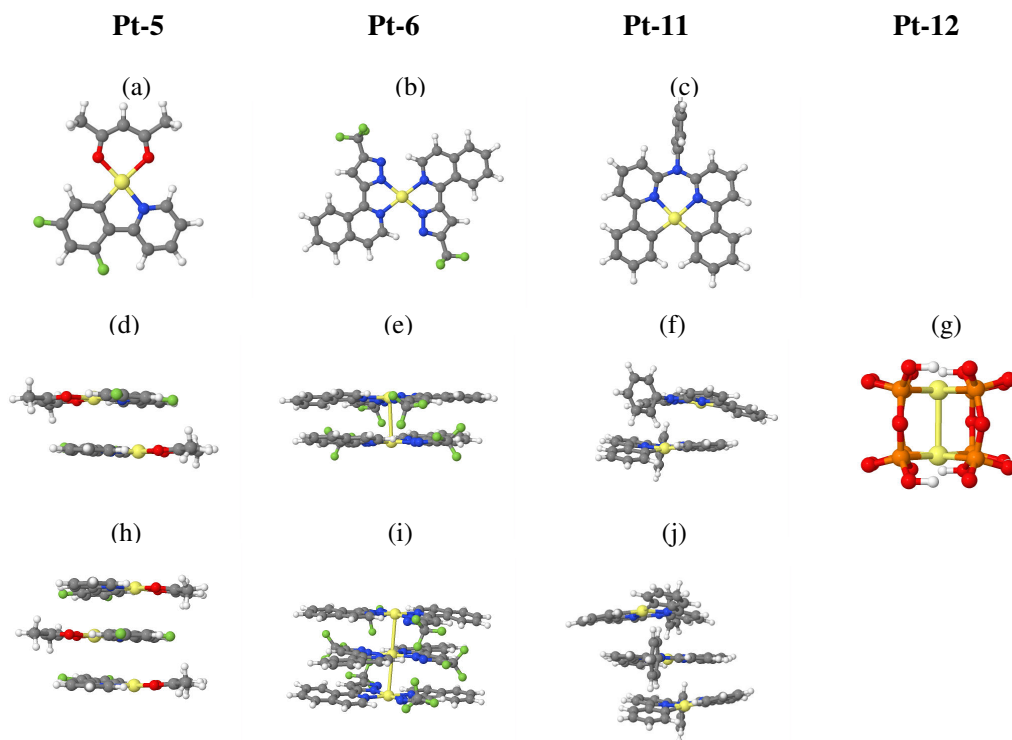


Figure 10: Optimised S_0 geometries for **Pt-5**, **Pt-6**, **Pt-11** and **Pt-12**. First row: monomers, second row: dimers, third row: trimers. Carbon atoms are depicted in grey, hydrogen in white, nitrogen in blue, oxygen in red, phosphorus in orange and platinum in yellow. **Pt-12** is a binuclear pincer complex resembling a dimer, however, no monomeric or trimeric structure is available.

The remaining complexes are also analysed together. Figure 10 displays the optimised S_0 for the two remaining bidentate complexes **Pt-5** and **Pt-6**, the tetradentate complex **Pt-11** and the binuclear pincer complex **Pt-12**. The monomers of **Pt-5** and **Pt-6** are square-planar, whereas **Pt-11** displays a flexible phenyl-group perpendicular to the main plane. For the dimer, **Pt-5** displays two parallel planes, whereas for **Pt-6** some stacking seems to occur. Previous computational studies on **Pt-6** report at least three different possible stacking geometries for the dimer and trimer.^[14] This geometry was chosen because it is the closest one to analyse possible $^3\text{MMLCT}$ and it is also the lowest in energy for the T_1 trimer. The flexible phenyl-group in **Pt-11** prevents parallel stacking leading to a crooked structure given in Figure 10f. **Pt-12** is presented along with the other dimers since it is a binuclear complex with the platinum's position being constrained by the

pyrophosphate ligands. In the trimer, **Pt-5** still stacks parallelly, but without close metallophilic contacts whereas this is for **Pt-6** still possible. For **Pt-11** the planes are strongly shifted due to the sterically demanding tetradentate ligand.

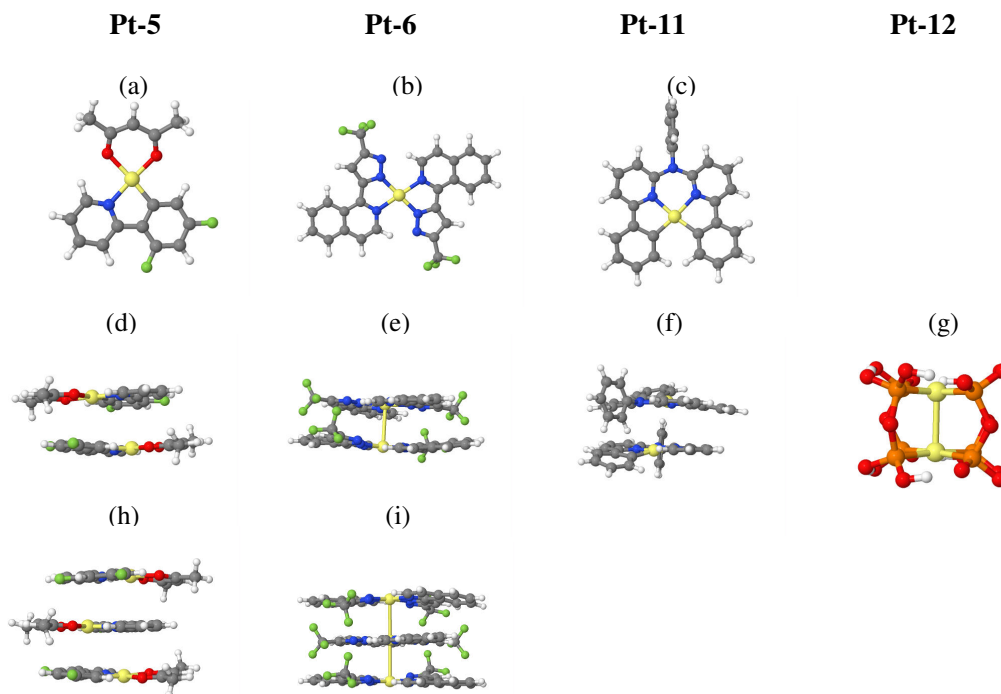


Figure 11: Optimised T_1 geometries for **Pt-5**, **Pt-6**, **Pt-11** and **Pt-12**. First row: monomers, second row: dimers, third row: trimers. Carbon atoms are depicted in grey, hydrogen in white, nitrogen in blue and platinum in yellow. No T_1 trimer was optimised for **Pt-11**. **Pt-12** is a binuclear pincer complex resembling a dimer, however, no monomeric or trimeric structure is available.

The optimised structures of the T_1 state for **Pt-5**, **Pt-6**, **Pt-7** and **Pt-8** are depicted in Figure 11. As for the previously discussed complexes, the monomers' geometries resemble the S_0 ones, except for **Pt-5** where a bending for acetylacetonate-ligand occurs that mostly vanishes when forming the dimer structure. As in the S_0 , **Pt-5** does also not show close metallophilic contacts in neither the dimer nor the trimer structure. The **Pt-6** dimer still depicts Pt $\cdots$ Pt interaction, whereas the **Pt-11** dimer is also in the T_1 sterically hindered to exhibit these. In **Pt-12**, the position of the metal centers does not alter significantly, but the oxygen linking the phosphate groups is bent more.

In the following paragraphs, the measured interplanar and interplatinum distances given in Table 2 are discussed. For **Pt-5**, the experimental Pt $\cdots$ Pt distance of 4.5 Å^[11] is quite well reproduced with 4.4 Å and 4.3 Å for the S_0 , respectively. The interplatinum distance for the T_1 is comparable to the S_0 in the trimer, whereas it is a bit smaller for the dimer with 4.2 Å. This change can be explained with differently shifted metal centers, as visualised in the Figures 11d and 11h. The

interplanar distance is consistent for S_0 and T_1 of both dimers and trimers with nearly 3.3 Å. This is still below the double van-der-Waals radius of Pt with approximately 3.5 Å, but significantly higher than values reported for the $^3\text{MMLCT}$ of **Pt-1** to **Pt-4**. Additionally, the platinum centers are not aligned linearly preventing the overlap of d-orbitals. This implies excimer emission either coming from π - π orbital interaction or d- π interaction.

The experimental data available for **Pt-6**^[21] reports high Pt···Pt distances of > 5.0 Å due to lacking of a close stacking scheme. For both the S_0 and T_1 dimer and the S_0 trimer, the interplatinum and interplane distances vary between 3.2 Å and 3.4 Å. Also here, despite the satisfying alignment of the metal centers, the distances are surprisingly too high to infer $^3\text{MMLCT}$ in these structures. As for **Pt-5**, this hints that π - π or d- π interaction is responsible for excimer emission. In the trimer, similar Pt···Pt and interplanar distances of 3.2 and 3.3 Å are reported with linear alignment of the platinum centers in Figure 11i.

Compared to most other complexes, **Pt-11** does not exhibit close stacking in the reported crystal structure,^[13] making any comparison between the computational data and the experiment needless. It also leads to the failure of optimising a stacking trimer structure in the T_1 state. Due to the bent non-connected phenyl rings of the tetradentate ligand shown in Figure 10f and 10j displaying an separation angle between 10 and 15°, the values for the "planes" have to be interpreted cautiously. The ligand's sterical hindrance also leads to highly shifted complexes resulting in Pt···Pt distances > 4.0 Å. Also the interplane distance is rather high with 3.6 Å for the S_0 and 3.4 Å for the T_1 , respectively. However, both interplatinum and interplane distances report closer stacking for the T_1 state compared to S_0 .

For **Pt-12**, experimental data for both the ground state as well as the excited state gained by time-resolved diffraction measurements is available.^[75] As similar studies performed with X-rays,^[76–78] it shows Pt···Pt contraction in the excited state of 0.2 to 0.3 Å. The computations report interplatinum distances of 3.0 Å in the S_0 and 2.8 Å in the T_1 , yielding a difference of 0.2 Å agreeing well with the experimental data. The contraction of the platinum centers leads to increased angle of the oxygen linking the phosphate groups and generally also distorts the hydrogen bonding within the different phosphate groups.

To conclude, stacking complex layers with less than 3.5 Å, which is twice the van-der-Waals radius of platinum, could be found for all complexes. Relating the experimental observations to the T_1 geometries implies that close Pt···Pt contacts of ≤ 3.0 Å in the T_1 state could be necessary for displaying $^3\text{MMLCT}$. However, there is no clear similarity between the S_0 and the T_1 geometries as they usually deviate significantly from each other, especially in the aggregates and excimers. This type of analysis, which is solely based on structural characteristics, is also not suitable to distinguish between the different types of excimer emission. In the next section, where the UV-vis absorption spectra based on the S_0 geometries will be discussed, the structural characteristics will be used to explain why this approach of analysis frequently fails.

Table 2: Distances in Å between the different complex layers for the dimers, trimers and tetramers of **Pt-5**, **Pt-6**, **Pt-11** and **Pt-12**. Pt...Pt indicates that the distances were measured directly between the Pt atoms, whereas "planes" indicates that planes covering the backbone of the complex were used to approximate the distance.

	Experiment ^[111] Pt...Pt	Dimer Computations				Trimer Computations			
		S ₀ Pt...Pt	T ₁ Pt...Pt	S ₀ planes	T ₁ planes	S ₀ Pt...Pt	T ₁ Pt...Pt	S ₀ planes	T ₁ planes
Pt-5	4.515	4.411	4.169	3.269	3.241	4.318	4.348	3.256	3.252
Pt-6	5.034	3.387	3.315	3.225	3.314	3.325	3.318	3.246	3.257
	5.034					3.325	3.323	3.245	3.225
Pt-7	3.223	3.974	4.098	3.307	3.197	3.881	2.843	3.319	2.982
	3.287					3.881	3.211	3.318	3.177
Pt-8	-	4.334	2.823	3.334	3.007	3.984	4.704	3.312	3.234
	-					4.654	2.786	3.207	3.016
Pt-9	3.295	4.118	2.795	3.300	2.910	4.129	4.142	3.284	3.281
						4.048	4.075	3.278	3.267
Pt-10	4.624	4.260	4.093	3.332	3.178	3.947	3.950	3.274	3.270
	4.877					4.062	4.048	3.277	2.262
Pt-11	-	4.692	4.081	3.622	3.450	4.542	-	3.680	-
	-					4.787	-	3.632	-
Pt-12	2.91 (S ₀) 2.63 (T ₁)	2.992	2.770	3.003	2.842				

4.2 UV-vis absorption spectra

Emission spectra are frequently used to experimentally distinguish excimers of excited monomers. Excimers usually exhibit a broad, structureless, red-shifted emission band.^[79] When this band is observed and crystal structures show close Pt...Pt contacts, ³MMLCT is usually assigned experimentally. Sometimes, additional DFT calculations are performed to check whether HOMO-LUMO gaps are narrow enough for this type of transition.^[10] In this section, computed UV-vis absorption spectra are used to investigate whether the broad, structureless, red-shifted band is visible and if so, whether it displays characteristics that allow alignment to one of the three possible excitation characters. It should be noted that only singlet excitations are included in UV-vis absorption spectra, as singlet-triplet excitations are spin-forbidden. Triplet ³MMLCT is usually connected to the transition from the lowest lying triplet state (T_1) to the ground state S_0 . In this chapter, special focus is laid on the $S_1 \rightarrow S_0$ transition, which corresponds to the lowest energy gap and therefore to the peak at the highest wavelength in the spectra presented in Figure 12. The computed wavelengths, oscillator strengths and characters of all twelve complexes are summarised in Table A4 in the appendix (Section 5).

For **Pt-1**, **Pt-2**, **Pt-3** and **Pt-4**, the presence of ³MMLCT was experimentally determined previously^[10] making them suitable candidates to check for the corresponding redshifted band. Their computed UV-vis-spectra are portrayed in Figure 12. All four complexes in this set depict very similar spectra as computed for the monomers (violet). The peak at the highest wavelength is always between 276 and 278 nm, whereas the peaks (or shoulders) of dimers (green), trimer (blue) and tetramer (orange) reach their maximum between 285 and 308 nm (see different red arrows in Figure 12). There is a general trend for the redshift being more pronounced in trimers compared to dimers. However, for tetramers, the peak's maximum is very close to the trimer's one. As has been discussed in Section 4.1, this is likely due to the less pronounced stacking behaviour.

The computed UV-vis absorption spectra of the remaining two bidentate complexes, **Pt-5** and **Pt-6**, are depicted in Figure 13. Contrarily to **Pt-1** to **Pt-4**, **Pt-5** was experimentally not predicted to show a MMLCT band at all.^[11] Agreeing with this result, the computed spectrum (Figure 13a) also lacks this additional band. Only the general red-shift and broadening/overlapping of peaks is depicted due to the formation of aggregated structures. For **Pt-6**, the previous computational study^[14] predicted the MMLCT band only for trimers but not for dimers. This is also represented in the computed UV-vis spectrum in Figure 13b: The peak at the highest wavelength remains at approximately 325 nm and only shifts in the trimer to approximately 370 nm (see red arrows). The four tridentate complexes **Pt-7** to **Pt-10** are analysed together due to their geometrical similarity. For **Pt-7** and **Pt-9** ³MMLCT has already been proposed experimentally, for **Pt-10** π - π^* interaction and the character of **Pt-8**'s excimer emission was not determined since the sample was polycrystalline impeding proper interpretation.^[12] In the computed UV-vis absorption spectra depicted in Figure 14, the clearest peak at higher wavelengths for **Pt-7** is at approximately 295 nm followed by a tiny shoulder towards higher wavelengths. Its dimers and trimers do not portray any

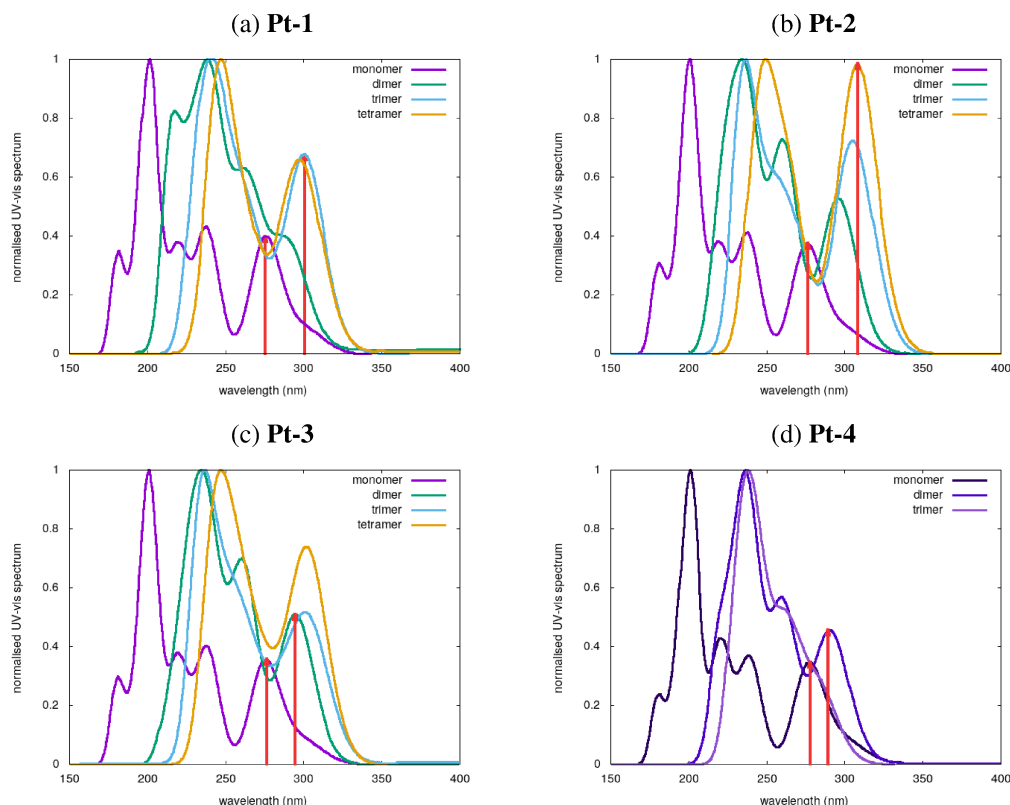


Figure 12: Computed normalised UV-vis spectra for the monomers, dimers, trimers and tetramers for **Pt-1**, **Pt-2**, **Pt-3** and **Pt-4**. The red arrows shall help to visualise the redshift, one is located at the peak with highest wavelength of the monomer and one at the redshifted peak in one of the aggregated structures. No tetramers were optimised for **Pt-4**. Level of theory: CAM-B3LYP-D3/MWB60(Pt)/6-31G(d) with 30 states.

clearly red-shifted band failing to reproduce the experimental findings. For **Pt-8**, no red-shifted peak can be spotted either. Here, this is most likely due to the large Pt...Pt distance of more than 4.3 Å in the dimer S_0 that shortens only in the T_1 to 2.8 Å, as a similar pattern occurs for the trimer. Also for **Pt-9**, the separated dimer and trimer S_0 structures prevent visualising the expected red-shifted peak in the UV-vis absorption spectra (dimer Pt...Pt distances in the S_0 : 4.1 Å, T_1 : 2.8 Å). As expected, **Pt-10** also lacks this band in the spectrum agreeing with the experimental results.

The tetradentate complex **Pt-11** (Figure 15a) shows no distinct red-shifted peak for both dimer and trimer that display almost identical spectra. For **Pt-12** in Figure 15b, there is no monomer absorption spectrum due to the binuclear nature of the complex. The spectrum shows a significant band at approximately 340 nm indicating the importance of low-lying excited states. For this structure, the MMLCT character was also observed for the $S_0 \rightarrow S_1$ absorption (see Table A4), although it is dark and therefore not visible in the spectrum.

To conclude, computationally determined UV-vis absorption spectra with TDDFT can sometimes

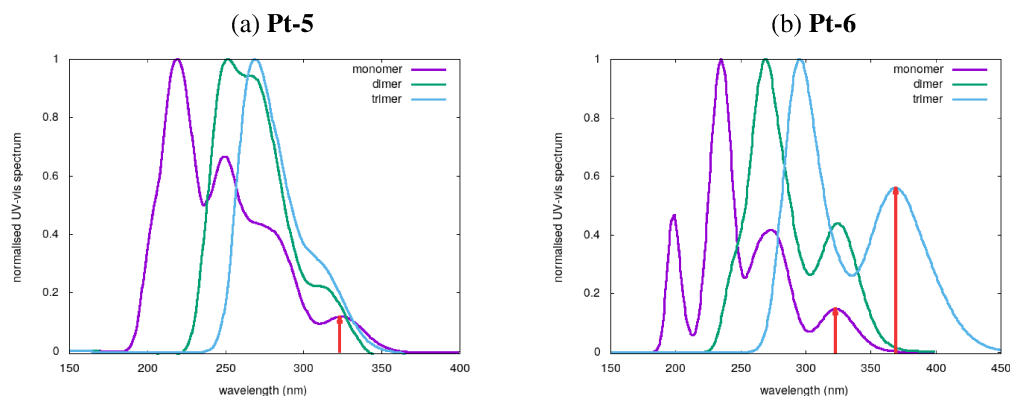


Figure 13: Computed normalised UV-vis spectra for the monomers, dimers and trimers for **Pt-5** and **Pt-6**. The red arrows shall help to visualise any potential redshift. In subfigure (a), there is only one since no red-shifted peak is observable. In subfigure (b), only the trimer displays one. Level of theory: CAM-B3LYP-D3/MWB60(Pt)/6-31G(d) with 30 states.

capture the $^3\text{MMLCT}$ band, where it was previously experimentally proposed. However, this only applies when closely stacking aggregates with small Pt $\cdots$ Pt distances already occur in the ground state since this is the structure the UV-vis absorption spectra get determined from. If no close Pt $\cdots$ Pt are exhibited, this approach fails and only confirms the general redshift expected for aggregating structures. The main problem of this analysis is that it is solely based on structural information and not on the wavefunction character making it unreliable.

4.3 Spin-density difference plots

The excimer emission discussed in this thesis is based on T_1 - S_0 transitions, where a spin flip is involved to proceed from the T_1 state to the S_0 state. One way to visualise this is plotting the spin density difference of the T_1 geometry, where this property is only non-zero for the involved single-occupied orbitals. This provides information about the excitation schemes presented in Figure 2.

The spin-density difference plots for the monomers, dimers, trimers and tetramers for **Pt-1** to **Pt-4** are visualised in Figure 16. The isovalues for all spin-density difference plots were chosen to portray the orbital character as clearly as possible. Changing the isovalue does not change the character of the interaction. In the following, they will be analysed together due to their similar geometry. Saito and al. already presented spin-density plots for the monomers (Figure 16a-16d) at a different level of theory that could be successfully reproduced in this work.^[10] The spin density is mostly localised on the NHC-ligand with minor contributions on the platinum center. In the dimers (Figure 16e-16h), all four complexes depict the spin density localised on the stacking platinum centers with contributions on the ligands. This suggests $^3\text{MMLCT}$ as the involvement of both metal centers and ligands is necessary here. Also for the trimers of **Pt-1** to **Pt-3** depicted in Figure 16i-16k, the overlapping d_{z^2} orbitals are visualised with π -orbitals

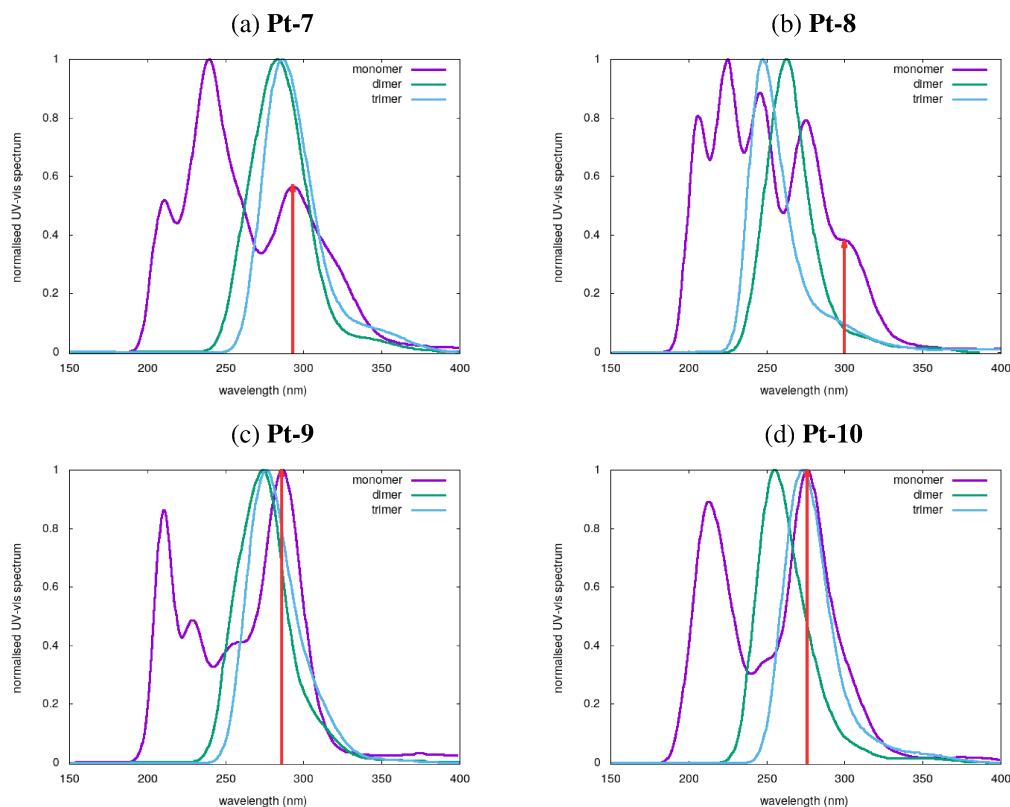


Figure 14: Computed normalised UV-vis absorption spectra for the monomers, dimers, trimers and tetramers for **Pt-7**, **Pt-8**, **Pt-9** and **Pt-10**. The red arrow visualises lowest-lying peak/shoulder with respect to the energy. Level of theory: CAM-B3LYP-D3/MWB60(Pt)/6-31G(d) with 30 states.

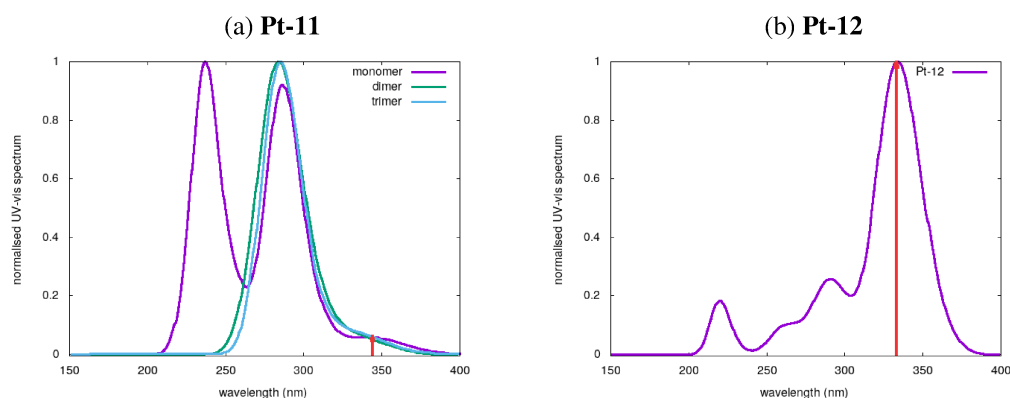


Figure 15: Computed normalised UV-vis spectra for the monomers, dimers and trimers for **Pt-11** and **Pt-12**. The red arrow visualises the peak lowest in energy for the monomer. Level of theory: CAM-B3LYP-D3/MWB60(Pt)/6-31G(d) with 30 states.

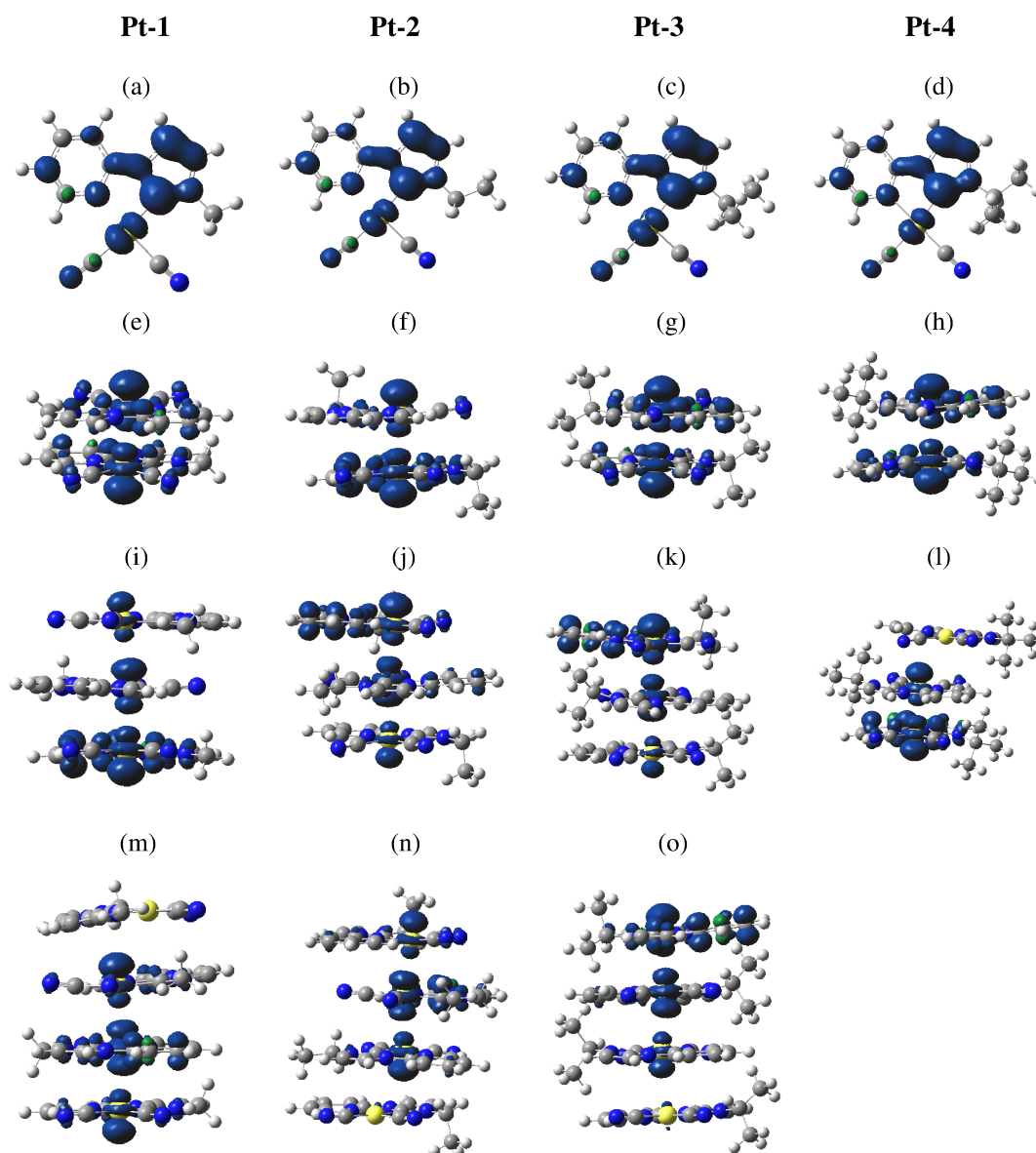


Figure 16: Spin density difference plots obtained at the T_1 optimised geometry with UCAM-B3LYP-D3/MWB60(Pt)/6-31G(d) level of theory for **Pt-1**, **Pt-2**, **Pt-3** and **Pt-4**. First row: monomers, second row: dimers, third row: trimers, fourth rows: tetramers. Carbon atoms are depicted in grey, hydrogen in white, nitrogen in blue and platinum in yellow. Note that no tetramers were investigated for **Pt-4**. Isovalue: 0.004

involved centered on only one ligand. The interlayer distances are not symmetric, the complex layer displaying shorter distances to the middle layer is usually the one with ligand contribution. In **Pt-4**, the sterically demanding tert-butyl group limits its ability to stack, which is also depicted in the spin density as the upper layer does not contribute to the spin density difference plot at all. This pattern is also observed for the investigated tetramers (Figure 16m-16o), where one

layer hardly contributes. Non-contributing layers in the spin density difference plot also hint the maximum number of layers possible to contribute to excimer emission. Qualitatively speaking, the sterical demand of the alkyl chain R does not influence the distribution of the spin density, only the formation of stacking structures as discussed in Section 4.1.

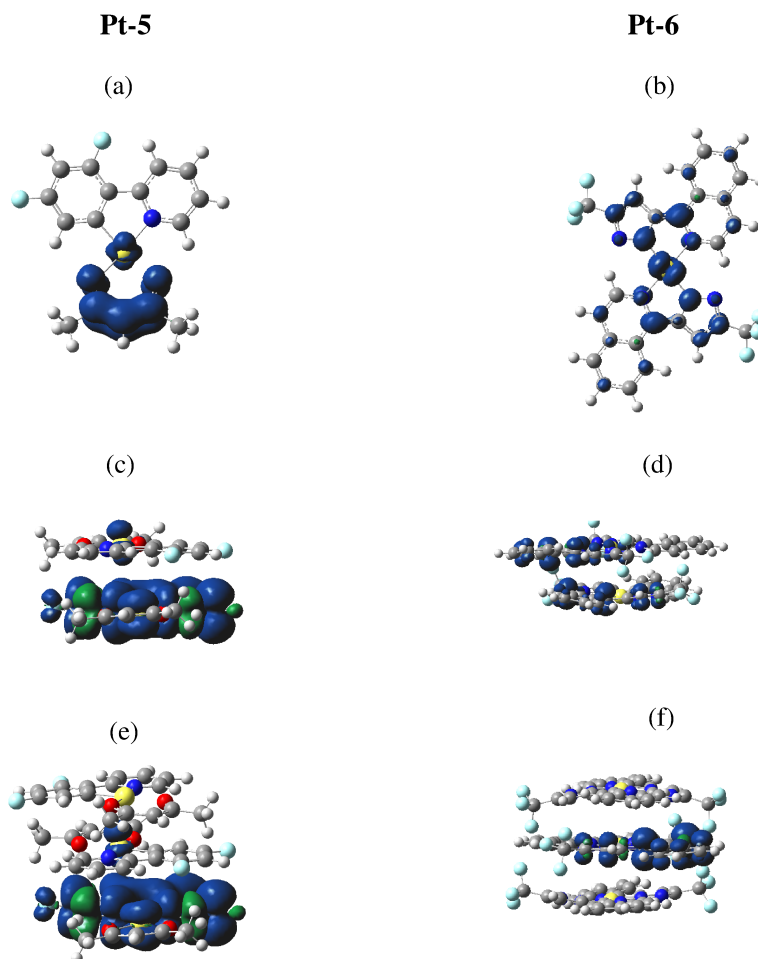


Figure 17: Spin density difference plots obtained at the T_1 optimised geometry with UCAM-B3LYP-D3/MWB60(Pt)/6-31G(d) level of theory for **Pt-5** and **Pt-6**. First row: monomers, second row: dimers, third row: trimers. Carbon atoms are depicted in grey, hydrogen in white, nitrogen in blue and platinum in yellow. Isovalue: 0.004, except for (c) and (e): 0.0008

The spin density difference plots for the remaining two bidentate complexes, **Pt-5** and **Pt-6**, are depicted in Figure 17. Both monomers show contributions coming from the platinum center as well as from the ligand matching the previously experimentally or computationally determined MLCT for these complexes.^[11,14] **Pt-5** displays d- π interaction in its dimeric and trimeric form (Figure 17c and 17e) whereas the orbitals involved for **Pt-6** are more ligand-centered.

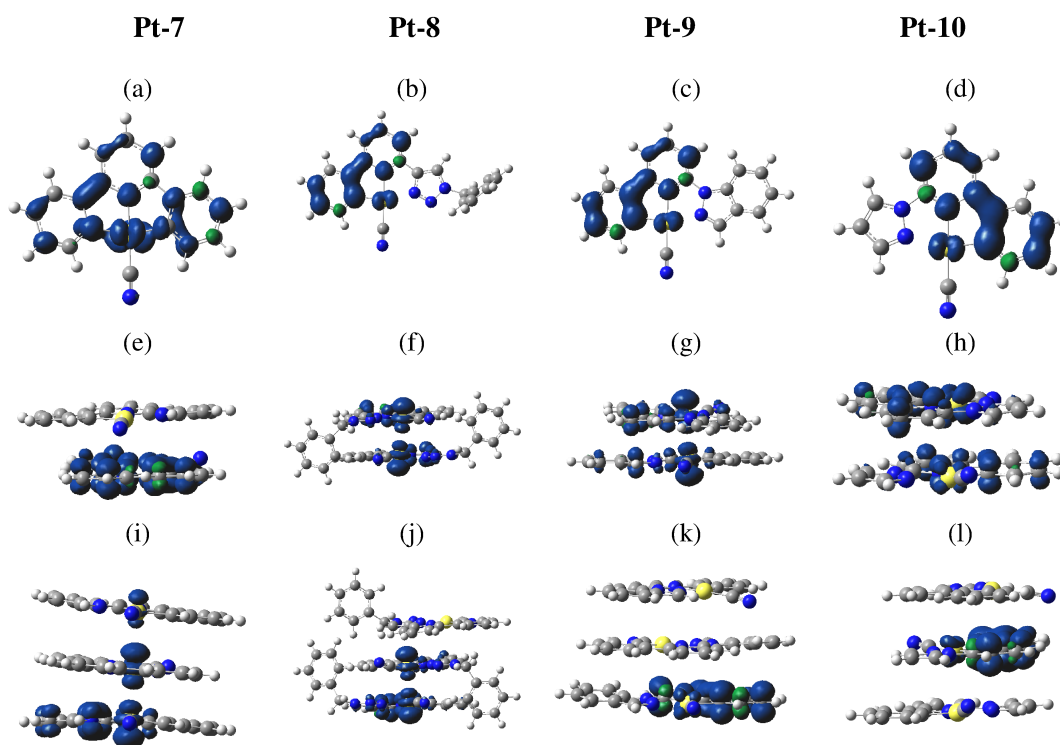


Figure 18: Spin density difference plots obtained at the T_1 optimised geometry with UCAM-B3LYP-D3/MWB60(Pt)/6-31G(d) level of theory for **Pt-7**, **Pt-8**, **Pt-9** and **Pt-10**. First row: monomers, second row: dimers, third row: trimers. Carbon atoms are depicted in grey, hydrogen in white, nitrogen in blue and platinum in yellow. Isovalue: 0.004

The four tridentate complexes included in this study, **Pt-7** to **Pt-10**, are analysed together due to their geometric similarity. For **Pt-7**, the spin density difference is located on both metal center and the whole ligand, whereas for **Pt-8** to **Pt-10** is situated only on the metal and the phenylpyridine ligand and not on the triazol, indazol or pyrazol ring. In the dimers, the orbitals are focused on only one layer in **Pt-7** while being spread over both layers in the other three complexes. In **Pt-8**, $^3\text{MMLCT}$ is exhibited due to the formed $d\sigma^*$ orbitals for both dimers and trimers. The dimer of **Pt-9** also shows $d\sigma^*$ orbitals, but not in trimer, where only ligand-centered orbitals are visible. **Pt-10** does not display any specific type of interaction. For the trimers, the spin density difference is either located on only one complex layer as for **Pt-7** or **Pt-10** or indicates $^3\text{MMLCT}$ as for **Pt-8**.

The spin density difference plots of **Pt-11** and **Pt-12** are depicted in Figure 19. In the **Pt-11** monomer, it is located on both the metal center and the ligand implying $^3\text{MLCT}$ and $\pi-\pi$ interaction. In the dimer, this changes to solely ligand contributions of a single layer. The binuclear complex **Pt-12** differs from all the other complexes in its construction showing the most distinct $d\sigma^*$ orbitals and only tiny contributions from the ligand.

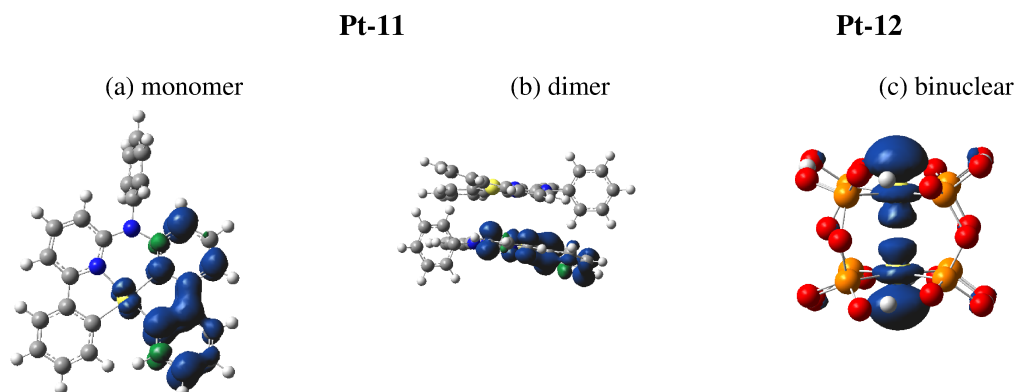


Figure 19: Spin density difference plots obtained at the T_1 optimised geometry with UCAM-B3LYP-D3/MWB60(Pt)/6-31G(d) level of theory for **Pt-11** and **Pt-12**. Carbon atoms are depicted in grey, hydrogen in white, nitrogen in blue, oxygen in red, phosphorus in orange and platinum in yellow. Isovalue: 0.004

To conclude, spin density difference plots are a useful tool to visualise the orbitals involved in the T_1 state, overall matching experimentally determined results: For **Pt-1** to **Pt-4**, **Pt-6**, **Pt-7** to **Pt-9**, $^3\text{MMLCT}$ was attributed by previous experimental or computational studies.^[10,12,14] Corresponding $d-\sigma^*$ and π^* orbitals were visualised for all of those complexes except for **Pt-6**. The reason for this deviation is still unknown. For **Pt-5**, **Pt-10**, **Pt-11** and **Pt-12** no $^3\text{MMLCT}$ is described by literature.^[11–13,15] The orbitals involved in the T_1 state for **Pt-5** point towards $d-\pi$ interaction, for **Pt-10** $\pi-\pi$ interaction, for **Pt-11** no interaction at all. For **Pt-12**, the term "MMLCT" is not used in the literature, but the influence of close stacking platinum centers in binuclear complexes is well described.^[15,80,81] The spin density difference plots allow assignment of the different proposed excitation schemes presented in Figure 2 and even for mixtures of those. However, this approach is solely qualitative since it is based on the visual inspection of spin density distribution plots. For quantitative assignments, a new type of analysis is necessary introduced in section 4.5.

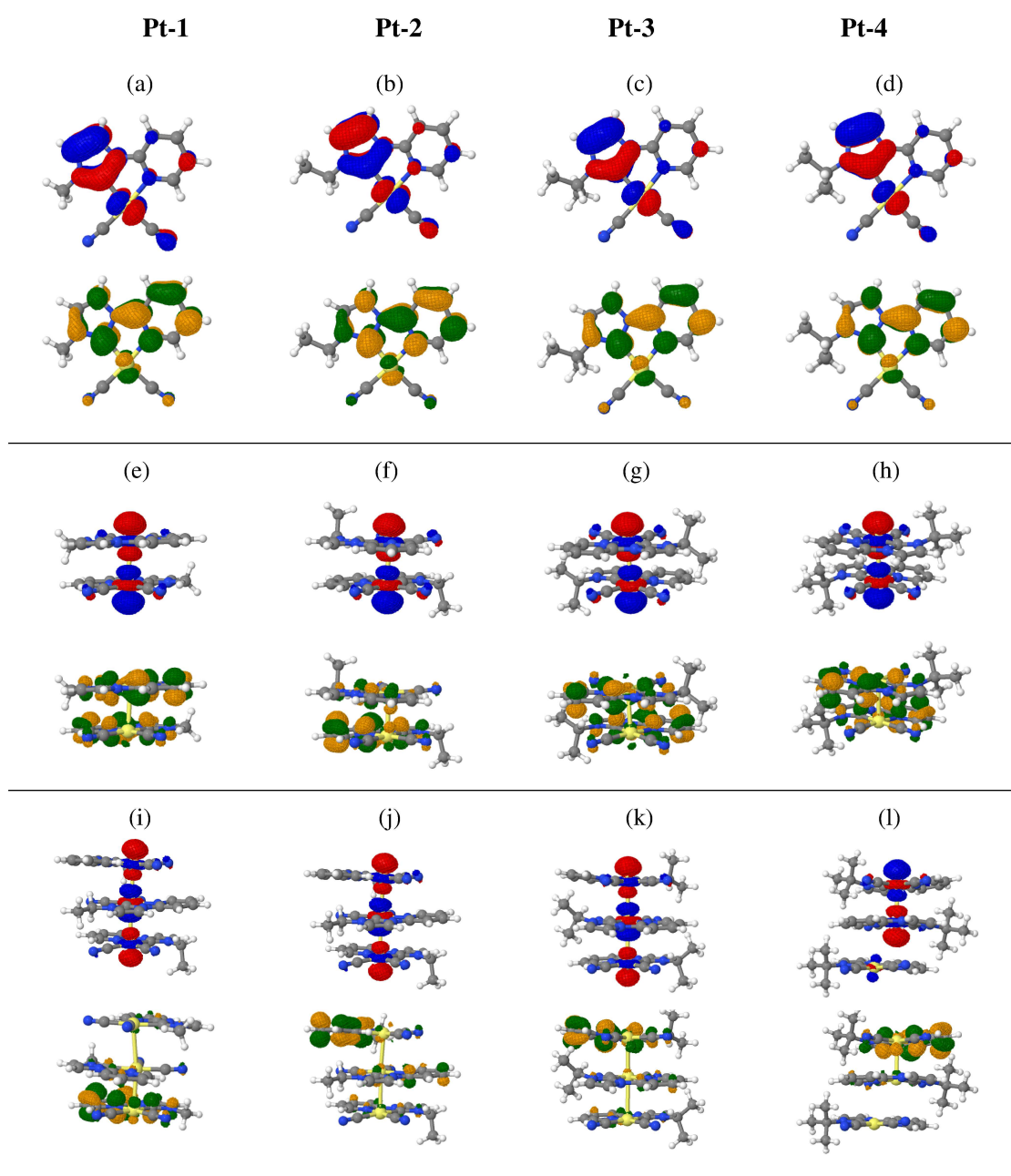
4.4 Natural transition orbitals (NTOs)

As discussed in Section 2.5.2, NTOs were developed to visualise the answer to the question "What got excited to where?"^[52] The spin density difference plots of the previous section are limited to triplet states as the total spin for singlet states adds up to 0. Additionally, the spin density are not derived from transition densities, but from the single-occupied orbitals in the T_1 state neglecting the multi-excitation character excited states typically have. To overcome those difficulties, the NTOs of all twelve complexes for monomers and excimers are presented and discussed in this section.

Figure 20 presents the occupied and virtual NTOs for **Pt-1** and **Pt-4** that are analysed together due to their similar structure. For the monomers, the orbitals are indistinguishable between **Pt-1**

to **Pt-4**. The occupied orbital is delocalized over the metal center, the phenylring connected to the alkyl group and the cyano group opposite to this ring. The virtual orbitals are spread over the whole NHC ligand and the metal center with only tiny contributions coming from the cyano group. This matches the description of the monomer HOMO-LUMO orbitals presented in Figure 2a, where a π and π^* orbital is involved.

Also in the dimers, the NTOs of **Pt-1** to **Pt-4** resemble each other. Due to the linear stacking of the metal centers, the d_{z^2} orbitals overlap to form $d\sigma$ orbitals as depicted for the occupied orbitals.



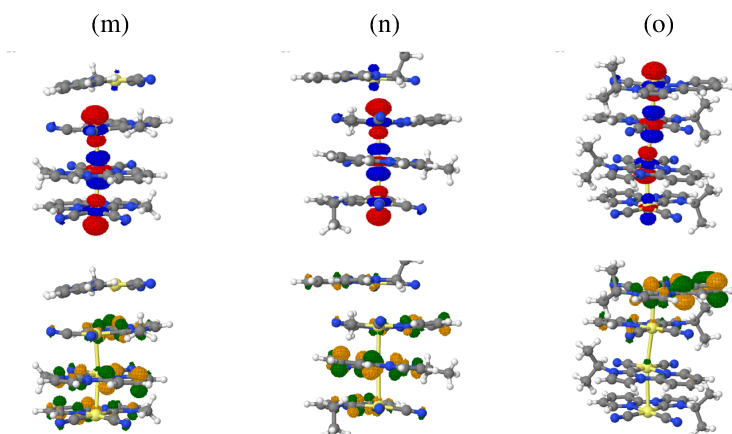


Figure 20: NTOs for **Pt-1**, **Pt-2**, **Pt-3** and **Pt-4**. Occupied orbitals are depicted in red/blue, virtual ones in yellow/green. (a) to (d): monomers, (e) to (h): dimers, (i) to (l): trimers, (m) to (o): tetramers. Carbon atoms are depicted in grey, hydrogen in white, nitrogen in blue and platinum in yellow. No tetramers were optimised for **Pt-4**.

The virtual orbitals display π^* orbitals, usually equally spread over both complex layers, except for **Pt-2** in Figure 20f where the lower layer is more dominant. Also these orbitals match the proposed scheme in Figure 2a. For the trimers presented in Figure 20i to 20l, the occupied orbitals also display d_{z^2} orbitals spread over all three layers, except for **Pt-4** where sterical hindrance from the butyl group prevents significant stacking. The virtual π^* orbitals are mostly located on one ligand, analysis of the interlayer distances reveals that this is the outer layer closer to the middle layer as the complexes are not symmetric.

In the tetramers, different possibilities for overlapping d_{z^2} orbitals exist: in **Pt-1** only three of the four layers stay linearly leading to only three contributing d_{z^2} orbitals. Also in **Pt-2** (Figure 20n), the fourth layer does not stack anymore, however and contrarily to **Pt-1**, there is still a small contribution visible. In **Pt-3** (Figure 20o) all four layers contribute to the NTO, nevertheless, also here the bottom layer is less involved than the others. For the virtual orbitals in the tetramers, they can be either spread of several layers as for **Pt-1** and **Pt-2** or mostly located on one as for **Pt-3**- which is rather surprising since this structure is the best-stacking one of the three. Based on the analysis of the NTOs, $^3\text{MMLCT}$ can be computationally validated for all four complexes **Pt-1** to **Pt-4** for their dimer, trimer and tetramer structures. The NTOs also hint the limit of the $^3\text{MMLCT}$'s feasibility, namely when the d_{z^2} orbitals do no longer overlap.

Figure 21 displays the occupied and virtual NTOs of the tridentate complexes **Pt-7** to **Pt-10** that are analysed together due to their similar geometrical structure. Also here, the NTOs in the monomers are located on both the metal center and the ligand, for both virtual and occupied orbitals. On the ligands, the orbitals are situated on the phenyl rings and not the different rests. In the dimer structure of **Pt-7** and **Pt-10**, the occupied NTO resembles π -orbitals spread over

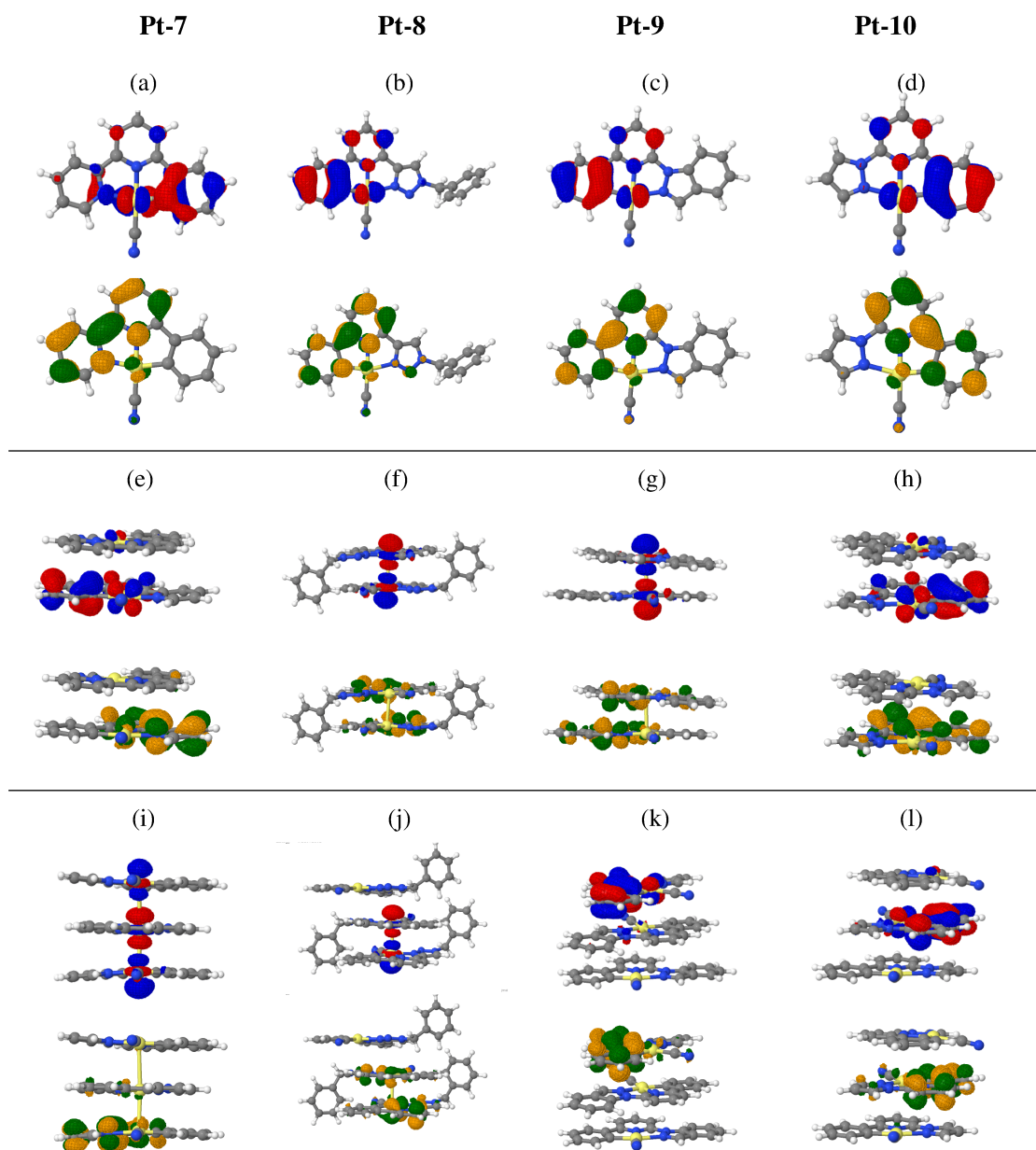


Figure 21: NTOs for **Pt-7**, **Pt-8**, **Pt-9** and **Pt-10**. Occupied orbitals are depicted in red/blue, virtual ones in yellow/green. (a) to (d): monomers, (e) to (h): dimers, (i) to (l): trimers. Carbon atoms are depicted in grey, hydrogen in white, nitrogen in blue and platinum in yellow.

the ligand of one layer and the platinum metal centers. The virtual NTO is solely located on the ligand. **Pt-8** and **Pt-9** show similar results despite their different substituents on the ligand core: As for **Pt-1** to **Pt-4**, the d_{z^2} overlap to form a $d\sigma$ -orbital. The virtual NTO with π^* character is spread on the ligands of both complex layers. Unlike **Pt-1** to **Pt-4**, the trimers of **Pt-7**, **Pt-9** and **Pt-10** show different orbital characters than their dimer structures. Here, **Pt-7** bears linear

stacking with resulting formation of a $d\sigma$ orbital and a virtual π^* NTO located on the ligand. **Pt-8** keeps the orbital characters also in its trimeric structure, however, only two layers are involved due to the bulkiness of the flexible phenyl group. In **Pt-9**, the occupied and virtual NTOs are solely located on the ligand of one layer, as well as for **Pt-10**.

Comparing the NTOs' characters of **Pt-7** to **Pt-10** with the proposed orbital scheme in Figure 2 reveals that **Pt-7**, **Pt-8** and **Pt-9** display $^3\text{MMLCT}$ due to orbital overlap in at least one of their dimeric or trimeric structure. For **Pt-10** and the remaining aggregated structures of **Pt-7** to **Pt-9**, π - π is visualised, with or without involvement of the platinum center. Nevertheless, these results match perfectly with the experimental conclusions drawn by Sivchik et al.:^[12] The crystal samples of **Pt-7** and **Pt-9** have been found to display $^3\text{MMLCT}$ emission, whereas **Pt-10** showed π - π intraligand transitions. The peaks in the emission spectrum of **Pt-8** could not be clearly assigned since it was a polycrystalline sample.

Figure 22 displays the NTOs of **Pt-5**, **Pt-6**, **Pt-11** and **Pt-12**. In the monomers, the occupied and virtual NTOs are spread over the platinum center and (parts of) the aromatic ring system. In the **Pt-5** dimer (Figure 22d), the occupied NTO shows d - π interaction with an d_{z^2} orbital in the upper layer and a π -orbital in the lower layer. In the virtual orbital, only the lower layer contributes with a π^* -orbital spread over both platinum center and the aromatic ring system. The **Pt-6** dimer only displays π -orbitals spread predominantly over both layers in both the occupied and the virtual orbital (see Figure 22e). In the **Pt-11** dimer (Figure 22f), the virtual orbital only shows a tiny contribution of a π^* orbital located on the platinum center in the upper layer that vanishes in the virtual NTO. This contribution is likely negligible compared to the more dominant π -orbitals spread over the lower layer in both occupied and virtual orbital. The binuclear pincer complex **Pt-12** depicts dominant contributions involving overlapping d_{z^2} orbitals forming $d\sigma^*$. The contributions located on the ligands are smaller. For **Pt-5**, the character of the NTOs in the trimer is equivalent to the one of the dimer: The upper layer does not contribute, the middle layer shows a d_{z^2} orbital in the occupied NTO and vanishes in the virtual NTO. Both lower layers display π -orbitals, pointing towards d - π orbital interaction. Also for **Pt-6**, the character remains the same with only π -orbitals being involved in the middle layer hinting π - π interaction.

To summarise, NTOs display similar orbitals as the spin density difference plots, generally agreeing with experimental results. Nevertheless, the NTOs can only be inspected visually and provide qualitative information. For quantitative information of excitation characters, a different approach needs to be used as will be presented in the next chapter.

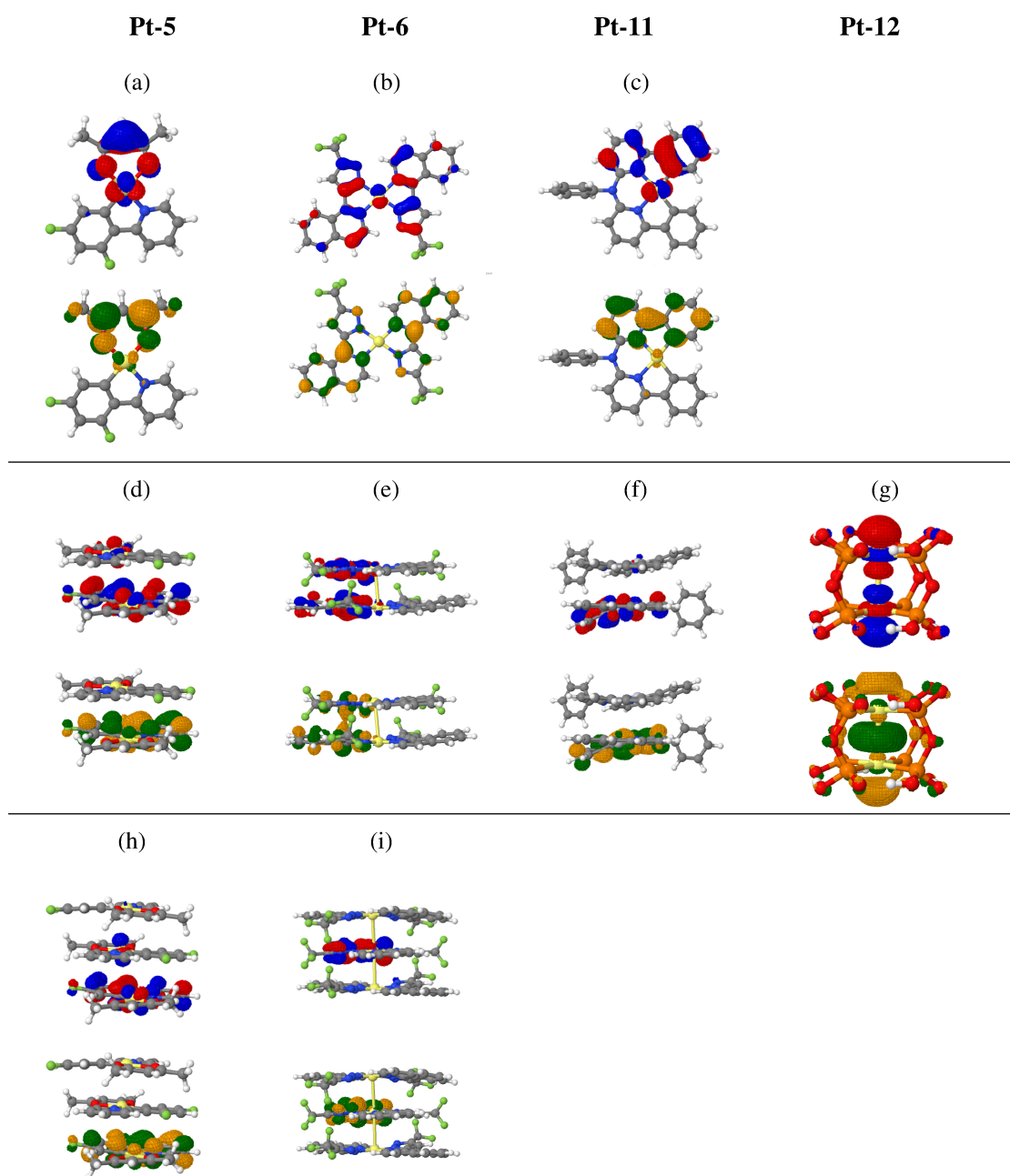


Figure 22: NTOs for **Pt-5**, **Pt-6**, **Pt-11** and **Pt-12**. Occupied orbitals are depicted in red/blue, virtual ones in yellow/green. (a) to (c): monomers, (d) to (g): dimers, (h) to (j): trimers. Carbon atoms are depicted in grey, hydrogen in white, nitrogen in blue, oxygen in red, phosphorus in orange and platinum in yellow.

4.5 1TDM analysis

The 1TDM was analysed with TheoDORE (Theoretical Density, Orbital Relaxation and Exciton analysis), a program developed by F. Plasser for fragment-based analysis of excited state using the 1TDM of the studied excited state.^[51] The coordinates of the electron-hole pair are accessible by integrating over the ground and the excited state wave functions. Each molecule or complex is divided in different fragments (decided by the user), which are connected to the position of the electron-hole pair. This allows computing of charge transfer between two fragments yielding numbers ranging between 0 (no excitation between these two fragments) and 1 (the electron-hole pair is entirely located on these two fragments).^[51]

In this investigation, the same fragmentation scheme was used for all complexes and excimers: Each metal center is chosen to be a single fragment to give access to analysing metal-to-metal charge transfer (MMCT) and each ligand is a new fragment, regardless whether it is a mono-, bi-, tri-, or tetradentate one. Also for **Pt-12**, each pyrophosphate unit was selected to be a single fragment. To give an example, the dimer of **Pt-1** consists of eight fragments: two coming from the two metal centers, four from the four cyano- and two from the two NHC-ligands. For better visualisation, a scheme is provided in Figure 23. In the following, the excited state character decomposition of T_1 is analysed separately for the monomers, dimers and trimers.

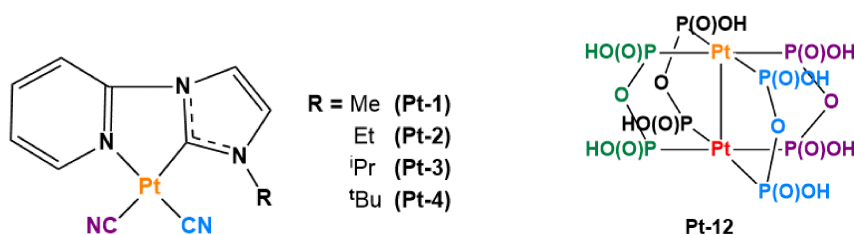


Figure 23: Fragmentation schemes for **Pt-1** to **Pt-4** and **Pt-12** as examples for all complexes. Each colour signifies a new fragment.

In Figure 24, the percentages of different excited state characters are given considering metal centered (MC), LC, ligand-to-metal charge transfer (LMCT), LLCT and MLCT. The values were determined for the T_1 state of the monomeric complexes **Pt-1** to **Pt-11**. **Pt-12** is not included because its binuclear structure resembles more a dimer than a monomer. Most complexes are of mixed character, except of **Pt-5**, **Pt-6** and **Pt-11** where LC dominates with > 80%. For all of these complexes, this is in accordance with the experimentally and/or previously computationally obtained data reporting LC and MLCT in diluted solution where dispersed monomers can be assumed.^[11,13,21] The four tridentate complexes **Pt-7** to **Pt-10** also show a mixture of MLCT and LC typical for Pt(II)-complexes although no spectral information in solution were reported by Sivchik et al.^[12] **Pt-1** to **Pt-4** show a more mixed behaviour than the other complexes, as LMCT and rising LLCT contributions influence the distribution. Especially for **Pt-2** and **Pt-3**, no dominant character can be reported anymore. Experimentally, MLCT and various LC transitions are reported.^[10] All eleven complexes only show minor contributions of MC.

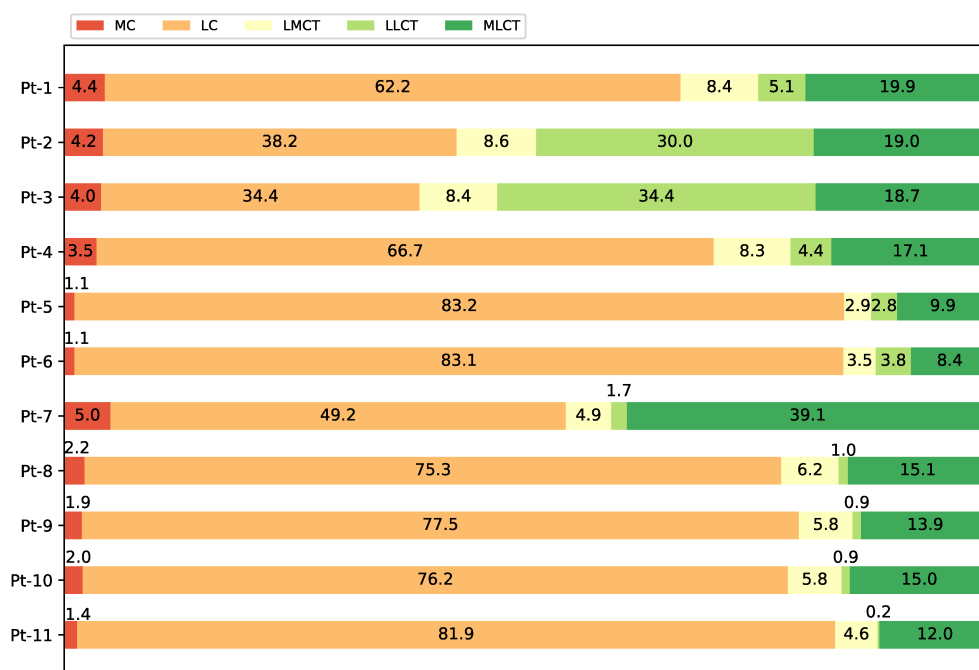


Figure 24: 1TDM analysis of the monomers of **Pt-1** to **Pt-11** (triplet geometry at the ground state PES). **Pt-12** is not included because its geometrical structure resembles a dimer more. Numbers given are percentages of the different transition characters. Summing up all percentages does not necessarily lead to 100% due to rounding differences.

For the analysis of the dimers, an additional excited state character was considered, the MMCT. This was motivated by the fact that TheoDORE can only analyse excitations between two fragments, however, for the $^3\text{MMLCT}$ at least three fragments are required: two metal centers and one ligand. The $^3\text{MMLCT}$ is therefore split in two processes, the MMCT and MLCT, since both are necessary to describe it.

With respect to the three different possible excitations leading to excimer emission discussed in Section 1, one can expect different excitation characters in the 1TDM. The d-d interaction leading to $^3\text{MMLCT}$ was discussed in the previous paragraph, for π - π interaction, LC or LLCT states are expected, whereas for d- π interaction MLCT character should be dominant. The 1TDM analysis for the dimers of **Pt-1** to **Pt-12** are displayed in Figure 25. **Pt-1** to **Pt-4** show a similar distribution in excitation characters due to their geometrical similarity. All of them experimentally display redshifted excimer emission that is assigned to $^3\text{MMLCT}$.^[10] This is confirmed here with MMCT characters > 10% and MLCT characters > 60%. Compared to the monomers, the MC became more dominant with values between 12 and 15%, too. Also the LC, which was prevalent especially in the monomers of **Pt-1** and **Pt-4** with 62% and 67%, respectively, only plays a minor role with < 3%. Also the LLCT with approximately 30% in the monomers of **Pt-2** and **Pt-3** is rather insignificant in the dimer analysis with less than 7%.

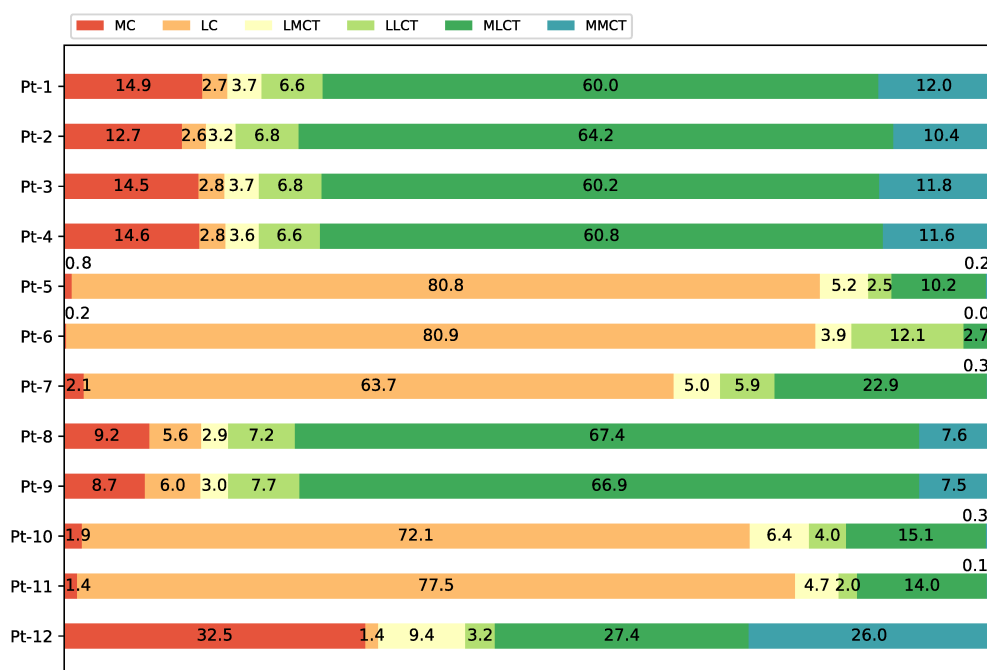


Figure 25: 1TDM analysis of the dimers of **Pt-1** to **Pt-12** (T_1 geometry at the ground state PES). Numbers given are percentages of the different transition characters. Summing up all percentages does not necessarily lead to 100% due to rounding differences.

Pt-8 and **Pt-9** show a similar profile with a prevalent MLCT character of approximately 67% and MMCT of 8% indicating $^3\text{MMLCT}$, too. For **Pt-9**, its redshifted excimer emission was assigned previously to $^3\text{MMLCT}$ as well.^[12] Additionally, the dominant LC character in the monomers with > 75% is reduced to approximately 6%. Summarising the complexes with a significant MMCT character, this is always accompanied by high percentages of MLCT.

The complexes **Pt-5**, **Pt-6**, **Pt-7**, **Pt-10** and **Pt-11** show a similar distribution in the dimers compared to the monomers with dominant LC. For **Pt-5**, the MMLCT responsible for excimer emission could be experimentally excluded.^[11] Adding the contributions of MLCT and LMCT yields 15% of d- π interaction that can be connected to structure presented in Figure 1c. The previously conducted computational study on **Pt-6**^[14] reported a mixed LC/MLCT state that can be partially confirmed here with 81% LC, but only 3% of MLCT. Experimentally $^3\text{MMLCT}$ is observed for **Pt-7** and $^3\text{MLCT}$ and π - π excitations for **Pt-10**.^[12] The latter one is well displayed in the distribution with 64% LC and 23% $^3\text{MLCT}$. **Pt-12** differs from the other eleven complexes since this type of dimer is not stabilised by intermolecular interactions, but covalent bonds from the pyrophosphate ligands forcing the Pt-centers to stack perfectly. This leads to 26% of MMCT and 33% MC. Together with 27% MLCT contribution, this suggests $^3\text{MMLCT}$.

Figure 26 displays the 1TDM analysis of the trimers of **Pt-1** to **Pt-11**. **Pt-12** is excluded because its structure resembles more a dimer than a trimer. For **Pt-1**, **Pt-2**, **Pt-3**, **Pt-4**, **Pt-5**, **Pt-8** and **Pt-10**

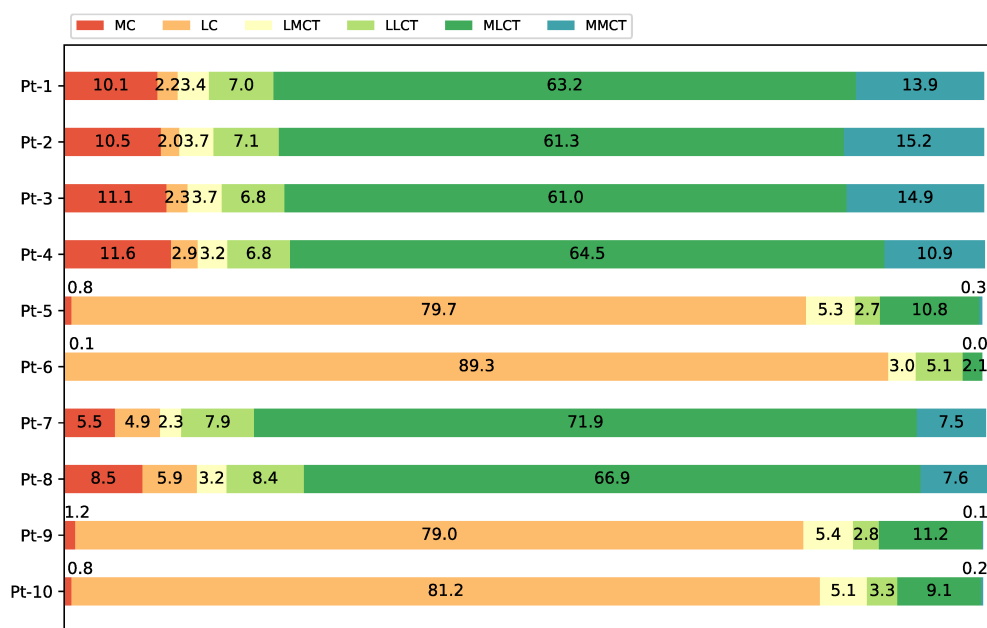


Figure 26: 1TDM analysis of the trimers of **Pt-1** to **Pt-11** (T_1 geometry at the ground state PES). Note that **Pt-12** is not included since it resembles more a dimer than trimer. Numbers given are percentages of the different transition characters. Summing up all percentages does not necessarily lead to 100% due to rounding differences.

the trimer excited character distributions are similar to those in the dimer. **Pt-1** to **Pt-4** still display dominant MLCT with slightly increasing MMCT and slightly decreasing MC. Qualitatively, also the excited state characters of the trimeric **Pt-6** resemble the dimer, however, the LC part increases to 89% and the LLCT is reduced to 5%. As indicated by spin density difference plot in Figure 18i and contrarily to the dimer, **Pt-7** displays 3 MMLCT in its trimeric structure with nearly 80 % combined MMCT and MLCT. On the other hand, **Pt-9** loses its 3 MMLCT character reported for dimers and now yields 79% of LC, well in agreement with the spin density difference plot in Figure 18k. For **Pt-10**, the LC character becomes even more dominant with 81% compared 72% in the monomer reducing the MLCT from 15% to 9%.

Figure 27 displays the 1TDM analysis for the tetramers of **Pt-1** to **Pt-3**. As for their respective dimeric and trimeric structure, the distribution of excited state characters is rather similar with approximately 60% of MLCT and 17% of MMCT.

To summarise, 1TDM with TheoDORÉ is a useful tool to get quantitative information about single excitation processes confirming the results of the spin-density difference plots. However, it can be difficult to assign the values to the three possible interactions discussed in Section 1, e.g. **Pt-5** qualitatively shows d- π -interaction in the spin-density difference plots, but only approximately 10% MLCT in the 1TDM analysis. Inversely, it is impossible to determine quantitative information from the spin-density difference plots, e.g. **Pt-12** shows 27% of MLCT

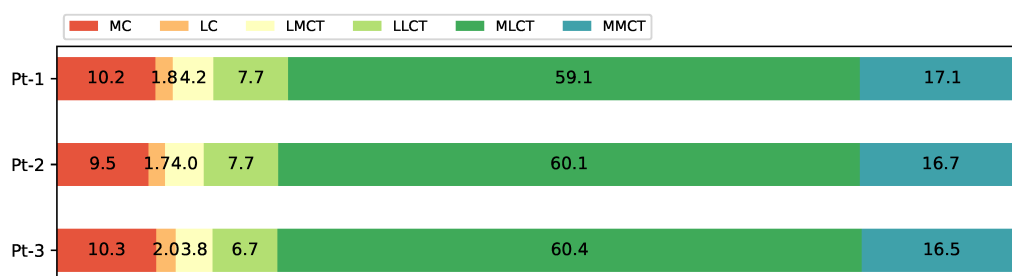


Figure 27: 1TDM analysis of the tetramers of **Pt-1** to **Pt-3** (T_1 geometry at the ground state PES). No tetramers were optimised for **Pt-4** to **Pt-12**. Numbers given are percentages of the different transition characters. Summing up all percentages does not necessarily lead to 100% due to rounding differences.

whereas the spin-density is only slightly located on the ligands. Here, the best approach to verify the data is to combine both analysis models to get a complete picture including qualitative and quantitative results.

4.6 Phosphorescent rate constants

Having developed an approach to classify complexes with respect to their excitation character, phosphorescent rate constants were computed to investigate how the emissive properties change. Therefore, the phosphorescent rate constants of monomers and excimers will be discussed and related to the different stacking interactions in the following section. All computed rate constants reported were calculated using Einstein's simplified formula for spontaneous radiative decay processes given in eq. 31 for all three triplet substates and then averaged according to eq. 32. The rate constants for all complexes **Pt-1** to **Pt-12** are listed in Table 3 together with the respective experimental values when available. For better visualisation, the rate constants were also portrayed in Figures 28, 29 and 30. Usually, all data was obtained using the T_1 geometry on the singlet PES, when this approach failed due to too high anharmonicities, the singlet geometry was taken.

Due to their similar geometry, **Pt-1** to **Pt-4** are analysed together. Their respective phosphorescent rate constants for the monomers, dimers, trimers and tetramers are presented in Figure 28. The monomers show all very similar rate constants between $1.5 \cdot 10^4$ and $2.8 \cdot 10^4 \text{ s}^{-1}$, with a slightly decreasing trend when going from the methyl-group to the bulkier tert-butyl group. The rate constants for the dimer range between $3.4 \cdot 10^5$ and $6.7 \cdot 10^5 \text{ s}^{-1}$, being more than 10 times higher than for monomer pointing towards the enormous influence the stacking leading to $^3\text{MMLCT}$ has. Since these rates were calculated based on eq. 31, only the oscillator strength or the energy gap serve as variables and can explain this significant increase of the rate constants. To give an example, the T_1 - S_0 energy gap for the **Pt-1** monomer, dimer, trimer and tetramer varies between 22500 and 25500 cm^{-1} . These fluctuations are not enough to describe an increase by a factor of 10, even if the energy gap scales quadratically as given by eq. 31. Therefore, the major cause for this increase is the oscillator strength being dependent on the transition dipole moment and the

Table 3: Phosphorescence rate constants in s^{-1} determined using eq. 31 for **Pt-1** to **Pt-11**. Note that tetramers were only optimised for **Pt-1** to **Pt-3**. An asterisk indicates that the rate constants were computed using the S_0 instead of the T_1 one.

	monomer	dimer	trimer	tetramer	experiment
Pt-1	2.77E+04	6.09E+05	2.40E+05	2.67E+05	1.80E+06 ^[10]
Pt-2	2.39E+04	3.39E+05	2.19E+05	1.88E+05	1.90E+06 ^[10]
Pt-3	2.17E+04	6.17E+05	6.69E+05	2.10E+05	2.20E+06 ^[10]
Pt-4	1.47E+04	6.69E+05	2.49E+05		8.00E+05 ^[10]
Pt-5	1.45E+04	1.17E+03	2.38E+03		0.85E+06 ^[11]
Pt-6	9.93E+03	1.82E+03	missing		/
Pt-7	7.28E+04	1.69E+04	1.47E+04		6.7E+04 ^[12]
Pt-8	5.16E+03	1.23E+05	8.62E+04		2.9E+04 ^[12]
Pt-9	3.60E+03	1.09E+05	1.47E+04*		1.4E+05 ^[12]
Pt-10	4.86E+03	3.15E+03	9.50E+02		2.8E+05 ^[12]
Pt-11	7.95E+03	5.09E+03	missing		

SOCs.

The trimer constants are also in the same range ($2.2 \cdot 10^5$ to $6.7 \cdot 10^5 \text{ s}^{-1}$) indicating that the formation of trimers does not alter the phosphorescent rate constants much. This trend is confirmed by the tetramers optimised for **Pt-1** to **Pt-3** as their rate constants vary between $1.9 \cdot 10^5$ and $2.7 \cdot 10^5$. This decrease is likely linked to the worse stacking behaviour leading to larger interlayer distances as reported in Section 4.1. The experimental values reported were determined by Saito et al.^[10] in solid crystal samples with uncountable complex layers constraining the orientation of single complexes and leading to better stacking than achieved computationally for much simplified dimers, trimers and tetramers. Nevertheless, the phosphorescent rate constants between $8.0 \cdot 10^5$ and $2.2 \cdot 10^6 \text{ s}^{-1}$ are less than 10 times as high for all dimers and trimer of **Pt-1** to **Pt-4**. For **Pt-4**, the experimental value is even comparable to the dimer phosphorescent rate constants. This is due to limited abilities of **Pt-4** to stack due to the sterically demanding tert-butyl group.

The four tridentate complexes **Pt-7** to **Pt-10** are analysed together due to their similar scaffold. **Pt-8** and **Pt-9** also display ³MMLCT as well as **Pt-1** to **Pt-4** and therefore show a similar pattern regarding their phosphorescent constants: The constants for the dimeric structure are more than ten times larger than for the monomers, with $1.2 \cdot 10^5$ and $1.1 \cdot 10^5 \text{ s}^{-1}$ compared to $5.2 \cdot 10^3$ and $3.6 \cdot 10^3 \text{ s}^{-1}$. The trimer rate constant of **Pt-8** is a bit lower probably due to stacking difficulties based on the sterically demanding ligand. **Pt-7** and **Pt-10** show a different pattern: The monomer shows the highest rate compared to the dimers and trimers and they also show less variance: it is between $1.5 \cdot 10^4$ and $7.3 \cdot 10^4 \text{ s}^{-1}$ for **Pt-7** and between $9.5 \cdot 10^2$ and $4.9 \cdot 10^3 \text{ s}^{-1}$ for **Pt-10**. The experimental values reported by Sivchik et al.^[12] were determined for solid state samples. For **Pt-7**, this value is close to the one reported for the monomer which is surprising since the

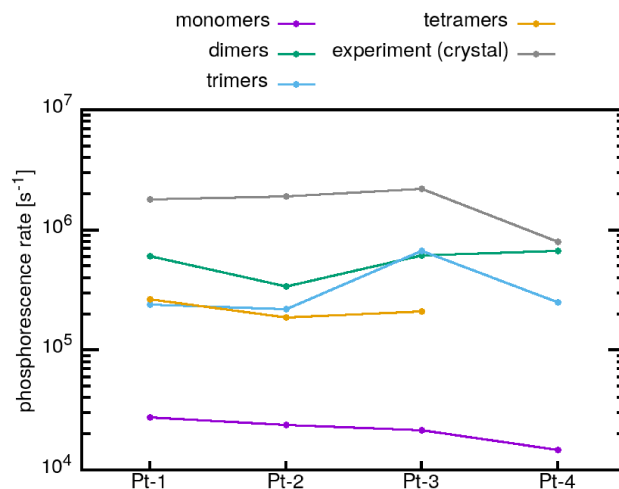


Figure 28: Phosphorescent rate constants in s^{-1} determined with Einstein's equation for **Pt-1** to **Pt-4**. No tetramer was optimised for **Pt-4**. Experimental data was measured by Saito et al.^[10]

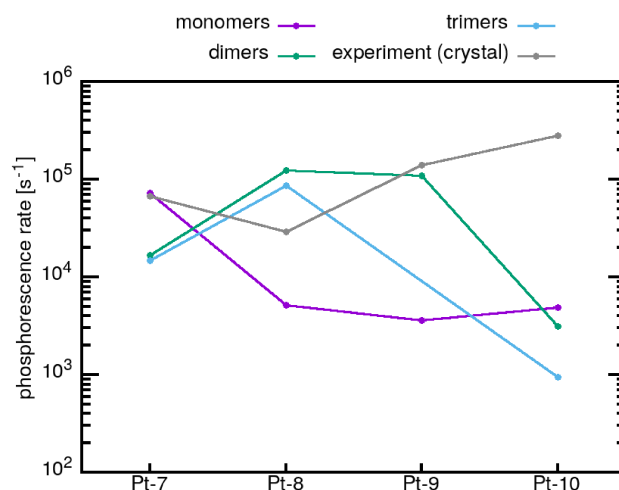


Figure 29: Phosphorescent rate constants in s^{-1} determined with Einstein's equation for **Pt-7** to **Pt-10**. Experimental data was measured by Sivchik et al.^[12]

monomer is the least similar to the crystal structure. In **Pt-8**, the rate is constant between monomer and dimer, whereas for **Pt-9** the experimental value is close to the dimeric one. In **Pt-10**, the experimentally determined rate constant surpasses the computed values by far.

Figure 30 visualises the computationally obtained phosphorescent rate constants for **Pt-5**, **Pt-6** and **Pt-11**. Note that no trimer was optimised for **Pt-11** and no rate constant could be obtained for the **Pt-6** trimer and **Pt-12** due to severe mixing of states. Also, experimental values to compare with

are only available for **Pt-5** and measured in solution, where dispersed monomers are expected.^[11] For **Pt-5**, the monomer rate constant is the same range as for the other bidendate complexes **Pt-1** to **Pt-4** and **Pt-6**. As for other complexes, where no $^3\text{MMLCT}$ can be rationalised based on the 1TDM analysis and NTO inspection, the phosphorescent rates decrease for both dimer and trimer. The experimental value, that should be close to the monomer, is approximately 60 times as high as for the experimental one. This can at least partially be explained the experimental setting carried out in solution which is not considered in the computations. Additionally, the rather different geometries of T_1 and S_0 lead to difficulties when using the harmonic approximation. In **Pt-6**, the dimer shows a higher rate constant compared to the monomer which usually serves as a sign for $^3\text{MMLCT}$. Indeed, the dimer (and trimer) structures arrange rather linearly with respect to the platinum centers, but do not stack closely enough to display overlapping $d\sigma^*$ orbitals in the NTO analysis. For **Pt-11**, the rate constants for both monomer and dimer are comparable following the pattern of non- $^3\text{MMLCT}$ displaying complexes.

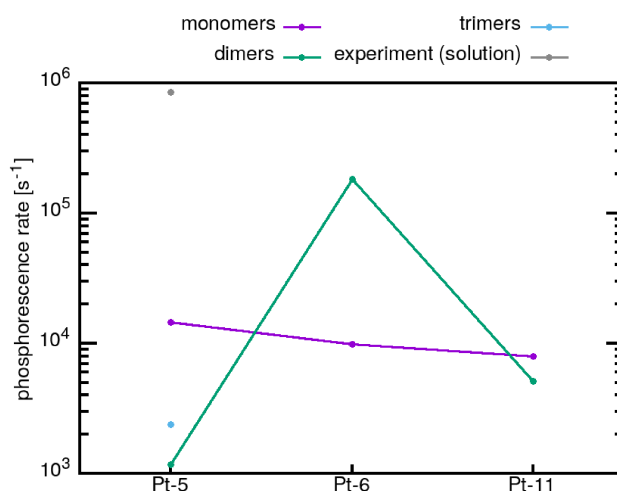


Figure 30: Phosphorescent rate constants in s^{-1} determined with Einstein's equation for **Pt-5**, **Pt-6** and **Pt-11**. Experimental data was measured by Cho et al.^[11] See text for missing data points.

To conclude, the $^3\text{MMLCT}$ has a significant influence on the phosphorescence rate constants of the excimers compared to the excited monomers by increasing it by at least a factor of 10. For the other two excimeric orbital interactions, $d-\pi$ and $\pi-\pi$, the rate constants remain at the same order of magnitude or decrease. Nevertheless, it is not possible to easily discriminate the latter two interactions from the $d-d$ orbital interaction leading to $^3\text{MMLCT}$ by comparing phosphorescence rate constants.

5 Conclusion

Square-planar platinum(II) complexes can arrange spontaneously to form supramolecular building blocks, such as dimers, trimers or even more complicated structures. These structures are usually defined as aggregates in the ground state and excimers in the excited state. This master thesis is an analysis of the excimeric structures of twelve different platinum(II) complexes including six bidentate, four tridentate, one tetradentate and one binuclear pincer complex. As previously proposed by literature,^[11] three different stacking mechanisms are possible, deriving from either d-d orbital interaction coming from the metal centers, π - π orbital interaction coming from the ligands and d- π orbital interaction coming from the metal center and the ligand. Dominant d-d orbital interaction is connected to close metallophilic Pt $\cdots$ Pt contacts leading to 3 MMLCT.

In this work, a computational protocol using (U)DFT and TDDFT is established with using the long-range exchange correlation functional including dispersion correction (U)CAM-B3LYP-D3, the ECP MWB60 for Pt and the 6-311G(d) basis set for all non-metal atoms. All monomeric, dimeric and trimeric structures were optimised for the S_0 and the T_1 . The highly stacking crystal structures are usually analysed using interplatinum distances. In the optimised aggregates and excimers, this constrain is missing leading to unreliable interplatinum distances. Therefore, the interplanar distances were determined additionally. The TDDFT calculations gave access to computed UV-vis absorption spectra and to analysing the ITDM with ITDM yielding quantitative values for different excited state characters. Visualising spin density difference plots and NTOs were used as a more qualitative approach to inspect orbitals. Finally, the influence of excimers on the phosphorescence rate constants compared to the excited monomers was investigated using Einstein's formula for spontaneous radiative decay.

Inspecting the geometrical parameters revealed that all twelve complexes are able to form aggregates with interplanar distances < 3.5 Å, which is twice the van-der-Waals radius of platinum. The S_0 geometry cannot be used to predict which type of stacking occurs in the T_1 state as no clear link between geometrical characteristics and wave function character has been found. In the T_1 state, only d-d stacking can be clearly distinguished from the other two possibilities by yielding interplatinum and interplanar distances of usually ≤ 3.0 Å. This was the case for **Pt-1** to **Pt-4** and **Pt-7** to **Pt-9**. Bulkier ligands do not necessarily prevent close stacking as revealed by **Pt-8** which has a flexible phenyl group. Additionally, it is both possible to have d-d stacking dimer but not a trimer - as for **Pt-4**, due to sterical hindrance from its ligand - but also to have a d-d stacking trimer without a d-d stacking dimer as for **Pt-7**. The computed UV-vis absorption spectra can also only sometimes be used to distinguish d-d orbital interaction from the other two possibilities, as the expected red-shifted peak is only sometimes visible as in the cases of **Pt-1** to **Pt-4** and **Pt-6**. This mismatching results can be attributed to the fact that the UV-vis absorption spectra have been calculated using the singlet geometry that do not generally allow to predict the T_1 structures as mentioned above. Next, the spin density difference plots were computed with the T_1 geometry and therefore more reliable in predicting the orbital interaction. d-d orbital interaction was correctly assigned for **Pt-1** to **Pt-4**, **Pt-7** to **Pt-10** and **Pt-12**. **Pt-5** shows d- π interaction, whereas **Pt-6**, **Pt-**

10 and **Pt-11** display π - π interaction. This information was validated in the NTO analysis where the occupied and virtual orbitals were visualised. They confirmed the proposed orbital interaction with respect to the stacking pattern. Also the quantitative analysis of the excited character matched the previous results: Due to technical settings, the $^3\text{MMLCT}$ that is connected to d-d orbital interaction had to be split in MMCT and MLCT. **Pt-1** to **Pt-4**, **Pt-7** to **Pt-9** and **Pt-12** showed contributions between 8% and 26% of $^3\text{MMCT}$ and 27% to 72% MLCT. For **Pt-5** displaying d- π interaction, approximately 10% of MLCT are reported and for **Pt-6**, **Pt-10** and **Pt-11** the biggest contribution is LC with at least 72%. Due to the similar results for d- π and π - π stacking, it is hardly possible to distinguish between these two interactions solely based on the 1TDM analysis. The comparison of phosphorescence rate constants also only allows to distinguish $^3\text{MMLCT}$ from the other possibilities: $^3\text{MMLCT}$ leads to an increase in phosphorescence rate constants by at least a factor of 10, whereas in the other cases the phosphorescence rate constants remains at the same order of magnitude or even declines. The experimentally reported values are usually measured in solid-phase crystal samples with uncountable complex layers which are hardly comparable to computed rate constants for dimers or trimers with just two or three complex layers.

To summarise, this computational study was able to validate experimental assignments of excitation types with the developed protocol. In the future, it can serve to find new square-planar platinum complexes displaying $^3\text{MMLCT}$ but also to characterise different stacking pattern and excited state characters for already existing complexes. For a qualitative approach, occupied and virtual NTOs are the orbitals that are the easiest to interpret and to assign to a stacking pattern. For a qualitative approach, the analysis of the 1TDM is a powerful tool to distinguish $^3\text{MMLCT}$ from the other two stacking patterns. UV-vis absorption spectra are to be interpreted carefully as well as interpreting data on the optimised geometries - as only d-d interaction can be discriminated in the T_1 state from the other interaction types.

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Additional information

5.1 UV-vis absorption spectra

Table 4: Computed absorption wavelength and oscillator strength of the $S_0 \rightarrow S_1$ excitation of the monomers (mon.), dimers (dim.), trimers (trim.) of **Pt-1** to **Pt-11**, the tetramers (tetr.) of **Pt-1** to **Pt-3** and the binuclear (binuc.) pincer complex **Pt-12**. The main configurations are presented with the corresponding percentage and were assigned to the respective transition(s).

Complex	State	λ [nm]	f	main configuration(s)	assignment
Pt-1 mon.	$S_0 \rightarrow S_1$	305	0.0100	HOMO $\rightarrow$ LUMO (66%)	MLCT/LLCT
Pt-1 dim.	$S_0 \rightarrow S_1$	295	0.0203	HOMO $\rightarrow$ LUMO (61%)	MLCT
Pt-1 trim.	$S_0 \rightarrow S_1$	303	0.1406	HOMO $\rightarrow$ LUMO (46%)	MMLCT
				HOMO-3 $\rightarrow$ LUMO (39 %)	MLCT
Pt-1 tetr.	$S_0 \rightarrow S_1$	303	0.1256	HOMO-1 $\rightarrow$ LUMO (43%)	MMLCT
				HOMO $\rightarrow$ LUMO (37%)	MLCT
Pt-2 mon.	$S_0 \rightarrow S_1$	304	0.0131	HOMO $\rightarrow$ LUMO (66 %)	MLCT
Pt-2 dim.	$S_0 \rightarrow S_1$	296	0.1124	HOMO $\rightarrow$ LUMO (46%)	MLCT
				HOMO-1 $\rightarrow$ LUMO (44%)	MMLCT
Pt-2 trim.	$S_0 \rightarrow S_1$	308	0.2072	HOMO-1 $\rightarrow$ LUMO (58%)	MMLCT
Pt-2 tetr.	$S_0 \rightarrow S_1$	309	0.2345	HOMO-10 $\rightarrow$ LUMO+2 (31%)	MLCT/LLCT
				HOMO-10 $\rightarrow$ LUMO (22%)	MLCT
				HOMO-4 $\rightarrow$ LUMO+2 (22%)	MLCT
Pt-3 mon.	$S_0 \rightarrow S_1$	303	0.0134	HOMO $\rightarrow$ LUMO (66%)	MLCT
Pt-3 dim.	$S_0 \rightarrow S_1$	297	0.0893	HOMO $\rightarrow$ LUMO (57%)	MLCT
Pt-3 trim.	$S_0 \rightarrow S_1$	306	0.1373	HOMO-1 $\rightarrow$ LUMO (49%)	MMLCT
				HOMO $\rightarrow$ LUMO (42 %)	MLCT
Pt-3 tetr.	$S_0 \rightarrow S_1$	304	0.2293	HOMO-1 $\rightarrow$ LUMO (47%)	MMLCT
				HOMO-3 $\rightarrow$ LUMO+1 (37%)	MLCT
				HOMO $\rightarrow$ LUMO+1 (37%)	MLCT
Pt-4 mon.	$S_0 \rightarrow S_1$	303	0.0122	HOMO $\rightarrow$ LUMO (66%)	MLCT
Pt-4 dim.	$S_0 \rightarrow S_1$	294	0.0527	HOMO $\rightarrow$ LUMO (57%)	MLCT
Pt-4 trim.	$S_0 \rightarrow S_1$	292	0.0122	HOMO-1 $\rightarrow$ LUMO+1 (45%)	MLCT
				HOMO $\rightarrow$ LUMO+1 (44 %)	MLCT
Pt-5 mon.	$S_0 \rightarrow S_1$	325	0.0532	HOMO $\rightarrow$ LUMO (58%)	MLCT
Pt-5 dim.	$S_0 \rightarrow S_1$	325	0.0000	HOMO $\rightarrow$ LUMO (57%)	MLCT

5.2 Coordinates of all optimised structures

Pt-5 trim.	$S_0 \rightarrow S_1$	325	0.0117	HOMO $\rightarrow$ LUMO (52%)	MLCT
Pt-6 mon.	$S_0 \rightarrow S_1$	359	0.1358	HOMO $\rightarrow$ LUMO (64%)	MLCT
Pt-6 dim.	$S_0 \rightarrow S_1$	368	0.0239	HOMO-1 $\rightarrow$ LUMO (40%)	MLCT
				HOMO-2 $\rightarrow$ LUMO (32%)	MLCT
Pt-6 trim.	$S_0 \rightarrow S_1$	392	0.0959	HOMO $\rightarrow$ LUMO (55%)	MMLCT
Pt-7 mon.	$S_0 \rightarrow S_1$	408	0.0025	HOMO $\rightarrow$ LUMO (64%)	MLCT
Pt-7 dim.	$S_0 \rightarrow S_1$	377	0.0005	HOMO $\rightarrow$ LUMO (62%)	MLCT
Pt-7 trim.	$S_0 \rightarrow S_1$	383	0.0000	HOMO $\rightarrow$ LUMO (48%)	MLCT
				HOMO-1 $\rightarrow$ LUMO+1 (44%)	MLCT
Pt-8 mon.	$S_0 \rightarrow S_1$	381	0.0031	HOMO $\rightarrow$ LUMO (65%)	MLCT
Pt-8 dim.	$S_0 \rightarrow S_1$	354	0.0001	HOMO $\rightarrow$ LUMO (62%)	MLCT
Pt-8 trim.	$S_0 \rightarrow S_1$	366	0.0048	HOMO $\rightarrow$ LUMO+1 (49%)	MLCT
				HOMO $\rightarrow$ LUMO (43%)	MLCT/LLCT
Pt-9 mon.	$S_0 \rightarrow S_1$	373	0.0075	HOMO $\rightarrow$ LUMO (61%)	MLCT
Pt-9 dim.	$S_0 \rightarrow S_1$	354	0.0027	HOMO-1 $\rightarrow$ LUMO+1 (54%)	MLCT
Pt-9 trim.	$S_0 \rightarrow S_1$	359	0.0030	HOMO $\rightarrow$ LUMO+1 (43%)	MLCT
				HOMO-1 $\rightarrow$ LUMO+1 (42%)	MLCT
Pt-10 mon.	$S_0 \rightarrow S_1$	377	0.0068	HOMO $\rightarrow$ LUMO (61%)	MLCT
Pt-10 dim.	$S_0 \rightarrow S_1$	349	0.0109	HOMO $\rightarrow$ LUMO (54%)	MLCT
Pt-10 trim.	$S_0 \rightarrow S_1$	359	0.0047	HOMO $\rightarrow$ LUMO+1 (47%)	MLCT
				HOMO $\rightarrow$ LUMO (27%)	MLCT
Pt-11 mon.	$S_0 \rightarrow S_1$	358	0.0169	HOMO $\rightarrow$ LUMO (66%)	MLCT
Pt-11 dim.	$S_0 \rightarrow S_1$	353	0.0097	HOMO $\rightarrow$ LUMO (39%)	MLCT
				HOMO-3 $\rightarrow$ LUMO (30%)	MLCT
				HOMO-2 $\rightarrow$ LUMO (27%)	MLCT/LLCT
Pt-11 trim.	$S_0 \rightarrow S_1$	350	0.0083	HOMO $\rightarrow$ LUMO+1 (47%)	MLCT
				HOMO $\rightarrow$ LUMO+2 (25%)	MLCT
Pt-12 binuc.	$S_0 \rightarrow S_1$	357	0.0000	HOMO $\rightarrow$ LUMO (70%)	MMLCT

5.2 Coordinates of all optimised structures

5.2.1 Pt-1

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Pt-1 monomer S_0

H 7.092073000 4.885087000 4.413598000

5.2 Coordinates of all optimised structures

H	8.855321000	4.920827000	0.486629000
C	7.806833000	4.902190000	2.378104000
Pt	12.179133000	4.920639000	4.546140000
N	14.722497000	4.927893000	6.336411000
N	10.333687000	4.913713000	3.494102000
N	13.681355000	4.948000000	1.775117000
C	13.240239000	4.938394000	2.851026000
N	9.526714000	4.895280000	5.646733000
C	13.801968000	4.925647000	5.626297000
N	10.763933000	4.893813000	7.401732000
C	8.658253000	4.882779000	6.729642000
H	7.585988000	4.875741000	6.630685000
C	9.440648000	4.881929000	7.825735000
H	9.182405000	4.873974000	8.872735000
C	10.837453000	4.902159000	6.063893000
C	9.239664000	4.901299000	4.273826000
C	10.185555000	4.920495000	2.160700000
H	11.109102000	4.930442000	1.592546000
C	7.953930000	4.895120000	3.758757000
C	8.934212000	4.915036000	1.566746000
C	11.895081000	4.896461000	8.325762000
H	12.823555000	4.906313000	7.759076000
H	11.840977000	5.785672000	8.957319000
H	11.853613000	3.999315000	8.946967000
H	6.813202000	4.897632000	1.943054000

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Pt-1 monomer T_1

H	-3.586115000	2.295710000	0.055682000
H	-4.482825000	-1.917185000	-0.044501000
C	-4.208839000	0.242027000	0.007954000
Pt	0.600311000	-0.635612000	-0.042614000
N	3.721102000	-0.640531000	-0.061142000
N	-1.495249000	-0.388647000	-0.023977000
N	0.229602000	-3.782033000	-0.119510000
C	0.467380000	-2.642803000	-0.092281000
N	-0.897945000	1.813526000	0.027633000
C	2.560945000	-0.697566000	-0.055747000
N	1.244192000	2.487800000	0.031736000
C	-0.878105000	3.171819000	0.061616000
H	-1.759273000	3.791537000	0.082514000
C	0.477452000	3.558745000	0.063219000

5.2 Coordinates of all optimised structures

H	0.880301000	4.561553000	0.085978000
C	0.460513000	1.308424000	0.006841000
C	-1.919659000	0.913172000	0.011152000
C	-2.424603000	-1.363659000	-0.042877000
H	-2.030999000	-2.372945000	-0.070499000
C	-3.283255000	1.255568000	0.027838000
C	-3.776237000	-1.097161000	-0.028162000
C	2.699957000	2.461620000	0.022338000
H	3.056733000	1.899740000	0.885431000
H	3.046161000	1.943495000	-0.871874000
H	3.067181000	3.488029000	0.045680000
H	-5.267905000	0.475749000	0.020105000

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Pt-1 dimer S_0

H	2.681405000	-1.981322000	2.628793000
H	4.412587000	1.858161000	1.749742000
C	3.709836000	-0.119654000	2.260617000
H	4.696501000	-0.533655000	2.433175000
Pt	-0.765396000	1.407476000	1.119134000
N	-3.647021000	1.746753000	-0.010520000
N	1.201836000	0.903468000	1.723119000
N	0.248930000	4.167319000	-0.046624000
C	-0.208333000	3.191837000	0.392627000
N	0.145926000	-1.080178000	2.212548000
C	-2.585886000	1.682640000	0.463855000
N	-1.978064000	-1.363394000	2.115093000
C	-0.084418000	-2.375481000	2.643962000
H	0.706673000	-3.064071000	2.884712000
C	-1.420187000	-2.547250000	2.589233000
H	-2.028837000	-3.403486000	2.831148000
C	-1.022385000	-0.457372000	1.868809000
C	1.357825000	-0.372456000	2.115059000
C	2.289045000	1.682341000	1.607766000
H	2.104348000	2.693255000	1.267086000
C	2.591898000	-0.930803000	2.388601000
C	3.557866000	1.207089000	1.880107000
C	-3.413769000	-1.148388000	1.996173000
H	-3.596483000	-0.247554000	1.415532000
H	-3.859575000	-2.005794000	1.489617000
H	-3.852660000	-1.039324000	2.990788000
Pt	1.104081000	-1.056160000	-1.212001000

5.2 Coordinates of all optimised structures

N	4.042574000	-0.027874000	-1.108486000
N	-0.935081000	-1.616441000	-1.325792000
N	1.789100000	-3.665748000	0.439346000
C	1.631181000	-2.729518000	-0.234191000
N	-1.099705000	0.505333000	-2.186206000
C	2.954222000	-0.434277000	-1.160884000
N	0.566091000	1.833385000	-2.437923000
C	-1.632042000	1.705929000	-2.638459000
H	-2.688943000	1.882443000	-2.734551000
C	-0.582357000	2.532440000	-2.792663000
H	-0.541110000	3.571868000	-3.072863000
C	0.265902000	0.593924000	-2.046002000
C	-1.754972000	-0.664362000	-1.804813000
C	-1.451533000	-2.797447000	-0.949621000
H	-0.736694000	-3.515304000	-0.566147000
C	-3.127665000	-0.841753000	-1.901107000
C	-2.805479000	-3.062703000	-1.040987000
C	1.885065000	2.455821000	-2.430402000
H	2.618537000	1.738261000	-2.072911000
H	2.140675000	2.766604000	-3.445758000
H	1.844654000	3.322122000	-1.767553000
H	-3.764595000	-0.033845000	-2.232291000
H	-3.184048000	-4.032189000	-0.739875000
C	-3.652164000	-2.064629000	-1.516675000
H	-4.721812000	-2.232694000	-1.582954000

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Pt-1 dimer T_1

H	5.097681000	-0.321201000	-0.929452000
H	4.053474000	3.673632000	0.287112000
C	4.745973000	1.729873000	-0.385443000
H	5.675311000	2.092651000	-0.809253000
Pt	0.548970000	-0.067109000	1.302895000
N	-1.918936000	-1.579165000	2.488371000
N	2.348905000	0.810175000	0.673411000
N	-0.482318000	2.734651000	2.383467000
C	-0.181194000	1.675437000	2.007434000
N	2.798866000	-1.357830000	0.088601000
C	-1.000807000	-1.010013000	2.058469000
N	1.468891000	-3.008761000	0.497605000
C	3.432845000	-2.501285000	-0.382616000
H	4.396492000	-2.484316000	-0.861318000

5.2 Coordinates of all optimised structures

C	2.590275000	-3.520843000	-0.129792000
H	2.674964000	-4.570565000	-0.359064000
C	1.569836000	-1.672537000	0.618012000
C	3.225548000	-0.037794000	0.085823000
C	2.665823000	2.122920000	0.727364000
H	1.929863000	2.755289000	1.205846000
C	4.432776000	0.387675000	-0.452929000
C	3.843357000	2.613464000	0.218382000
C	0.293710000	-3.812732000	0.787715000
H	-0.414112000	-3.224898000	1.366716000
H	-0.158576000	-4.119806000	-0.157262000
H	0.591033000	-4.691915000	1.363693000
Pt	-0.548999000	0.067011000	-1.302896000
N	1.919051000	1.578808000	-2.488386000
N	-2.349040000	-0.810058000	-0.673411000
N	0.482049000	-2.734889000	-2.383328000
C	0.181040000	-1.675632000	-2.007322000
N	-2.798714000	1.357995000	-0.088551000
C	1.000854000	1.009752000	-2.058501000
N	-1.468565000	3.008775000	-0.497573000
C	-3.432474000	2.501493000	0.382857000
H	-4.396048000	2.484607000	0.861708000
C	-2.589806000	3.520960000	0.130004000
H	-2.674323000	4.570675000	0.359370000
C	-1.569672000	1.672573000	-0.618017000
C	-3.225559000	0.038009000	-0.085797000
C	-2.666159000	-2.122746000	-0.727463000
H	-1.930289000	-2.755191000	-1.205980000
C	-4.432868000	-0.387309000	0.452898000
C	-3.843777000	-2.613145000	-0.218537000
C	-0.293406000	3.812687000	-0.787956000
H	0.414751000	3.224418000	-1.366103000
H	-0.590593000	4.691271000	-1.364923000
H	0.158431000	4.120707000	0.156926000
H	-5.097708000	0.321649000	0.929391000
H	-4.054047000	-3.673279000	-0.287321000
C	-4.746262000	-1.729457000	0.385329000
H	-5.675676000	-2.092118000	0.809075000
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Pt-1 trimer S_0			
H	-1.671353000	-4.139550000	-1.028488000

5.2 Coordinates of all optimised structures

H	-2.059719000	-3.868847000	3.250983000
C	-1.932707000	-4.174954000	1.109037000
H	-2.348394000	-5.176565000	1.124305000
Pt	-3.245349000	0.431533000	-1.211368000
Pt	0.001516000	0.287789000	0.812918000
N	-3.872392000	-2.444067000	-2.224466000
N	1.390726000	3.034331000	0.301204000
N	-2.668243000	2.255224000	-0.294243000
N	-0.869239000	-1.627116000	1.060563000
N	-2.134780000	1.474325000	-3.980433000
N	-0.420213000	0.969687000	3.882136000
C	-2.600989000	1.018607000	-3.016849000
C	-0.213953000	0.772289000	2.752810000
N	-3.327961000	1.092811000	1.576724000
N	-0.528922000	-1.688344000	-1.204677000
C	-3.686975000	-1.342183000	-1.899518000
C	0.852873000	2.017670000	0.481271000
N	-4.275695000	-0.831017000	1.525175000
N	0.359823000	-0.101020000	-2.334598000
C	-3.599318000	0.767230000	2.895416000
C	-0.527785000	-2.112256000	-2.525518000
H	-3.300251000	1.381576000	3.726950000
H	-0.942829000	-3.051977000	-2.843026000
C	-4.201106000	-0.438066000	2.857870000
C	0.031790000	-1.112008000	-3.227822000
H	-4.574991000	-1.062018000	3.653537000
C	-3.729397000	0.095849000	0.727308000
C	0.018858000	-0.435684000	-1.090410000
C	-2.736800000	2.252466000	1.047364000
C	-0.999085000	-2.339705000	-0.071031000
C	-2.128450000	3.315739000	-0.913844000
C	-1.252348000	-2.178431000	2.224118000
H	-1.127579000	-1.552587000	3.098446000
C	-2.262049000	3.291108000	1.826753000
C	-1.550173000	-3.612201000	-0.093375000
C	-1.645529000	4.402933000	-0.209266000
C	-1.778917000	-3.452413000	2.290887000
C	-4.924905000	-2.061947000	1.092097000
C	0.996108000	1.132052000	-2.764911000
H	-4.690661000	-2.243938000	0.046100000
H	1.933119000	0.876305000	-3.263372000
H	-4.552280000	-2.889529000	1.697239000

5.2 Coordinates of all optimised structures

H	0.322145000	1.645437000	-3.453622000
H	-6.006309000	-1.968506000	1.216651000
Pt	3.204983000	-1.149316000	-0.337761000
N	1.706395000	-3.733370000	0.545681000
N	4.111898000	0.711210000	-0.793312000
N	3.242514000	-1.854297000	-3.414789000
C	3.217928000	-1.715176000	-2.259927000
N	3.720464000	1.039048000	1.444612000
C	2.304085000	-2.799183000	0.192924000
N	2.839587000	-0.418504000	2.747043000
C	3.578123000	1.660367000	2.676587000
H	3.841208000	2.688657000	2.853054000
C	3.028095000	0.740061000	3.489889000
H	2.709238000	0.807889000	4.516916000
C	3.239107000	-0.244985000	1.481548000
C	4.187626000	1.567199000	0.238083000
C	4.544566000	1.106498000	-2.001889000
H	4.453077000	0.369997000	-2.791135000
C	4.684653000	2.853582000	0.106599000
C	5.059624000	2.371562000	-2.214502000
C	2.226720000	-1.617143000	3.301872000
H	2.007996000	-2.314184000	2.497083000
H	2.912191000	-2.083041000	4.013809000
H	1.304996000	-1.325881000	3.807677000
C	-1.703490000	4.382367000	1.177921000
H	-1.296467000	5.202106000	1.758866000
H	-2.078972000	3.248451000	-1.993536000
H	-1.198266000	5.230832000	-0.744288000
H	-2.278987000	3.224675000	2.906118000
H	0.237094000	-1.018300000	-4.280390000
H	1.193333000	1.755362000	-1.897155000
C	5.123485000	3.256931000	-1.143521000
H	5.508799000	4.261477000	-1.280299000
H	4.702547000	3.526871000	0.952536000
H	5.396021000	2.653397000	-3.204684000

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Pt-1 trimer T_1

H	0.203352000	-4.930520000	-1.614707000
H	-0.115204000	-4.758498000	2.674278000
C	0.020069000	-5.029337000	0.530239000
H	0.017324000	-6.112938000	0.564369000

5.2 Coordinates of all optimised structures

Pt	-2.947915000	-0.283439000	-0.551882000
Pt	0.062238000	-0.188849000	0.160912000
N	-3.060179000	-3.366713000	-0.109261000
N	0.023633000	2.879109000	-0.446732000
N	-3.034048000	1.825346000	-0.729689000
N	0.028766000	-2.273107000	0.439523000
N	-2.609152000	-0.554146000	-3.687578000
N	-0.504478000	0.441185000	3.224659000
C	-2.737858000	-0.548380000	-2.531370000
C	-0.266637000	0.246687000	2.103250000
N	-3.311967000	1.641121000	1.541548000
N	0.226799000	-2.221683000	-1.842985000
C	-3.014437000	-2.219312000	-0.290534000
C	0.037138000	1.738779000	-0.221050000
N	-3.411178000	-0.224751000	2.597428000
N	0.446119000	-0.412000000	-2.984518000
C	-3.504749000	1.963402000	2.876478000
C	0.366035000	-2.613029000	-3.162831000
H	-3.565384000	2.975328000	3.237944000
H	0.371703000	-3.643422000	-3.471719000
C	-3.558827000	0.788876000	3.531719000
C	0.486660000	-1.475877000	-3.874593000
H	-3.659985000	0.575214000	4.583062000
C	-3.243278000	0.282685000	1.372713000
C	0.277890000	-0.862967000	-1.736258000
C	-3.177818000	2.482938000	0.432349000
C	0.120584000	-2.998832000	-0.687862000
C	-2.915404000	2.529741000	-1.864568000
C	-0.051359000	-2.908622000	1.620154000
H	-0.078198000	-2.275768000	2.495143000
C	-3.191458000	3.864664000	0.512053000
C	0.118371000	-4.380481000	-0.687715000
C	-2.928400000	3.911070000	-1.872252000
C	-0.062139000	-4.284536000	1.702435000
C	-3.264566000	-1.623894000	2.973721000
C	0.355061000	0.975707000	-3.407415000
H	-3.268983000	-2.242098000	2.079585000
H	0.990609000	1.117894000	-4.280461000
H	-2.316328000	-1.738562000	3.502884000
H	-0.683878000	1.193269000	-3.659988000
H	-4.093979000	-1.910267000	3.623249000
Pt	2.873397000	-0.377200000	0.531245000

5.2 Coordinates of all optimised structures

N	2.559544000	-2.050016000	3.157500000
N	3.191175000	0.866226000	-1.103347000
N	3.182324000	-2.978577000	-1.268684000
C	3.073350000	-2.067905000	-0.553329000
N	2.961864000	2.484580000	0.513119000
C	2.681450000	-1.434720000	2.179160000
N	2.708565000	2.010544000	2.611822000
C	2.883831000	3.694659000	1.185921000
H	2.927089000	4.646421000	0.685883000
C	2.730389000	3.385412000	2.492809000
H	2.635313000	4.027318000	3.353873000
C	2.831368000	1.441959000	1.392759000
C	3.141410000	2.212682000	-0.834726000
C	3.465396000	0.487313000	-2.385514000
H	3.522632000	-0.582020000	-2.544701000
C	3.286063000	3.176326000	-1.820938000
C	3.654316000	1.392549000	-3.393166000
C	2.634771000	1.282565000	3.873385000
H	3.480600000	0.599899000	3.952775000
H	2.669298000	2.010492000	4.685103000
H	1.707635000	0.715646000	3.924456000
C	-3.058991000	4.585444000	-0.664349000
H	-3.054978000	5.669440000	-0.634098000
H	-2.810942000	1.941254000	-2.767104000
H	-2.823539000	4.442649000	-2.809763000
H	-3.287480000	4.362342000	1.468027000
H	0.580219000	-1.317109000	-4.935975000
H	0.696232000	1.625800000	-2.607105000
C	3.542564000	2.775625000	-3.119708000
H	3.665188000	3.510853000	-3.906254000
H	3.198650000	4.225303000	-1.564758000
H	3.881577000	1.035139000	-4.390925000

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Pt-1 tetramer S_0

H	1.381149000	2.564455000	-3.156650000
H	0.469242000	4.582059000	0.534459000
C	0.916652000	3.732011000	-1.404527000
H	0.707086000	4.637393000	-1.962906000
H	-5.677530000	4.224754000	-0.775799000
H	-6.201917000	3.542317000	3.441265000
C	-5.981111000	4.061247000	1.351097000

5.2 Coordinates of all optimised structures

H	-6.171701000	5.120041000	1.488767000
Pt	5.063292000	0.502412000	-0.610497000
Pt	1.658071000	-0.507741000	0.876648000
N	4.510889000	2.350631000	-3.053183000
N	1.879769000	-3.439730000	1.912546000
N	5.129518000	-0.683559000	1.147681000
N	1.404112000	1.409761000	0.004699000
N	5.755319000	-2.019016000	-2.389130000
N	1.229766000	0.679957000	3.784052000
C	5.529577000	-1.036691000	-1.807839000
C	1.351095000	0.167456000	2.745402000
N	4.423252000	1.301620000	2.067799000
N	1.858177000	0.206506000	-1.897627000
C	4.792504000	1.656690000	-2.162582000
C	1.823180000	-2.336798000	1.545577000
N	4.294229000	3.148343000	0.983870000
N	2.403683000	-1.867551000	-1.906417000
C	4.017853000	2.254593000	2.987665000
C	2.165689000	-0.099854000	-3.212938000
H	3.772205000	2.019993000	4.008930000
H	2.148379000	0.627963000	-4.004778000
C	3.945461000	3.414194000	2.304504000
C	2.510890000	-1.401484000	-3.212609000
H	3.666737000	4.404037000	2.628118000
H	2.868287000	-2.035356000	-4.006952000
C	4.576821000	1.849609000	0.822252000
C	2.013188000	-0.887911000	-1.086761000
C	4.681016000	-0.067334000	2.254145000
C	1.512514000	1.438022000	-1.334722000
C	5.404115000	-1.996155000	1.204058000
C	1.046772000	2.529991000	0.652187000
H	5.743790000	-2.440591000	0.276843000
H	0.954811000	2.438216000	1.726637000
C	4.475105000	-0.726699000	3.452101000
C	1.287722000	2.582235000	-2.080513000
C	5.235708000	-2.727178000	2.365108000
C	0.794818000	3.710176000	-0.018860000
C	4.373620000	4.178942000	-0.043305000
C	2.784980000	-3.221496000	-1.527910000
H	2.593403000	-3.364271000	-0.468068000
H	4.500525000	3.708857000	-1.015348000
H	2.188245000	-3.931754000	-2.102365000

5.2 Coordinates of all optimised structures

H	3.447362000	4.755332000	-0.038816000
H	3.845642000	-3.351167000	-1.750150000
H	5.221585000	4.836196000	0.162833000
Pt	-1.618115000	0.152327000	-0.888313000
Pt	-4.979109000	-0.634964000	0.520012000
N	-2.457950000	3.061042000	-0.134682000
N	-4.099284000	-3.480313000	-0.394994000
N	-1.135955000	-1.871571000	-1.287721000
N	-5.471310000	1.370437000	0.994900000
N	-1.345937000	0.871591000	-3.962257000
N	-4.946141000	-1.300528000	3.606755000
C	-1.462955000	0.683262000	-2.819246000
C	-4.980533000	-1.176097000	2.450249000
N	-1.392176000	-2.014387000	0.985955000
N	-5.181314000	1.597974000	-1.270475000
C	-2.124910000	1.981331000	-0.415595000
C	-4.468315000	-2.438077000	-0.031849000
N	-1.853433000	-0.352836000	2.256195000
N	-4.664240000	-0.007789000	-2.593460000
C	-1.418964000	-2.516025000	2.278078000
C	-5.000583000	2.172242000	-2.520628000
H	-5.078622000	3.230003000	-2.701917000
C	-1.710612000	-1.468901000	3.069801000
C	-4.678793000	1.159575000	-3.346109000
H	-1.854515000	-1.408134000	4.135022000
H	-4.408261000	1.159963000	-4.389098000
C	-1.662361000	-0.669911000	0.974509000
C	-4.948936000	0.246636000	-1.310927000
C	-1.112387000	-2.670784000	-0.208199000
C	-5.464079000	2.214143000	-0.049130000
C	-0.890281000	-2.402780000	-2.497143000
C	-5.734249000	1.852437000	2.220565000
H	-0.908208000	-1.705263000	-3.325112000
H	-5.722045000	1.120771000	3.019349000
C	-0.828636000	-4.025286000	-0.287694000
C	-5.714741000	3.570124000	0.084156000
C	-0.623370000	-3.747065000	-2.663326000
C	-5.995497000	3.192372000	2.437277000
C	-2.181385000	0.958125000	2.790004000
C	-4.307784000	-1.301309000	-3.159256000
H	-4.187015000	-2.023937000	-2.356617000
H	-2.329258000	1.652594000	1.967487000

5.2 Coordinates of all optimised structures

H	-5.097437000	-1.634484000	-3.836791000
H	-3.099610000	0.866998000	3.373128000
H	-3.370963000	-1.187133000	-3.706434000
H	-1.356969000	1.293439000	3.423341000
H	4.050062000	-0.209462000	4.301498000
H	5.445078000	-3.789266000	2.364555000
C	4.753771000	-2.084428000	3.498446000
H	4.570798000	-2.639722000	4.411198000
H	-0.800589000	-4.632649000	0.605588000
H	-0.440733000	-4.139410000	-3.656521000
C	-0.592527000	-4.567061000	-1.537402000
H	-0.383318000	-5.627034000	-1.632202000
H	-1.215668000	-3.545026000	2.515051000

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Pt-1 tetramer T_1

H	-2.009407000	3.536913000	2.688246000
H	-1.027159000	4.822170000	-1.307023000
C	-1.535334000	4.357433000	0.751880000
H	-1.600468000	5.389279000	1.079504000
H	4.638927000	4.753887000	-0.556908000
H	5.121101000	2.565305000	-4.231226000
C	4.901639000	3.822619000	-2.481301000
H	4.964041000	4.760703000	-3.021502000
Pt	-4.883277000	0.265052000	0.572454000
Pt	-1.249987000	-0.330403000	-0.495048000
N	-4.871226000	2.635447000	2.592806000
N	-1.331149000	-3.423895000	-0.925692000
N	-4.678204000	-1.239260000	-0.907224000
N	-1.372444000	1.725015000	-0.079024000
N	-5.223841000	-1.925691000	2.828326000
N	-1.101655000	0.053504000	-3.644899000
C	-5.137192000	-1.060221000	2.055522000
C	-1.076326000	-0.102763000	-2.491909000
N	-4.256954000	0.611865000	-2.204121000
N	-1.818936000	0.914347000	2.017643000
C	-4.939554000	1.737101000	1.856282000
C	-1.301375000	-2.270946000	-0.775237000
N	-4.475240000	2.632106000	-1.515431000
N	-1.883131000	-1.183186000	2.496808000
C	-3.969061000	1.418170000	-3.293341000
C	-2.170426000	0.835825000	3.355429000

5.2 Coordinates of all optimised structures

H	-3.633153000	1.029590000	-4.238876000
H	-2.402273000	1.700509000	3.951257000
C	-4.114010000	2.685209000	-2.858426000
C	-2.217330000	-0.478239000	3.646473000
H	-3.977325000	3.623701000	-3.370820000
H	-2.499803000	-0.987414000	4.552901000
C	-4.553500000	1.362730000	-1.097593000
C	-1.651964000	-0.336214000	1.484175000
C	-4.300464000	-0.789634000	-2.116362000
C	-1.650133000	2.030087000	1.206105000
C	-4.778553000	-2.562665000	-0.709330000
C	-1.161403000	2.726440000	-0.955678000
H	-5.068777000	-2.863611000	0.289469000
H	-0.917588000	2.423699000	-1.963895000
C	-3.982404000	-1.632151000	-3.165236000
C	-1.755682000	3.335669000	1.657378000
C	-4.501896000	-3.472067000	-1.712854000
C	-1.228599000	4.049228000	-0.575260000
C	-4.788819000	3.815635000	-0.725817000
C	-1.970514000	-2.634162000	2.406199000
H	-1.376347000	-2.982719000	1.567496000
H	-4.833664000	3.545360000	0.326183000
H	-1.582979000	-3.063293000	3.330037000
H	-4.004724000	4.558249000	-0.876847000
H	-3.016479000	-2.917490000	2.279273000
H	-5.752679000	4.221682000	-1.042120000
Pt	1.570887000	-0.131540000	0.001052000
Pt	4.504114000	-0.276395000	0.121685000
N	1.763724000	2.375772000	-1.856459000
N	4.490124000	-2.666083000	2.127822000
N	1.433483000	-1.836515000	1.195528000
N	4.722973000	1.429542000	-1.103536000
N	1.179724000	1.790352000	2.508625000
N	4.946017000	-2.137219000	-2.404029000
C	1.345272000	1.134866000	1.560963000
C	4.776158000	-1.536149000	-1.422258000
N	1.739523000	-2.858723000	-0.829046000
N	4.452688000	2.474975000	0.918668000
C	1.689624000	1.427556000	-1.187287000
C	4.496447000	-1.787551000	1.365909000
N	1.873049000	-1.780024000	-2.692739000
N	4.222669000	1.437365000	2.789382000

5.2 Coordinates of all optimised structures

C	1.839274000	-3.815446000	-1.828857000
C	4.323352000	3.454559000	1.894051000
H	4.332283000	4.508483000	1.676188000
C	1.932403000	-3.132193000	-2.984688000
C	4.173010000	2.795326000	3.058448000
H	2.051674000	-3.480746000	-3.997197000
H	4.012647000	3.165042000	4.058004000
C	1.761869000	-1.599021000	-1.369383000
C	4.372778000	1.221866000	1.474852000
C	1.562441000	-3.011990000	0.535491000
C	4.634973000	2.607210000	-0.457708000
C	1.297198000	-1.864657000	2.540891000
C	4.892281000	1.435055000	-2.437583000
H	1.206705000	-0.897546000	3.016635000
H	4.950683000	0.458280000	-2.900468000
C	1.520451000	-4.238275000	1.184717000
C	4.723939000	3.827236000	-1.109439000
C	1.271330000	-3.039914000	3.247783000
C	4.987649000	2.607049000	-3.157370000
C	2.067929000	-0.747819000	-3.695753000
C	3.970099000	0.424180000	3.802115000
H	4.128331000	-0.562233000	3.373037000
H	1.929237000	0.227480000	-3.239426000
H	4.655977000	0.571312000	4.639275000
H	3.081883000	-0.839865000	-4.092195000
H	2.936703000	0.524831000	4.139535000
H	1.324340000	-0.864879000	-4.484477000
H	-3.611703000	-1.233389000	-4.099385000
H	-4.572592000	-4.532477000	-1.507687000
C	-4.084869000	-2.998621000	-2.949766000
H	-3.817024000	-3.688424000	-3.741989000
H	1.611912000	-5.154717000	0.616950000
H	1.172030000	-3.011732000	4.326281000
C	1.374232000	-4.254798000	2.556757000
H	1.354016000	-5.198252000	3.089792000
H	1.828248000	-4.872572000	-1.631005000

5.2.2 Pt-2

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Pt-2 monomer S_0

Pt	4.418802000	5.043950000	11.209647000
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5.2 Coordinates of all optimised structures

N	6.869694000	4.771724000	9.314441000
C	5.987920000	4.882369000	10.063695000
N	2.915221000	4.379077000	8.493916000
C	3.025346000	4.663152000	9.797317000
N	2.614158000	5.185191000	12.324255000
N	1.731297000	4.700482000	10.257691000
N	6.025705000	5.702963000	13.842016000
C	5.545186000	5.453359000	12.812810000
C	1.581705000	4.250304000	8.128436000
H	1.291797000	4.024005000	7.114711000
C	1.286773000	5.525967000	14.272384000
H	1.246913000	5.748489000	15.331538000
C	0.229308000	5.023837000	12.175625000
C	1.493672000	4.973474000	11.612661000
C	0.132399000	5.306103000	13.531708000
C	0.831458000	4.446141000	9.230933000
H	-0.236089000	4.421199000	9.369719000
C	2.514270000	5.457254000	13.634045000
H	3.456485000	5.617444000	14.146413000
C	4.039588000	4.299817000	7.550143000
H	3.720375000	3.640306000	6.739194000
H	4.875476000	3.835636000	8.070266000
C	4.435397000	5.675156000	7.037833000
H	5.268656000	5.576134000	6.337984000
H	4.772527000	6.299224000	7.867858000
H	3.601438000	6.166403000	6.526096000
H	-0.653914000	4.847632000	11.575057000
H	-0.843440000	5.352719000	14.003049000

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Pt-2 monomer T_1

Pt	-0.057996000	-0.913169000	0.001459000
N	2.528342000	-2.660072000	0.001714000
N	2.205401000	1.343969000	-0.000129000
N	-1.669955000	0.449077000	0.000661000
N	0.041262000	1.958276000	-0.000338000
N	-2.106894000	-3.331230000	0.002051000
C	1.535107000	-2.057438000	0.001640000
C	0.898381000	0.788680000	0.000342000
C	-1.279532000	-2.512527000	0.001855000
C	2.153213000	2.658984000	-0.000954000
C	-3.964326000	1.113298000	0.000214000

5.2 Coordinates of all optimised structures

C	-2.256819000	2.806142000	-0.000863000
C	-1.307392000	1.769114000	-0.000190000
C	-3.587765000	2.469500000	-0.000662000
C	0.805483000	3.080887000	-0.001142000
C	-2.982728000	0.146549000	0.000851000
C	3.397923000	0.489017000	0.000360000
C	4.693437000	1.275163000	-0.001130000
H	3.034044000	3.282793000	-0.001446000
H	-5.005746000	0.817617000	0.000402000
H	-1.936685000	3.841470000	-0.001538000
H	-4.342961000	3.248071000	-0.001175000
H	0.411832000	4.083945000	-0.001733000
H	-3.209699000	-0.913062000	0.001551000
H	3.317111000	-0.166004000	-0.868893000
H	3.317907000	-0.163991000	0.871216000
H	5.523904000	0.566038000	-0.000892000
H	4.794860000	1.903415000	0.889672000
H	4.793802000	1.901651000	-0.893290000

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Pt-2 dimer S_0

Pt	-1.216493000	0.454332000	-1.400168000
N	1.542509000	0.937769000	-2.767113000
C	0.491644000	0.766270000	-2.297596000
N	-0.079607000	-2.501265000	-1.133486000
C	-0.974451000	-1.517928000	-1.003312000
N	-2.998568000	-0.004744000	-0.348670000
N	-1.993451000	-2.065725000	-0.270336000
N	-2.054049000	3.503383000	-1.460575000
C	-1.691388000	2.400452000	-1.542539000
C	-0.505625000	-3.647238000	-0.475547000
H	0.120150000	-4.521150000	-0.405442000
C	-5.082445000	0.475887000	0.700953000
H	-5.858534000	1.198952000	0.919846000
C	-4.139810000	-1.725137000	0.863124000
C	-3.077527000	-1.268213000	0.100284000
C	-5.153711000	-0.833026000	1.167333000
C	-1.705578000	-3.379731000	0.073279000
H	-2.343028000	-3.980643000	0.698049000
C	-3.987595000	0.854696000	-0.052357000
H	-3.860711000	1.859179000	-0.437465000
C	1.198797000	-2.391410000	-1.838916000

5.2 Coordinates of all optimised structures

H	1.864887000	-3.124525000	-1.380487000
H	1.595942000	-1.399151000	-1.636722000
C	1.036370000	-2.605030000	-3.334790000
H	2.009942000	-2.522020000	-3.825122000
H	0.382271000	-1.837688000	-3.755804000
H	0.618101000	-3.592514000	-3.553523000
Pt	1.216480000	-0.454617000	1.399510000
N	-1.542061000	-0.938999000	2.767016000
C	-0.491363000	-0.767147000	2.297258000
N	0.079171000	2.501088000	1.134681000
C	0.973901000	1.517770000	1.003405000
N	2.998248000	0.005279000	0.347679000
N	1.992683000	2.066083000	0.270542000
N	2.056182000	-3.503129000	1.461264000
C	1.692566000	-2.400436000	1.542331000
C	0.505169000	3.647630000	0.477741000
H	-0.120102000	4.522036000	0.409089000
C	5.082600000	-0.474074000	-0.701573000
H	5.858948000	-1.196786000	-0.920716000
C	4.139403000	1.726788000	-0.862596000
C	3.076975000	1.269047000	-0.100459000
C	5.153656000	0.835161000	-1.167059000
C	1.704957000	3.380503000	-0.071626000
H	2.342332000	3.981929000	-0.695980000
C	3.987622000	-0.853680000	0.051153000
H	3.860938000	-1.858436000	0.435612000
C	-1.199088000	2.390769000	1.840310000
H	-1.864884000	3.125068000	1.383318000
H	-1.596953000	1.399106000	1.636535000
C	-1.036106000	2.602087000	3.336445000
H	-2.009560000	2.518888000	3.826983000
H	-0.382246000	1.833868000	3.756193000
H	-0.617306000	3.589082000	3.556375000
H	-4.156049000	-2.741901000	1.231144000
H	-5.992625000	-1.157954000	1.773029000
H	5.992698000	1.160737000	-1.772229000
H	4.155556000	2.743842000	-1.229823000

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Pt-2 dimer T_1

Pt	-0.609663000	-0.136708000	1.301192000
N	1.426691000	1.933542000	2.450705000

5.2 Coordinates of all optimised structures

C	0.676023000	1.142178000	2.049761000
N	-1.949884000	2.529454000	0.211256000
C	-1.845615000	1.209606000	0.431546000
N	-2.147534000	-1.373601000	0.563704000
N	-2.953527000	0.654976000	-0.147985000
N	0.859211000	-2.516933000	2.793718000
C	0.368488000	-1.623436000	2.235924000
C	-3.102829000	2.801802000	-0.513259000
H	-3.363370000	3.807628000	-0.801066000
C	-3.205796000	-3.448893000	0.076541000
H	-3.193976000	-4.528126000	0.159286000
C	-4.163782000	-1.399137000	-0.731285000
C	-3.117901000	-0.732073000	-0.119665000
C	-4.203485000	-2.780675000	-0.628549000
C	-3.727633000	1.631264000	-0.753874000
H	-4.616722000	1.409755000	-1.318163000
C	-2.189219000	-2.716305000	0.653788000
H	-1.370356000	-3.177618000	1.188399000
C	-1.087381000	3.555772000	0.804193000
H	-1.152755000	4.432717000	0.157439000
H	-0.063246000	3.192699000	0.770509000
C	-1.498851000	3.874736000	2.233006000
H	-0.838981000	4.645326000	2.639725000
H	-1.401175000	2.987567000	2.862417000
H	-2.531158000	4.235764000	2.279022000
Pt	0.643162000	-0.500052000	-1.200907000
N	0.167975000	-3.593621000	-1.164984000
C	0.351162000	-2.446365000	-1.178092000
N	3.208666000	-1.291319000	0.488775000
C	2.379361000	-0.463191000	-0.175741000
N	1.131768000	1.517399000	-1.285936000
N	2.914542000	0.790427000	-0.032441000
N	-1.969539000	-0.059229000	-2.963056000
C	-1.015313000	-0.282422000	-2.336868000
C	4.237428000	-0.566567000	1.058070000
H	5.000467000	-1.045447000	1.650511000
C	0.855401000	3.805769000	-1.930724000
H	0.291293000	4.542623000	-2.490738000
C	2.694708000	3.189323000	-0.507549000
C	2.263108000	1.874924000	-0.598433000
C	1.989082000	4.174723000	-1.173923000
C	4.061444000	0.735809000	0.747271000

5.2 Coordinates of all optimised structures

H	4.616802000	1.611778000	1.033512000
C	0.457876000	2.496954000	-1.956020000
H	-0.411042000	2.161648000	-2.507642000
C	3.120200000	-2.753488000	0.507027000
H	3.614483000	-3.086270000	1.421731000
H	2.072142000	-3.023171000	0.593753000
C	3.746642000	-3.364807000	-0.736928000
H	3.669267000	-4.454125000	-0.688167000
H	3.214262000	-3.032815000	-1.631712000
H	4.803009000	-3.092115000	-0.829275000
H	-4.905879000	-0.854734000	-1.299768000
H	-5.002515000	-3.333372000	-1.110054000
H	2.309671000	5.208361000	-1.119564000
H	3.569571000	3.428550000	0.084017000

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Pt	-0.017769000	-0.827689000	0.641632000
Pt	3.292897000	0.348257000	-0.682828000
N	-0.165907000	1.965928000	2.026742000
N	3.234485000	-2.570671000	-1.768443000
C	-0.115720000	0.925009000	1.506763000
C	3.294716000	-1.471867000	-1.391234000
N	0.006496000	0.916745000	-2.017413000
N	3.112530000	-1.178791000	2.098786000
C	3.190436000	-0.121547000	1.285138000
N	0.085225000	-2.660004000	-0.419898000
N	3.212103000	2.264910000	0.224115000
N	0.061501000	-1.219279000	-2.200435000
N	3.051597000	0.965562000	2.109214000
N	-0.018466000	-2.385941000	3.405238000
N	3.214574000	1.736252000	-3.520397000
C	-0.036045000	-1.744008000	2.433461000
C	3.284653000	1.126599000	-2.531672000
C	0.025573000	0.619388000	-3.372247000
C	2.902453000	-0.778033000	3.411048000
H	0.012617000	1.382401000	-4.128539000
H	2.748043000	-1.494918000	4.200246000
C	0.191408000	-5.028186000	-0.657772000
C	3.088566000	4.643529000	0.257230000
H	0.233199000	-6.001438000	-0.184151000
H	3.111895000	5.574793000	-0.295283000

5.2 Coordinates of all optimised structures

C	0.145000000	-3.630418000	-2.606375000
C	2.883348000	3.404225000	2.303461000
C	0.096751000	-2.537700000	-1.756553000
C	3.046486000	2.247931000	1.557381000
C	0.193481000	-4.890916000	-2.044136000
C	2.904120000	4.617634000	1.636031000
C	0.060782000	-0.720978000	-3.493599000
C	2.858624000	0.567809000	3.425483000
H	0.084945000	-1.346382000	-4.368232000
H	2.675315000	1.258024000	4.230293000
C	0.135838000	-3.890598000	0.119849000
C	3.235723000	3.445445000	-0.416515000
H	3.362408000	3.387389000	-1.490994000
C	-0.035386000	2.258283000	-1.429216000
C	3.198048000	-2.577753000	1.671490000
H	0.756989000	2.300074000	-0.684562000
H	2.669304000	-3.161829000	2.427218000
H	-0.981524000	2.349568000	-0.897081000
H	2.654757000	-2.664379000	0.733087000
C	0.118523000	3.360395000	-2.459514000
C	4.639519000	-3.025172000	1.494756000
H	0.135292000	4.321041000	-1.935776000
H	4.661737000	-4.071440000	1.178997000
H	-0.725308000	3.367936000	-3.154794000
H	5.124709000	-2.431084000	0.716886000
H	1.054005000	3.253601000	-3.016255000
H	5.204703000	-2.928251000	2.427131000
Pt	-3.302256000	0.294086000	-0.834923000
N	-3.019624000	-2.474353000	-2.234383000
C	-3.164060000	-1.431054000	-1.740759000
N	-3.286731000	-1.543924000	1.755494000
C	-3.339859000	-0.397551000	1.067360000
N	-3.390181000	2.093371000	0.287506000
N	-3.321793000	0.587938000	2.018081000
N	-3.024788000	2.003216000	-3.479516000
C	-3.169562000	1.283107000	-2.576874000
C	-3.204271000	-1.292242000	3.118735000
H	-3.092016000	-2.078381000	3.843889000
C	-3.416462000	4.454064000	0.605102000
H	-3.444960000	5.442449000	0.163094000
C	-3.332491000	2.990743000	2.505724000
C	-3.347411000	1.926325000	1.619336000

5.2 Coordinates of all optimised structures

C	-3.365773000	4.272921000	1.983254000
C	-3.225575000	0.043738000	3.290395000
H	-3.149062000	0.637436000	4.184592000
C	-3.424546000	3.339225000	-0.212523000
H	-3.448455000	3.404333000	-1.293999000
C	-3.243036000	-2.866619000	1.110936000
H	-4.170666000	-2.991640000	0.549938000
H	-2.436194000	-2.834412000	0.382003000
C	-3.032326000	-3.999133000	2.098187000
H	-2.973065000	-4.934799000	1.536066000
H	-2.100532000	-3.872754000	2.656394000
H	-3.863353000	-4.090525000	2.804558000
H	2.720101000	3.351579000	3.371191000
H	2.771181000	5.539468000	2.191924000
H	-3.273994000	2.818576000	3.571931000
H	-3.347459000	5.126984000	2.651594000
C	0.021334000	-0.203096000	-1.289850000
H	0.145292000	-3.490549000	-3.678137000
H	0.234554000	-5.765004000	-2.684452000
H	0.127232000	-3.924602000	1.202048000

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Pt	0.073600000	0.022348000	-0.054530000
Pt	-2.716168000	-0.317111000	1.107932000
N	1.050124000	1.443559000	2.553718000
N	-3.213001000	-3.192649000	0.005672000
C	0.675972000	0.916796000	1.587518000
C	-3.037537000	-2.130989000	0.446010000
N	0.685655000	-2.552779000	1.672084000
N	-3.875739000	0.463610000	-1.738091000
C	-3.389696000	0.686809000	-0.510019000
N	-0.579599000	-1.067171000	-1.724474000
N	-2.509505000	1.693013000	1.724353000
N	-0.098675000	-2.815080000	-0.324089000
N	-3.388144000	2.046174000	-0.367275000
N	-0.640257000	2.867429000	-1.285357000
N	-1.903656000	-1.445209000	3.954767000
C	-0.328544000	1.838797000	-0.841596000
C	-2.184297000	-1.082298000	2.885992000
C	0.515694000	-3.915557000	1.457733000
C	-4.161445000	1.667255000	-2.371069000

5.2 Coordinates of all optimised structures

H	0.742542000	-4.645905000	2.214156000
H	-4.549458000	1.699241000	-3.376419000
C	-1.274103000	-1.353835000	-3.982167000
C	-1.858669000	3.452011000	3.189078000
H	-1.514544000	-0.899914000	-4.935603000
H	-1.431195000	3.745522000	4.139354000
C	-0.923415000	-3.276670000	-2.585999000
C	-2.768414000	3.968949000	1.027098000
C	-0.553630000	-2.407511000	-1.572480000
C	-2.883347000	2.608191000	0.811333000
C	-1.286027000	-2.739851000	-3.806694000
C	-2.246315000	4.391995000	2.240588000
C	0.028892000	-4.084411000	0.211375000
C	-3.843419000	2.663478000	-1.520059000
H	-0.245091000	-4.976573000	-0.323192000
H	-3.868390000	3.731840000	-1.645486000
C	-0.923085000	-0.549543000	-2.922049000
C	-1.998367000	2.109176000	2.894451000
H	-1.694261000	1.327867000	3.577813000
C	1.130709000	-1.911343000	2.919849000
C	-4.209638000	-0.854373000	-2.286438000
H	0.328510000	-1.257923000	3.250366000
H	-4.152144000	-0.767091000	-3.373396000
H	1.991255000	-1.291964000	2.682272000
H	-3.442590000	-1.553544000	-1.962848000
C	1.459571000	-2.909774000	4.009996000
C	-5.582166000	-1.318484000	-1.825745000
H	1.799750000	-2.354816000	4.887642000
H	-5.800838000	-2.298563000	-2.257308000
H	2.259966000	-3.596169000	3.715634000
H	-5.598225000	-1.421702000	-0.738557000
H	0.574825000	-3.480448000	4.304843000
H	-6.364095000	-0.616689000	-2.132760000
Pt	2.647764000	-0.060195000	-1.270706000
N	1.571131000	1.061011000	-3.981774000
C	1.978192000	0.650278000	-2.973343000
N	2.936035000	3.024923000	-0.533766000
C	3.058213000	1.694368000	-0.354219000
N	3.536336000	-0.714842000	0.503054000
N	3.645958000	1.547246000	0.877501000
N	2.370644000	-3.049220000	-2.297398000
C	2.456647000	-1.930139000	-1.991768000

5.2 Coordinates of all optimised structures

C	3.425772000	3.698719000	0.572089000
H	3.409498000	4.772875000	0.639693000
C	4.412001000	-2.326772000	2.035339000
H	4.618906000	-3.366336000	2.259217000
C	4.470438000	0.009378000	2.603821000
C	3.894616000	0.274348000	1.369278000
C	4.733811000	-1.304908000	2.946862000
C	3.863426000	2.785156000	1.462300000
H	4.269487000	2.904243000	2.451602000
C	3.812014000	-1.999912000	0.845340000
H	3.522604000	-2.743768000	0.113790000
C	2.478836000	3.663744000	-1.774838000
H	3.345159000	3.772192000	-2.435771000
H	1.783441000	2.977516000	-2.247696000
C	1.802256000	5.000614000	-1.528833000
H	1.403391000	5.363829000	-2.479149000
H	0.964132000	4.880655000	-0.839699000
H	2.492005000	5.760728000	-1.147935000
H	-3.049484000	4.674609000	0.257022000
H	-2.133463000	5.452667000	2.436940000
H	4.703165000	0.822658000	3.279562000
H	5.184517000	-1.537731000	3.904705000
C	0.300528000	-1.874727000	0.581984000
H	-0.898992000	-4.345028000	-2.422354000
H	-1.558908000	-3.397050000	-4.624775000
H	-0.880727000	0.527661000	-2.998698000

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H	-0.574192000	-0.771674000	4.578829000
H	0.172105000	-3.138818000	4.746900000
H	6.213161000	-2.755141000	2.604713000
H	6.654112000	-4.776062000	1.226793000
Pt	-1.576516000	-0.692637000	-0.397102000
Pt	-5.099316000	-0.087463000	0.724486000
N	-2.477026000	1.011153000	-2.850633000
N	-3.957580000	-1.786808000	3.072682000
C	-2.131499000	0.364079000	-1.946548000
C	-4.424311000	-1.147437000	2.220352000
N	-2.204794000	2.015267000	1.139304000
N	-4.375347000	-2.707667000	-0.922668000
C	-1.798488000	0.747400000	1.011875000

5.2 Coordinates of all optimised structures

C	-4.830784000	-1.465524000	-0.736503000
N	-0.998688000	-1.707927000	1.375484000
N	-5.728316000	0.972494000	-1.003308000
N	-1.456535000	0.354252000	2.272917000
N	-5.092111000	-0.995335000	-1.997299000
N	-1.069722000	-3.306552000	-2.119370000
N	-5.484553000	2.533212000	2.451087000
C	-1.268161000	-2.305583000	-1.558707000
C	-5.358052000	1.508008000	1.914786000
C	-2.136645000	2.416384000	2.468296000
C	-4.322651000	-3.016978000	-2.274821000
H	-2.468994000	3.384918000	2.795914000
H	-3.915623000	-3.951525000	-2.623167000
C	-0.184698000	-3.539330000	2.660989000
C	-6.487092000	2.871700000	-2.225291000
H	0.146072000	-4.569761000	2.687974000
H	-6.856369000	3.889800000	-2.210015000
C	-0.584164000	-1.422563000	3.715483000
C	-5.824801000	0.881865000	-3.393625000
C	-1.001622000	-0.951173000	2.484917000
C	-5.558275000	0.310123000	-2.159696000
C	-0.169425000	-2.740726000	3.798200000
C	-6.293820000	2.184365000	-3.419775000
C	-1.660951000	1.376766000	3.182161000
C	-4.767957000	-1.945030000	-2.957224000
H	-1.454074000	1.282292000	4.233403000
H	-4.844268000	-1.766173000	-4.015575000
C	-0.599123000	-2.985622000	1.466370000
C	-6.189309000	2.233982000	-1.035887000
H	-0.614773000	-3.546030000	0.540199000
H	-6.295908000	2.713673000	-0.070216000
C	-3.946708000	-3.615883000	0.144204000
H	-3.248601000	-4.319000000	-0.314151000
H	-3.401164000	-3.023802000	0.875629000
C	-5.127704000	-4.314243000	0.797552000
H	-4.768033000	-4.982051000	1.584681000
H	-5.790514000	-3.579047000	1.259821000
H	-5.695227000	-4.903227000	0.070180000
Pt	4.904517000	0.394569000	-1.156969000
Pt	1.752703000	0.406547000	0.885444000
N	3.754465000	3.187414000	-1.921000000
N	2.887402000	-2.282293000	1.984959000

5.2 Coordinates of all optimised structures

C	4.215805000	2.149262000	-1.669556000
C	2.439829000	-1.286491000	1.581817000
N	4.855968000	1.684070000	1.748052000
N	1.742074000	-1.183103000	-1.864529000
C	5.095914000	0.742099000	0.830725000
C	1.588017000	-0.125796000	-1.065632000
N	5.606755000	-1.476568000	-0.448659000
N	1.060499000	2.200971000	-0.014659000
N	5.489191000	-0.355695000	1.550806000
N	1.149447000	0.879403000	-1.885014000
N	4.610844000	-0.848263000	-4.048738000
N	1.807274000	1.759377000	3.754008000
C	4.720031000	-0.285193000	-3.036112000
C	1.798570000	1.198781000	2.733559000
C	5.063213000	1.190394000	3.029006000
C	1.397826000	-0.863339000	-3.170658000
H	4.854953000	1.786019000	3.902309000
H	1.464074000	-1.575624000	-3.972506000
C	6.225311000	-3.769721000	-0.630853000
C	0.469297000	4.507517000	-0.073094000
H	6.401105000	-4.628665000	-1.266750000
H	0.323308000	5.435760000	0.465853000
C	6.133846000	-2.721232000	1.526829000
C	0.482142000	3.223862000	-2.101556000
C	5.755911000	-1.553276000	0.884249000
C	0.883129000	2.132789000	-1.345113000
C	6.367992000	-3.844192000	0.751312000
C	0.283385000	4.427960000	-1.451394000
C	5.456202000	-0.092323000	2.913410000
C	1.024828000	0.429948000	-3.190550000
H	5.668696000	-0.833857000	3.663483000
H	0.679684000	1.050242000	-3.998366000
C	5.840651000	-2.568487000	-1.195830000
C	0.853946000	3.371460000	0.611452000
H	5.693854000	-2.441375000	-2.261581000
H	1.010028000	3.358433000	1.683241000
C	4.399726000	3.045495000	1.459313000
H	3.092177000	-2.313965000	-0.790059000
H	3.681001000	2.981162000	0.645590000
H	1.430844000	-2.885488000	-0.723433000
C	5.554026000	3.957487000	1.077985000
C	2.480967000	-3.463815000	-2.518412000

5.2 Coordinates of all optimised structures

H	5.175018000	4.962416000	0.874221000
H	2.895385000	-4.380580000	-2.089451000
H	6.037636000	3.591787000	0.169212000
H	1.559633000	-3.729965000	-3.043154000
H	6.295636000	4.018987000	1.880640000
H	3.207127000	-3.051708000	-3.225442000
H	-5.644731000	0.330377000	-4.306345000
H	-6.501995000	2.662011000	-4.370991000
H	0.349993000	3.129263000	-3.170188000
H	-0.013615000	5.303051000	-2.018863000
H	-3.517380000	2.253580000	-0.438476000
C	-2.703959000	2.815978000	0.014897000
H	-1.908689000	2.873765000	-0.726673000
C	-3.172483000	4.197314000	0.428768000
H	-2.357074000	4.791705000	0.852286000
H	-3.991794000	4.137686000	1.149875000
H	-3.532950000	4.718688000	-0.462544000
C	2.200997000	-2.493073000	-1.387878000
H	3.874108000	3.388908000	2.352475000

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Pt-2 tetramer T_1

H	-1.620281000	3.555001000	-3.633977000
H	-1.441689000	5.692320000	-2.378006000
H	3.812433000	-4.004827000	-3.140835000
H	3.723355000	-2.805625000	-5.320004000
Pt	-1.281756000	0.391198000	0.309940000
Pt	-4.793843000	-0.167166000	-0.501233000
N	-1.667958000	-2.492179000	1.442356000
N	-4.471466000	2.811211000	-1.357251000
C	-1.493231000	-1.431358000	0.999237000
C	-4.625119000	1.697272000	-1.059052000
N	-1.793940000	-1.027689000	-2.477193000
N	-4.262404000	1.068753000	2.376805000
C	-1.576538000	-0.000787000	-1.649711000
C	-4.518114000	0.105508000	1.486320000
N	-1.274908000	2.327543000	-0.519317000
N	-4.936290000	-2.149730000	0.241342000
N	-1.616756000	1.118165000	-2.434279000
N	-4.512435000	-1.056249000	2.212931000
N	-1.097993000	1.598317000	3.241252000
N	-5.141934000	-1.259357000	-3.449750000

5.2 Coordinates of all optimised structures

C	-1.134183000	1.084354000	2.197799000
C	-5.039988000	-0.759125000	-2.403975000
C	-1.966083000	-0.566161000	-3.774237000
C	-4.071374000	0.532187000	3.641583000
H	-2.192719000	-1.226555000	-4.591474000
H	-3.789686000	1.150170000	4.477670000
C	-1.248553000	4.708541000	-0.465451000
C	-5.180047000	-4.514058000	0.080707000
H	-1.177726000	5.616885000	0.120341000
H	-5.361501000	-5.381042000	-0.542497000
C	-1.492468000	3.561342000	-2.560208000
C	-4.729878000	-3.498550000	2.208116000
C	-1.452992000	2.368782000	-1.853481000
C	-4.726525000	-2.272928000	1.562071000
C	-1.395624000	4.744796000	-1.853036000
C	-4.956730000	-4.633695000	1.449039000
C	-1.848907000	0.775550000	-3.755876000
C	-4.223814000	-0.802967000	3.546966000
H	-1.920777000	1.498824000	-4.548618000
H	-4.117999000	-1.578266000	4.285658000
C	-1.180145000	3.484764000	0.163398000
C	-5.161168000	-3.255060000	-0.488338000
H	-1.041169000	3.384665000	1.232412000
H	-5.316972000	-3.088000000	-1.547458000
C	-4.171716000	2.497590000	2.067226000
H	-3.526602000	2.936959000	2.829784000
H	-3.669978000	2.590286000	1.106316000
C	-5.543494000	3.149776000	2.016675000
H	-5.435089000	4.212269000	1.783600000
H	-6.148322000	2.695193000	1.228835000
H	-6.066244000	3.052545000	2.973535000
Pt	4.520890000	0.036335000	-0.156806000
Pt	1.549854000	0.113616000	-0.112494000
N	4.972542000	1.090551000	2.745626000
N	1.428288000	1.206648000	-3.042682000
C	4.826675000	0.719964000	1.653058000
C	1.483443000	0.798743000	-1.955495000
N	4.360649000	-2.727789000	1.387095000
N	2.025065000	3.173468000	0.517533000
C	4.364654000	-1.917564000	0.317053000
C	1.850140000	1.871198000	0.812410000
N	4.300823000	-0.853834000	-2.054493000

5.2 Coordinates of all optimised structures

N	1.616158000	-0.471174000	1.886102000
N	4.233569000	-2.748529000	-0.762481000
N	1.967494000	1.774003000	2.171922000
N	5.105730000	2.907766000	-1.367576000
N	1.252696000	-2.848562000	-1.237218000
C	4.866389000	1.879039000	-0.880159000
C	1.321901000	-1.756342000	-0.842832000
C	4.213208000	-4.050343000	0.988495000
C	2.266160000	3.884148000	1.684466000
H	4.174512000	-4.854733000	1.705303000
H	2.462984000	4.941917000	1.679160000
C	4.039674000	-0.870849000	-4.420905000
C	1.414366000	-1.996655000	3.707394000
H	3.980743000	-0.306389000	-5.342802000
H	1.203275000	-3.004537000	4.044180000
C	3.953979000	-2.933675000	-3.193899000
C	1.921962000	0.312167000	4.139990000
C	4.159181000	-2.194085000	-2.042719000
C	1.846727000	0.532377000	2.772841000
C	3.894814000	-2.255691000	-4.401153000
C	1.707668000	-0.966126000	4.616113000
C	4.118473000	-4.067952000	-0.356224000
C	2.230466000	3.019146000	2.719730000
H	3.947257000	-4.880675000	-1.040290000
H	2.388080000	3.173416000	3.772416000
C	4.234922000	-0.202201000	-3.229435000
C	1.383427000	-1.718622000	2.364561000
H	4.332132000	0.873450000	-3.174380000
H	1.153041000	-2.468433000	1.620494000
C	4.654185000	-2.310110000	2.760319000
H	2.748459000	3.124859000	-1.422028000
H	4.176464000	-1.347802000	2.926120000
H	1.047187000	3.528627000	-1.284748000
C	6.151655000	-2.212374000	3.006086000
C	2.398622000	5.172900000	-0.914274000
H	6.333798000	-1.901584000	4.038101000
H	2.382190000	5.485148000	-1.961290000
H	6.591927000	-1.459529000	2.348778000
H	1.692722000	5.804683000	-0.364513000
H	6.647008000	-3.173581000	2.835103000
H	3.411548000	5.338247000	-0.538041000
H	-4.532606000	-3.561625000	3.269685000

H	-4.952983000	-5.608727000	1.923987000
H	2.131861000	1.136499000	4.808226000
H	1.750514000	-1.162519000	5.681404000
H	-2.730788000	-2.406007000	-1.261189000
C	-1.951663000	-2.417219000	-2.021535000
H	-1.020643000	-2.715213000	-1.543756000
C	-2.315176000	-3.367878000	-3.145484000
H	-1.524978000	-3.420158000	-3.900748000
H	-3.258706000	-3.086197000	-3.621356000
H	-2.426084000	-4.369203000	-2.720174000
C	2.029543000	3.705377000	-0.852799000
H	4.180080000	-3.039731000	3.419961000

5.2.3 Pt-3

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Pt-3 monomer S_0

Pt	5.033164000	1.735557000	9.043282000
C	3.595333000	1.419019000	7.688317000
N	3.671979000	1.543343000	10.664204000
N	2.639204000	1.219843000	7.056995000
N	7.237723000	2.046422000	6.870521000
N	5.603665000	1.915729000	11.852802000
C	6.245371000	2.012523000	10.641556000
C	6.380759000	1.925095000	7.646494000
N	7.526757000	2.250262000	10.950034000
C	4.223177000	1.673975000	11.882821000
C	6.497666000	2.083409000	12.901105000
H	6.209962000	2.049717000	13.938269000
C	2.123452000	1.333235000	12.942291000
H	1.518048000	1.251483000	13.838635000
C	7.700476000	2.287120000	12.328283000
H	8.660575000	2.464843000	12.782077000
C	3.486011000	1.576528000	13.051480000
H	3.959976000	1.688008000	14.018269000
C	9.704533000	3.302277000	10.432374000
H	9.295339000	4.266178000	10.748845000
H	10.398041000	3.483334000	9.607972000
H	10.284682000	2.873859000	11.256909000
C	9.131308000	0.971222000	9.602507000
H	9.579517000	0.491503000	10.480024000
H	9.889188000	1.048600000	8.819158000

5.2 Coordinates of all optimised structures

H	8.321347000	0.346627000	9.220246000
C	8.611550000	2.361040000	9.945994000
H	8.140018000	2.783652000	9.060800000
C	2.354886000	1.308508000	10.564870000
H	1.976929000	1.212631000	9.553048000
C	1.548050000	1.197128000	11.685301000
H	0.488787000	1.006785000	11.564277000

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Pt-3 monomer T_1

Pt	-0.189595000	-0.910326000	-0.084929000
N	-1.801583000	0.446267000	0.023629000
N	-2.231718000	-3.328394000	0.066926000
N	2.368041000	-2.682626000	-0.329736000
N	-0.098464000	1.961367000	-0.058791000
N	2.070554000	1.362800000	-0.134152000
C	-1.408066000	-2.508570000	0.004313000
C	0.767603000	0.796452000	-0.074398000
C	1.386656000	-2.067478000	-0.235470000
C	-1.444362000	1.767042000	0.009758000
C	0.654033000	3.088142000	-0.146782000
C	-3.724002000	2.459170000	0.131823000
C	2.004435000	2.675677000	-0.183785000
C	-2.395973000	2.800610000	0.063717000
C	4.495944000	1.272434000	-0.609511000
C	3.487468000	0.052508000	1.374086000
C	3.288951000	0.527716000	-0.062354000
C	-3.111404000	0.138769000	0.094702000
C	-4.095187000	1.101784000	0.147812000
H	0.249835000	4.085551000	-0.202425000
H	-4.480668000	3.235052000	0.176379000
H	2.878841000	3.305555000	-0.246123000
H	-2.079473000	3.837025000	0.058055000
H	4.318214000	1.649164000	-1.621416000
H	5.337107000	0.577328000	-0.653159000
H	4.796089000	2.104621000	0.037145000
H	3.718794000	0.897543000	2.032102000
H	4.315707000	-0.659053000	1.402154000
H	2.597651000	-0.462244000	1.738628000
H	3.073576000	-0.340151000	-0.686172000
H	-3.334520000	-0.921535000	0.105384000
H	-5.134067000	0.802064000	0.201383000

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Pt-3 trimer S_0

Pt	-0.214327000	-1.885798000	-0.423083000
C	-1.634763000	-2.442981000	-1.724791000
N	-1.497066000	-2.122420000	1.247018000
N	-2.561365000	-2.731242000	-2.367225000
N	1.749986000	-1.301913000	-2.769935000
N	0.352686000	-1.303260000	2.329052000
C	0.985074000	-1.320371000	1.115053000
C	1.021794000	-1.560619000	-1.900146000
N	2.227693000	-0.891994000	1.365091000
C	-0.977414000	-1.719640000	2.418259000
C	1.199836000	-0.831534000	3.320318000
H	0.889745000	-0.674327000	4.338661000
C	-3.011336000	-2.171652000	3.555884000
H	-3.608869000	-2.172435000	4.460836000
C	2.374542000	-0.580189000	2.711331000
H	3.276881000	-0.150435000	3.108469000
C	-1.702547000	-1.723242000	3.598486000
H	-1.265218000	-1.349549000	4.513766000
C	4.413447000	0.112738000	0.776387000
H	4.043566000	1.074334000	1.138734000
H	5.072530000	0.286677000	-0.078287000
H	5.017335000	-0.350033000	1.564270000
C	3.776463000	-2.202156000	-0.017078000
H	4.256073000	-2.665380000	0.852083000
H	4.506163000	-2.141445000	-0.828734000
H	2.953551000	-2.835196000	-0.353265000
C	3.281945000	-0.802531000	0.330198000
H	2.790475000	-0.372612000	-0.542197000
C	-2.765259000	-2.565078000	1.214578000
H	-3.122152000	-2.880900000	0.242321000
C	-3.552167000	-2.606703000	2.349617000
H	-4.570820000	-2.968627000	2.282355000
Pt	0.214327000	1.885798000	0.423083000
C	1.634763000	2.442981000	1.724791000
N	1.497066000	2.122420000	-1.247018000
N	2.561365000	2.731242000	2.367225000
N	-1.749986000	1.301913000	2.769935000
N	-0.352686000	1.303260000	-2.329052000
C	-0.985074000	1.320371000	-1.115053000

5.2 Coordinates of all optimised structures

C	-1.021794000	1.560619000	1.900146000
N	-2.227693000	0.891994000	-1.365091000
C	0.977414000	1.719640000	-2.418259000
C	-1.199836000	0.831534000	-3.320318000
H	-0.889745000	0.674327000	-4.338661000
C	3.011336000	2.171652000	-3.555884000
H	3.608869000	2.172435000	-4.460836000
C	-2.374542000	0.580189000	-2.711331000
H	-3.276881000	0.150435000	-3.108469000
C	1.702547000	1.723242000	-3.598486000
H	1.265218000	1.349549000	-4.513766000
C	-4.413447000	-0.112738000	-0.776387000
H	-4.043566000	-1.074334000	-1.138734000
H	-5.072530000	-0.286677000	0.078287000
H	-5.017335000	0.350033000	-1.564270000
C	-3.776463000	2.202156000	0.017078000
H	-4.256073000	2.665380000	-0.852083000
H	-4.506163000	2.141445000	0.828734000
H	-2.953551000	2.835196000	0.353265000
C	-3.281945000	0.802531000	-0.330198000
H	-2.790475000	0.372612000	0.542197000
C	2.765259000	2.565078000	-1.214578000
H	3.122152000	2.880900000	-0.242321000
C	3.552167000	2.606703000	-2.349617000
H	4.570820000	2.968627000	-2.282355000

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Pt-3 dimer T_1

Pt	0.359650000	-0.495874000	-1.273103000
C	-1.304012000	0.048170000	-2.279067000
N	-0.402309000	-2.385306000	-0.790278000
N	-2.299743000	0.244150000	-2.848253000
N	1.739038000	2.153520000	-2.203131000
N	1.660549000	-2.593162000	0.180227000
C	1.925380000	-1.339791000	-0.316797000
C	1.225341000	1.168104000	-1.862368000
N	3.201338000	-1.079828000	0.025087000
C	0.422404000	-3.168925000	-0.050458000
C	2.773333000	-3.088500000	0.849990000
H	2.781289000	-4.040227000	1.352300000
C	-1.207348000	-4.898166000	0.089602000
H	-1.527666000	-5.872591000	0.439774000

5.2 Coordinates of all optimised structures

C	3.723477000	-2.136827000	0.746382000
H	4.720223000	-2.115391000	1.151457000
C	0.050628000	-4.429460000	0.402256000
H	0.735521000	-5.014272000	1.002948000
C	4.995314000	0.489574000	0.683432000
H	4.591637000	0.477976000	1.698360000
H	5.384510000	1.488093000	0.466153000
H	5.839558000	-0.205505000	0.617910000
C	4.455748000	0.048516000	-1.755511000
H	5.215803000	-0.738207000	-1.815401000
H	4.908673000	0.997539000	-2.053896000
H	3.653297000	-0.173973000	-2.461569000
C	3.912851000	0.160241000	-0.335216000
H	3.152882000	0.939764000	-0.307214000
C	-1.635997000	-2.858545000	-1.088636000
H	-2.251617000	-2.197787000	-1.684900000
C	-2.067825000	-4.092213000	-0.672321000
H	-3.062297000	-4.427208000	-0.940938000
Pt	-0.299079000	0.556069000	1.276876000
C	1.420975000	0.170738000	2.253201000
N	0.306653000	2.487971000	0.712374000
N	2.434303000	0.065611000	2.814592000
N	-1.453152000	-2.149133000	2.335433000
N	-1.820277000	2.528241000	-0.138385000
C	-1.959253000	1.258867000	0.364222000
C	-1.023128000	-1.140587000	1.949790000
N	-3.221237000	0.898820000	0.081708000
C	-0.606572000	3.189446000	0.003598000
C	-3.001438000	2.939845000	-0.741971000
H	-3.110981000	3.890795000	-1.233823000
C	0.901911000	5.003932000	-0.290276000
H	1.140863000	5.981118000	-0.694116000
C	-3.866734000	1.916409000	-0.598900000
H	-4.878989000	1.816302000	-0.950718000
C	-0.342991000	4.449116000	-0.515462000
H	-1.094259000	4.968739000	-1.096207000
C	-4.769059000	-0.875662000	-0.655345000
H	-4.317252000	-0.780980000	-1.646052000
H	-5.019894000	-1.924380000	-0.472855000
H	-5.707615000	-0.311231000	-0.638271000
C	-4.446738000	-0.342625000	1.810174000
H	-5.280997000	0.367377000	1.818320000

5.2 Coordinates of all optimised structures

H	-4.825150000	-1.329534000	2.088975000
H	-3.711900000	-0.042067000	2.560313000
C	-3.806667000	-0.408821000	0.429182000
H	-2.961966000	-1.093262000	0.469799000
C	1.520617000	3.039077000	0.922036000
H	2.212616000	2.431886000	1.491595000
C	1.849198000	4.286141000	0.445339000
H	2.836568000	4.687381000	0.636864000

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Pt-3 trimer S_0

Pt	3.203159000	0.519167000	-1.219032000
Pt	0.237353000	0.092837000	0.858665000
C	3.135619000	-0.588241000	-2.888295000
C	0.070916000	1.330939000	2.433952000
N	4.169034000	-1.014544000	-0.116562000
N	-0.637206000	1.480027000	-0.480346000
N	3.127805000	-1.367107000	-3.752753000
N	-0.141152000	2.089869000	3.291917000
N	1.690427000	2.865516000	-2.600623000
N	1.637956000	-1.996166000	2.703449000
N	3.806600000	0.479741000	1.586401000
N	-0.493771000	-0.325921000	-1.884719000
C	3.322698000	1.338156000	0.634600000
C	0.148405000	-0.983481000	-0.868255000
C	2.277715000	1.985987000	-2.116277000
C	1.091899000	-1.236745000	2.011075000
N	3.002779000	2.452227000	1.303834000
N	0.440279000	-2.188110000	-1.366347000
C	4.264651000	-0.783808000	1.203347000
C	-0.871972000	1.004333000	-1.714380000
C	3.752968000	1.057307000	2.845646000
C	-0.622364000	-1.140608000	-2.998252000
H	4.031144000	0.537930000	3.746168000
H	-1.143081000	-0.839928000	-3.890344000
C	5.227637000	-2.921301000	1.577025000
C	-1.677371000	3.110402000	-2.449090000
H	5.624094000	-3.676059000	2.247265000
H	-2.080174000	3.749416000	-3.226994000
C	3.253707000	2.295073000	2.661333000
C	-0.038645000	-2.306078000	-2.666224000
H	3.014561000	3.056469000	3.382511000

5.2 Coordinates of all optimised structures

H	0.074284000	-3.207774000	-3.240446000
C	4.778583000	-1.715516000	2.089768000
C	-1.417064000	1.780879000	-2.724104000
H	4.795106000	-1.514518000	3.151901000
H	-1.626709000	1.353137000	-3.693571000
C	1.795336000	4.588789000	1.643007000
C	1.998749000	-4.077126000	-1.651532000
H	1.043400000	4.051995000	2.226812000
H	2.519952000	-3.462576000	-2.389733000
H	1.303588000	5.391492000	1.086721000
H	2.731542000	-4.672533000	-1.100043000
H	2.505694000	5.060825000	2.330380000
H	1.341053000	-4.777172000	-2.176117000
C	3.645482000	4.379405000	-0.072629000
C	0.315053000	-4.069081000	0.231788000
H	4.402255000	4.715674000	0.644677000
H	-0.472294000	-4.548435000	-0.354672000
H	3.262106000	5.249374000	-0.612083000
H	0.916611000	-4.833617000	0.732930000
H	4.110189000	3.712426000	-0.801105000
H	-0.138796000	-3.446550000	1.001305000
C	2.498708000	3.678421000	0.646307000
C	1.218254000	-3.226213000	-0.655675000
H	1.781769000	3.331289000	-0.096275000
H	1.915555000	-2.670356000	-0.028764000
C	4.618484000	-2.180119000	-0.608840000
C	-0.904159000	2.769714000	-0.218717000
H	4.513596000	-2.302564000	-1.679451000
H	-0.699618000	3.091943000	0.793724000
C	5.158817000	-3.156290000	0.207477000
C	-1.410194000	3.618753000	-1.180951000
H	5.507093000	-4.085153000	-0.227366000
H	-1.584449000	4.660462000	-0.939593000
Pt	-3.399829000	-1.149167000	-0.342806000
C	-3.025840000	-2.998139000	-1.022195000
N	-2.807485000	-1.608344000	1.638386000
N	-2.752667000	-4.093004000	-1.303909000
N	-3.992642000	-0.141082000	-3.229218000
N	-3.172688000	0.647361000	1.879406000
C	-3.655367000	0.624867000	0.599765000
C	-3.825172000	-0.559685000	-2.156774000
N	-4.144099000	1.853878000	0.387785000

5.2 Coordinates of all optimised structures

C	-2.692378000	-0.543412000	2.450020000
C	-3.337310000	1.898685000	2.450048000
H	-2.960681000	2.153132000	3.425824000
C	-1.732223000	-1.864794000	4.168504000
H	-1.275704000	-1.956816000	5.147363000
C	-3.954658000	2.649613000	1.514401000
H	-4.255999000	3.682013000	1.548841000
C	-2.158045000	-0.622299000	3.723043000
H	-2.019152000	0.269479000	4.318349000
C	-6.241299000	1.533261000	-0.850055000
H	-6.119667000	0.449775000	-0.799767000
H	-6.767249000	1.770077000	-1.778632000
H	-6.853724000	1.866024000	-0.004790000
C	-5.025186000	3.742286000	-0.954043000
H	-5.697272000	4.148947000	-0.191061000
H	-5.458663000	3.976331000	-1.929267000
H	-4.059005000	4.247371000	-0.883415000
C	-4.885740000	2.231713000	-0.839021000
H	-4.287558000	1.857674000	-1.669247000
C	-2.412971000	-2.809941000	2.085128000
H	-2.524269000	-3.626017000	1.382254000
C	-1.874212000	-2.976767000	3.347906000
H	-1.544080000	-3.958521000	3.663229000

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Pt	2.869003000	0.414502000	-0.595294000
Pt	0.072086000	-0.048128000	-0.207240000
C	2.957634000	-0.783185000	-2.217129000
C	-0.149376000	1.561276000	0.989896000
N	3.482000000	-1.086063000	0.714475000
N	-0.408643000	1.009530000	-1.964283000
N	3.030542000	-1.558718000	-3.081735000
N	-0.327116000	2.525249000	1.616369000
N	2.324933000	2.891414000	-2.426994000
N	0.521720000	-1.769110000	2.362213000
N	3.151908000	0.578465000	2.253547000
N	-0.307722000	-1.108503000	-2.832247000
C	2.903407000	1.392222000	1.174929000
C	0.117000000	-1.521009000	-1.600980000
C	2.513854000	1.958266000	-1.759344000
C	0.367666000	-1.147043000	1.392419000

5.2 Coordinates of all optimised structures

N	2.740994000	2.632345000	1.690683000
N	0.374959000	-2.823726000	-1.728452000
C	3.475221000	-0.748707000	2.040257000
C	-0.525999000	0.248051000	-3.065721000
C	3.104164000	1.313731000	3.431009000
C	-0.339227000	-2.174140000	-3.715830000
H	3.243821000	0.872852000	4.402786000
H	-0.663985000	-2.081893000	-4.737323000
C	4.216574000	-2.918293000	2.697540000
C	-1.037766000	2.141562000	-4.401118000
H	4.489085000	-3.636247000	3.462190000
H	-1.283685000	2.584418000	-5.359526000
C	2.850352000	2.589253000	3.064532000
C	0.081155000	-3.243984000	-3.016438000
H	2.725735000	3.466046000	3.676123000
H	0.195474000	-4.268928000	-3.322282000
C	3.820252000	-1.645051000	3.045088000
C	-0.826960000	0.777027000	-4.307935000
H	3.772270000	-1.335782000	4.082043000
H	-0.907789000	0.133784000	-5.173632000
C	1.880806000	4.951949000	1.671004000
C	2.062704000	-4.562768000	-1.347569000
H	0.952410000	4.593453000	2.119426000
H	2.694315000	-3.991646000	-2.032801000
H	1.646112000	5.774525000	0.989969000
H	2.686591000	-4.993300000	-0.560047000
H	2.539588000	5.354916000	2.448403000
H	1.606039000	-5.393397000	-1.895483000
C	3.895656000	4.282958000	0.292913000
C	-0.028180000	-4.461807000	0.080020000
H	4.579368000	4.588916000	1.092734000
H	-0.659303000	-5.057059000	-0.584663000
H	3.746718000	5.127127000	-0.385470000
H	0.483139000	-5.122228000	0.786887000
H	4.353658000	3.474103000	-0.279130000
H	-0.661776000	-3.782254000	0.644617000
C	2.555091000	3.844745000	0.873780000
C	1.008137000	-3.670275000	-0.701333000
H	1.893991000	3.545496000	0.062758000
H	1.497825000	-2.970151000	-0.026957000
C	3.899513000	-2.340173000	0.388494000
C	-0.600322000	2.333515000	-2.066543000

5.2 Coordinates of all optimised structures

H	3.921478000	-2.552572000	-0.671795000
H	-0.468619000	2.896471000	-1.153525000
C	4.265762000	-3.264203000	1.328380000
C	-0.927961000	2.932822000	-3.263040000
H	4.599229000	-4.244130000	1.008132000
H	-1.064933000	4.006007000	-3.303067000
Pt	-3.005106000	-0.684733000	-0.061994000
C	-2.894245000	-2.445158000	-1.021081000
N	-2.759832000	-1.548118000	1.855533000
N	-2.816759000	-3.509905000	-1.482414000
N	-3.699756000	0.737957000	-2.746621000
N	-2.975879000	0.649689000	2.478262000
C	-3.140222000	0.935441000	1.149327000
C	-3.423575000	0.194879000	-1.756584000
N	-3.368299000	2.251124000	1.100786000
C	-2.730092000	-0.669844000	2.871889000
C	-3.102709000	1.796147000	3.246021000
H	-2.985220000	1.807559000	4.315867000
C	-2.313707000	-2.400497000	4.443475000
H	-2.116702000	-2.730441000	5.457511000
C	-3.349882000	2.794837000	2.376363000
H	-3.483309000	3.848189000	2.552310000
C	-2.497421000	-1.051228000	4.181642000
H	-2.449344000	-0.312814000	4.971273000
C	-5.043104000	3.115322000	-0.476612000
H	-5.476533000	2.118534000	-0.584624000
H	-5.173907000	3.642029000	-1.425438000
H	-5.583356000	3.662357000	0.303983000
C	-2.871088000	4.373381000	-0.050373000
H	-3.417827000	5.065861000	0.598639000
H	-2.837890000	4.821772000	-1.047012000
H	-1.851146000	4.267053000	0.328280000
C	-3.560004000	3.017641000	-0.146628000
H	-3.071773000	2.426328000	-0.917922000
C	-2.608789000	-2.853437000	2.120875000
H	-2.670981000	-3.510677000	1.263327000
C	-2.386172000	-3.318223000	3.402875000
H	-2.255726000	-4.379685000	3.571976000

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Pt	-0.335544000	-5.502284000	-0.435782000
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5.2 Coordinates of all optimised structures

Pt	-0.362302000	-1.845046000	0.468128000
C	-1.665590000	-6.109368000	-1.808027000
C	0.988537000	-1.162700000	1.792030000
N	-1.648988000	-5.921872000	1.175251000
N	0.905752000	-1.512363000	-1.196595000
N	-2.551497000	-6.450119000	-2.481525000
N	1.827854000	-0.731712000	2.474677000
N	1.679519000	-4.663374000	-2.658540000
N	-2.294351000	-2.560911000	2.810599000
N	0.083393000	-4.992175000	2.357451000
N	-0.934519000	-2.299078000	-2.310396000
C	0.758911000	-4.907680000	1.168486000
C	-1.534489000	-2.427665000	-1.091201000
C	0.927791000	-5.013522000	-1.842801000
C	-1.582895000	-2.265519000	1.937945000
N	1.948619000	-4.381724000	1.483067000
N	-2.752510000	-2.917562000	-1.354453000
C	-1.206820000	-5.525767000	2.379952000
C	0.364406000	-1.794956000	-2.389979000
C	0.848593000	-4.485851000	3.397209000
C	-1.778907000	-2.711392000	-3.324292000
H	0.490242000	-4.400288000	4.408264000
H	-1.495106000	-2.720496000	-4.361843000
C	-3.229285000	-6.204028000	3.422578000
C	2.338562000	-1.131145000	-3.525389000
H	-3.853894000	-6.297735000	4.304166000
H	2.896558000	-0.972540000	-4.440980000
C	2.017430000	-4.109602000	2.843709000
C	-2.918826000	-3.098635000	-2.721825000
H	2.867058000	-3.625615000	3.291576000
H	-3.809304000	-3.530718000	-3.142032000
C	-1.967861000	-5.644463000	3.531537000
C	1.041340000	-1.607108000	-3.582361000
H	-1.595384000	-5.276186000	4.477297000
H	0.569051000	-1.842641000	-4.525872000
C	4.051926000	-3.158287000	1.018576000
C	-4.786522000	-4.216312000	-0.810048000
H	3.581593000	-2.249070000	1.399913000
H	-4.298449000	-5.090140000	-1.247513000
H	4.720303000	-2.889638000	0.196282000
H	-5.392766000	-4.535903000	0.041968000
H	4.669492000	-3.594662000	1.811217000

5.2 Coordinates of all optimised structures

H	-5.468242000	-3.788465000	-1.552689000
C	3.661859000	-5.488952000	0.117423000
C	-4.434484000	-1.879847000	0.092419000
H	4.152472000	-5.940798000	0.986641000
H	-4.954337000	-1.424091000	-0.756693000
H	4.409185000	-5.329541000	-0.664141000
H	-5.156079000	-2.067945000	0.892508000
H	2.912569000	-6.179677000	-0.272883000
H	-3.684363000	-1.184371000	0.466964000
C	3.027444000	-4.155342000	0.494893000
C	-3.773493000	-3.187891000	-0.324284000
H	2.530694000	-3.738565000	-0.380384000
H	-3.225600000	-3.594205000	0.525502000
C	-2.869979000	-6.473280000	1.078298000
C	2.164929000	-1.048553000	-1.150181000
H	-3.164099000	-6.775737000	0.081119000
H	2.538071000	-0.820508000	-0.161224000
C	-3.688097000	-6.632768000	2.180672000
C	2.916173000	-0.856711000	-2.290831000
H	-4.667174000	-7.080328000	2.060993000
H	3.922530000	-0.465930000	-2.213209000
Pt	0.362302000	1.845046000	-0.468128000
Pt	0.335544000	5.502284000	0.435782000
C	-0.988537000	1.162700000	-1.792030000
C	1.665590000	6.109368000	1.808027000
N	-0.905752000	1.512363000	1.196595000
N	1.648988000	5.921872000	-1.175251000
N	-1.827854000	0.731712000	-2.474677000
N	2.551497000	6.450119000	2.481525000
N	2.294351000	2.560911000	-2.810599000
N	-1.679519000	4.663374000	2.658540000
N	0.934519000	2.299078000	2.310396000
N	-0.083393000	4.992175000	-2.357451000
C	1.534489000	2.427665000	1.091201000
C	-0.758911000	4.907680000	-1.168486000
C	1.582895000	2.265519000	-1.937945000
C	-0.927791000	5.013522000	1.842801000
N	2.752510000	2.917562000	1.354453000
N	-1.948619000	4.381724000	-1.483067000
C	-0.364406000	1.794956000	2.389979000
C	1.206820000	5.525767000	-2.379952000
C	1.778907000	2.711392000	3.324292000

5.2 Coordinates of all optimised structures

C	-0.848593000	4.485851000	-3.397209000
H	1.495106000	2.720496000	4.361843000
H	-0.490242000	4.400288000	-4.408264000
C	-2.338562000	1.131145000	3.525389000
C	3.229285000	6.204028000	-3.422578000
H	-2.896558000	0.972540000	4.440980000
H	3.853894000	6.297735000	-4.304166000
C	2.918826000	3.098635000	2.721825000
C	-2.017430000	4.109602000	-2.843709000
H	3.809304000	3.530718000	3.142032000
H	-2.867058000	3.625615000	-3.291576000
C	-1.041340000	1.607108000	3.582361000
C	1.967861000	5.644463000	-3.531537000
H	-0.569051000	1.842641000	4.525872000
H	1.595384000	5.276186000	-4.477297000
C	4.786522000	4.216312000	0.810048000
C	-4.051926000	3.158287000	-1.018576000
H	4.298449000	5.090140000	1.247513000
H	-3.581593000	2.249070000	-1.399913000
H	5.392766000	4.535903000	-0.041968000
H	-4.720303000	2.889638000	-0.196282000
H	5.468242000	3.788465000	1.552689000
H	-4.669492000	3.594662000	-1.811217000
C	4.434484000	1.879847000	-0.092419000
C	-3.661859000	5.488952000	-0.117423000
H	4.954337000	1.424091000	0.756693000
H	-4.152472000	5.940798000	-0.986641000
H	5.156079000	2.067945000	-0.892508000
H	-4.409185000	5.329541000	0.664141000
H	3.684363000	1.184371000	-0.466964000
H	-2.912569000	6.179677000	0.272883000
C	3.773493000	3.187891000	0.324284000
C	-3.027444000	4.155342000	-0.494893000
H	3.225600000	3.594205000	-0.525502000
H	-2.530694000	3.738565000	0.380384000
C	-2.164929000	1.048553000	1.150181000
C	2.869979000	6.473280000	-1.078298000
H	-2.538071000	0.820508000	0.161224000
H	3.164099000	6.775737000	-0.081119000
C	-2.916173000	0.856711000	2.290831000
C	3.688097000	6.632768000	-2.180672000
H	-3.922530000	0.465930000	2.213209000

5.2 Coordinates of all optimised structures

H	4.667174000	7.080328000	-2.060993000
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Pt	4.480242000	-0.106163000	-0.558456000
Pt	1.618675000	-0.035856000	-0.207466000
C	4.389865000	-1.143442000	-2.287071000
C	1.671878000	1.395742000	1.211520000
N	4.743374000	-1.813065000	0.610949000
N	1.437258000	1.300794000	-1.822595000
N	4.340715000	-1.833130000	-3.223610000
N	1.653702000	2.249810000	2.001099000
N	4.504376000	2.578821000	-2.161760000
N	1.711798000	-2.174725000	2.067563000
N	4.703212000	-0.262263000	2.295295000
N	1.165603000	-0.670251000	-2.957446000
C	4.641262000	0.679331000	1.296117000
C	1.433358000	-1.306096000	-1.777384000
C	4.479929000	1.573000000	-1.578032000
C	1.668377000	-1.381408000	1.219253000
N	4.690393000	1.873595000	1.927517000
N	1.431645000	-2.611074000	-2.065982000
C	4.770904000	-1.602108000	1.959634000
C	1.230051000	0.719935000	-3.017734000
C	4.754586000	0.356983000	3.537819000
C	0.972644000	-1.592366000	-3.972827000
H	4.776141000	-0.189520000	4.464688000
H	0.748000000	-1.311805000	-4.986861000
C	5.042023000	-3.926588000	2.416024000
C	1.181871000	2.827716000	-4.109389000
H	5.146622000	-4.750475000	3.112308000
H	1.086565000	3.425607000	-5.008628000
C	4.747013000	1.685139000	3.292953000
C	1.133859000	-2.802014000	-3.405863000
H	4.758831000	2.509744000	3.984425000
H	1.075439000	-3.783783000	-3.842046000
C	4.907655000	-2.635611000	2.879120000
C	1.107506000	1.448129000	-4.188086000
H	4.901310000	-2.417688000	3.939976000
H	0.953003000	0.945080000	-5.133206000
C	4.217232000	4.295055000	2.117469000
C	2.721037000	-4.690327000	-1.861468000

5.2 Coordinates of all optimised structures

H	3.234235000	4.049233000	2.523725000
H	3.487342000	-4.176047000	-2.446679000
H	4.132440000	5.202345000	1.512917000
H	3.205283000	-5.325902000	-1.115265000
H	4.911665000	4.516752000	2.935564000
H	2.147827000	-5.344359000	-2.527189000
C	6.141657000	3.434504000	0.715565000
C	0.600244000	-4.356866000	-0.520660000
H	6.838677000	3.551144000	1.553035000
H	-0.068279000	-4.753968000	-1.289579000
H	6.152781000	4.349645000	0.117715000
H	0.929580000	-5.172931000	0.129275000
H	6.481504000	2.616775000	0.077705000
H	0.047147000	-3.639375000	0.080227000
C	4.730145000	3.170200000	1.229291000
C	1.819245000	-3.691937000	-1.141890000
H	4.057419000	3.057837000	0.380699000
H	2.387852000	-3.198893000	-0.356195000
C	4.895693000	-3.090167000	0.171407000
C	1.525332000	2.637351000	-1.759352000
H	4.897401000	-3.205232000	-0.903876000
H	1.722026000	3.043004000	-0.778606000
C	5.042393000	-4.152093000	1.022938000
C	1.389615000	3.433572000	-2.874690000
H	5.169952000	-5.147571000	0.614408000
H	1.478252000	4.508181000	-2.777900000
Pt	-1.424489000	0.245850000	-0.077700000
Pt	-4.707352000	0.209581000	0.737461000
C	-1.609781000	-1.430039000	-1.173744000
C	-4.653057000	1.993324000	1.656439000
N	-1.401891000	-0.763991000	1.774290000
N	-4.906121000	1.073012000	-1.189416000
N	-1.754114000	-2.428959000	-1.753115000
N	-4.583865000	3.083456000	2.057830000
N	-1.834436000	1.916304000	-2.682465000
N	-4.562140000	-1.274679000	3.474352000
N	-1.432232000	1.394909000	2.546348000
N	-4.878262000	-1.139975000	-1.793874000
C	-1.365562000	1.796639000	1.241703000
C	-4.746334000	-1.428207000	-0.460750000
C	-1.643888000	1.297148000	-1.716564000
C	-4.617540000	-0.702106000	2.463409000

5.2 Coordinates of all optimised structures

N	-1.334366000	3.131606000	1.290907000
N	-4.685946000	-2.762522000	-0.401980000
C	-1.408894000	0.033514000	2.854156000
C	-4.925602000	0.196540000	-2.206286000
C	-1.454352000	2.484782000	3.397508000
C	-4.906027000	-2.299973000	-2.549902000
H	-1.534136000	2.396161000	4.466732000
H	-4.971687000	-2.304808000	-3.624152000
C	-1.409298000	-1.836020000	4.316967000
C	-5.054903000	1.949652000	-3.802355000
H	-1.416500000	-2.253501000	5.317246000
H	-5.091388000	2.291771000	-4.830644000
C	-1.397789000	3.569806000	2.605125000
C	-4.789114000	-3.313698000	-1.671569000
H	-1.412707000	4.616243000	2.856416000
H	-4.733810000	-4.374760000	-1.842783000
C	-1.399072000	-0.461948000	4.145489000
C	-4.992477000	0.591209000	-3.530949000
H	-1.407034000	0.209859000	4.992971000
H	-4.977532000	-0.141247000	-4.327273000
C	-2.399297000	4.874695000	-0.091194000
C	-3.539397000	-4.700996000	0.591018000
H	-3.274111000	4.248566000	-0.257737000
H	-2.655928000	-4.377224000	0.033432000
H	-2.244536000	5.509234000	-0.968950000
H	-3.223718000	-5.112242000	1.553713000
H	-2.614811000	5.519068000	0.766612000
H	-4.022109000	-5.511793000	0.035056000
C	0.079210000	4.920416000	0.389736000
C	-5.836478000	-3.964613000	1.408121000
H	-0.132791000	5.704668000	1.123832000
H	-6.365691000	-4.623904000	0.711164000
H	0.361605000	5.413368000	-0.545096000
H	-5.684003000	-4.502150000	2.347728000
H	0.919187000	4.329783000	0.760149000
H	-6.456656000	-3.090115000	1.618004000
C	-1.147796000	4.041205000	0.149343000
C	-4.490850000	-3.535672000	0.839706000
H	-0.975233000	3.394464000	-0.708743000
H	-4.029064000	-2.839509000	1.536347000
C	-1.416113000	-2.091152000	1.951147000
C	-4.983658000	2.382874000	-1.459697000

H	-1.420823000	-2.676993000	1.044490000
H	-4.975449000	3.029975000	-0.592839000
C	-1.422752000	-2.665965000	3.203862000
C	-5.063958000	2.860309000	-2.754045000
H	-1.426523000	-3.744397000	3.298678000
H	-5.109989000	3.927686000	-2.929835000

5.2.4 Pt-4

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Pt-4 monomer S_0

Pt	4.615530000	1.720115000	9.123020000
N	5.485227000	1.566405000	11.050256000
N	3.271093000	1.595473000	11.663627000
N	7.526536000	1.706017000	7.935199000
N	1.586672000	1.735591000	10.331514000
N	3.392563000	1.945990000	6.269068000
C	2.935621000	1.693754000	10.329819000
C	6.412108000	1.719477000	8.266453000
C	3.846355000	1.861674000	7.335359000
C	1.009921000	3.163529000	8.411998000
H	2.045973000	3.224954000	8.090868000
H	0.385422000	3.248103000	7.518850000
H	0.784776000	4.005710000	9.074861000
C	6.799997000	1.507813000	11.315808000
H	7.450725000	1.544217000	10.449825000
C	7.277977000	1.407849000	12.611258000
H	8.346110000	1.363047000	12.784414000
C	0.700904000	1.843308000	9.119135000
C	2.145898000	1.577176000	12.469211000
H	2.180505000	1.505303000	13.542625000
C	4.611896000	1.527140000	12.065513000
C	0.929530000	0.610293000	8.243986000
H	0.304629000	0.682606000	7.350042000
H	1.961018000	0.526719000	7.913299000
C	6.368086000	1.367541000	13.660021000
H	6.710220000	1.289489000	14.686413000
C	1.098392000	1.664844000	11.632040000
H	0.048976000	1.682222000	11.861130000
C	-0.765171000	1.860459000	9.560665000
H	-1.000982000	2.722582000	10.192282000
H	-1.379941000	1.938739000	8.661411000

5.2 Coordinates of all optimised structures

H	-1.057064000	0.939777000	10.075401000
C	5.008214000	1.427829000	13.390344000
H	4.280083000	1.398185000	14.190147000
H	0.649404000	-0.295652000	8.791831000

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Pt-4 monomer T_1

Pt	-0.368575000	-0.910339000	0.000438000
N	-1.914934000	0.521599000	0.000840000
N	-0.146702000	1.957678000	0.000420000
N	-2.574974000	-3.174224000	0.000982000
N	2.032782000	1.342659000	-0.000107000
N	1.885703000	-3.068820000	-0.000131000
C	0.706384000	0.761675000	-0.000074000
C	-1.697761000	-2.410055000	0.000750000
C	1.044953000	-2.267115000	0.000115000
C	3.354356000	-0.276477000	-1.280870000
C	-3.238595000	0.270958000	0.001102000
C	-4.181139000	1.276481000	0.001132000
C	3.310399000	0.561614000	-0.000676000
C	0.615517000	3.075746000	0.000856000
C	-1.499992000	1.818783000	0.000620000
C	3.355376000	-0.276641000	1.279381000
C	-3.749940000	2.613767000	0.000770000
C	1.956950000	2.655452000	0.000487000
C	4.496777000	1.527482000	-0.001087000
C	-2.405609000	2.895006000	0.000491000
H	2.518351000	-0.966484000	-1.349971000
H	4.271204000	-0.871378000	-1.282213000
H	3.361333000	0.377896000	-2.158801000
H	-3.509438000	-0.777752000	0.001276000
H	-5.233461000	1.022315000	0.001376000
H	0.225441000	4.080203000	0.001766000
H	3.362791000	0.377625000	2.157389000
H	4.272362000	-0.871331000	1.280048000
H	2.519561000	-0.966833000	1.348935000
H	-4.471809000	3.423456000	0.000655000
H	2.823989000	3.295673000	0.000596000
H	4.521445000	2.158608000	-0.895539000
H	5.410241000	0.929438000	-0.001675000
H	4.522374000	2.158248000	0.893591000
H	-2.046449000	3.917022000	0.000064000

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Pt-4 dimer S_0

Pt	0.977999000	0.908492000	-1.484711000
N	2.625890000	1.406180000	-0.264841000
N	0.945444000	2.332849000	0.988594000
N	2.822715000	-1.119301000	-3.044032000
N	-1.019218000	2.809134000	0.257333000
N	-1.441059000	-0.002294000	-3.226284000
C	0.107195000	2.157614000	-0.087036000
C	2.085187000	-0.364406000	-2.553794000
C	-0.553999000	0.377593000	-2.576298000
C	-3.041250000	1.769745000	-0.679365000
H	-2.469958000	0.954256000	-1.116011000
H	-3.924980000	1.935017000	-1.303172000
H	-3.360677000	1.494009000	0.326971000
C	3.914029000	1.111174000	-0.505594000
H	4.115385000	0.647974000	-1.463096000
C	4.901923000	1.352882000	0.428714000
H	5.930214000	1.101866000	0.199275000
C	-2.216094000	3.049677000	-0.615633000
C	0.317298000	3.018642000	2.011935000
H	0.765638000	3.186044000	2.975256000
C	2.291688000	1.971864000	0.902770000
C	-1.738197000	3.512946000	-1.992869000
H	-2.610750000	3.731713000	-2.614597000
H	-1.149929000	2.754413000	-2.503340000
C	4.539601000	1.890301000	1.660592000
H	5.285137000	2.057410000	2.430308000
C	-0.910443000	3.309513000	1.553378000
H	-1.727693000	3.784060000	2.062365000
C	-3.070234000	4.160240000	0.003749000
H	-3.522427000	3.853946000	0.950910000
H	-3.885595000	4.382687000	-0.688625000
H	-2.498674000	5.081294000	0.154093000
C	3.215852000	2.209544000	1.908728000
H	2.900687000	2.600809000	2.865100000
Pt	-0.978001000	-0.908432000	1.484664000
N	-2.625861000	-1.406147000	0.264789000
N	-0.945358000	-2.332771000	-0.988616000
N	-2.823012000	1.119116000	3.043956000
N	1.019239000	-2.809166000	-0.257245000

5.2 Coordinates of all optimised structures

N	1.440969000	0.002400000	3.226307000
C	-0.107154000	-2.157576000	0.087057000
C	-2.085350000	0.364307000	2.553788000
C	0.553953000	-0.377536000	2.576291000
C	3.041286000	-1.769662000	0.679223000
H	2.470039000	-0.954180000	1.115932000
H	3.925152000	-1.934872000	1.302854000
H	3.360507000	-1.493999000	-0.327201000
C	-3.914030000	-1.111314000	0.505588000
H	-4.115393000	-0.648097000	1.463083000
C	-4.901930000	-1.353225000	-0.428657000
H	-5.930247000	-1.102346000	-0.199183000
C	2.216140000	-3.049621000	0.615707000
C	-0.317216000	-3.018630000	-2.011910000
H	-0.765537000	-3.186078000	-2.975231000
C	-2.291625000	-1.971856000	-0.902800000
C	1.738236000	-3.512723000	1.992990000
H	2.610790000	-3.731175000	2.614827000
H	1.149768000	-2.754221000	2.503274000
C	-4.539575000	-1.890625000	-1.660537000
H	-5.285120000	-2.057877000	-2.430215000
C	0.910478000	-3.309587000	-1.553282000
H	1.727713000	-3.784182000	-2.062244000
C	3.070270000	-4.160279000	-0.003519000
H	3.522568000	-3.854107000	-0.950670000
H	3.885558000	-4.382709000	0.688947000
H	2.498669000	-5.081314000	-0.153824000
C	-3.215792000	-2.209690000	-1.908718000
H	-2.900606000	-2.600920000	-2.865095000
H	-1.140048000	4.425539000	-1.902689000
H	1.140296000	-4.425465000	1.902936000

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Pt-4 dimer T_1

Pt	-0.580447000	0.458195000	-1.228076000
N	-0.281522000	2.480175000	-0.781876000
N	-2.198792000	2.150263000	0.420363000
N	2.107067000	0.391492000	-2.903919000
N	-3.526329000	0.457846000	0.174102000
N	-1.074792000	-2.460756000	-2.227131000
C	-2.299376000	0.914556000	-0.183483000
C	1.122238000	0.349097000	-2.286343000

5.2 Coordinates of all optimised structures

C	-0.924668000	-1.377956000	-1.832497000
C	-3.490657000	-2.002607000	0.196270000
H	-2.456357000	-2.018142000	-0.130132000
H	-3.973414000	-2.905588000	-0.189341000
H	-3.522068000	-2.007902000	1.287761000
C	0.715277000	3.267831000	-1.247200000
H	1.378618000	2.801344000	-1.961845000
C	0.870146000	4.569484000	-0.837811000
H	1.684350000	5.159986000	-1.239532000
C	-4.212628000	-0.770286000	-0.336219000
C	-3.314252000	2.415147000	1.195961000
H	-3.417645000	3.299604000	1.799607000
C	-1.161909000	3.011111000	0.094782000
C	-4.234487000	-0.714602000	-1.865944000
H	-4.754619000	-1.595636000	-2.251826000
H	-3.233636000	-0.713137000	-2.291409000
C	-0.030268000	5.103720000	0.092541000
H	0.077786000	6.122860000	0.445563000
C	-4.127865000	1.357870000	1.041576000
H	-5.082025000	1.172333000	1.497473000
C	-5.658845000	-0.795634000	0.166272000
H	-5.715355000	-0.876329000	1.255532000
H	-6.141387000	-1.682346000	-0.251337000
H	-6.228708000	0.077914000	-0.165026000
C	-1.061437000	4.315636000	0.560520000
H	-1.772681000	4.694992000	1.282161000
Pt	0.580404000	-0.458372000	1.228132000
N	0.281703000	-2.480348000	0.781485000
N	2.199126000	-2.150042000	-0.420397000
N	-2.106961000	-0.392374000	2.904195000
N	3.526415000	-0.457529000	-0.173756000
N	1.074253000	2.460488000	2.227632000
C	2.299485000	-0.914397000	0.183590000
C	-1.122225000	-0.349690000	2.286492000
C	0.924324000	1.377717000	1.832848000
C	3.490169000	2.002896000	-0.195922000
H	2.455824000	2.018198000	0.130351000
H	3.972666000	2.905994000	0.189734000
H	3.521689000	2.008181000	-1.287409000
C	-0.715160000	-3.268081000	1.246441000
H	-1.378565000	-2.801718000	1.961095000
C	-0.870009000	-4.569630000	0.836662000

5.2 Coordinates of all optimised structures

H	-1.684304000	-5.160219000	1.238069000
C	4.212415000	0.770755000	0.336620000
C	3.314737000	-2.414758000	-1.195820000
H	3.418334000	-3.299161000	-1.799510000
C	1.162205000	-3.011015000	-0.095163000
C	4.234200000	0.715049000	1.866342000
H	4.754086000	1.596210000	2.252265000
H	3.233326000	0.713331000	2.291752000
C	0.030517000	-5.103588000	-0.093696000
H	-0.077516000	-6.122615000	-0.447053000
C	4.128215000	-1.357414000	-1.041203000
H	5.082440000	-1.171734000	-1.496906000
C	5.658643000	0.796431000	-0.165817000
H	5.715177000	0.877121000	-1.255075000
H	6.140960000	1.683262000	0.251799000
H	6.228700000	-0.076976000	0.165520000
C	1.061794000	-4.315393000	-0.561297000
H	1.773121000	-4.694554000	-1.282957000
H	-4.767050000	0.179977000	-2.205171000
H	4.766972000	-0.179398000	2.205586000

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Pt-4 trimer S_0

Pt	0.143314000	0.865356000	0.743575000
Pt	3.453053000	-0.500837000	-1.254984000
N	-0.027274000	-0.702324000	-0.653719000
N	3.274654000	1.588909000	-1.021924000
N	-0.909745000	0.994296000	-1.920782000
N	3.671965000	1.022963000	1.165824000
N	1.044311000	-1.141431000	3.012133000
N	2.471694000	-0.182019000	-4.232277000
N	-1.336938000	2.989215000	-1.241635000
N	4.166335000	-0.936537000	1.898212000
N	0.891897000	3.154229000	2.723560000
N	3.784533000	-3.565959000	-1.714292000
C	-0.739865000	1.842383000	-0.856451000
C	3.863504000	-0.279005000	0.762520000
C	0.788572000	-0.363338000	2.184921000
C	2.881283000	-0.385289000	-3.162523000
C	0.536299000	2.331019000	1.981726000
C	3.683946000	-2.423195000	-1.525150000
C	0.011222000	4.806714000	-0.309093000

5.2 Coordinates of all optimised structures

C	3.314104000	-3.243947000	1.665030000
H	0.626720000	4.118739000	0.265551000
H	3.001293000	-3.082695000	0.637426000
H	-0.013304000	5.762154000	0.223196000
H	3.581257000	-4.300378000	1.762558000
H	0.469506000	4.964885000	-1.290049000
H	2.489633000	-3.012290000	2.342564000
C	0.455462000	-1.945951000	-0.490058000
C	3.092099000	2.475674000	-2.014899000
H	0.803886000	-2.186537000	0.504141000
H	2.946797000	2.049825000	-2.999832000
C	0.532825000	-2.841427000	-1.537439000
C	3.095654000	3.837569000	-1.781660000
H	0.985652000	-3.811390000	-1.379734000
H	2.954582000	4.522548000	-2.608797000
C	-1.410494000	4.276518000	-0.470329000
C	4.531447000	-2.389128000	2.017072000
C	-1.612788000	1.596565000	-2.944548000
C	3.815103000	1.158589000	2.534329000
H	-1.930644000	1.070630000	-3.827907000
H	3.607305000	2.074502000	3.060565000
C	-0.452854000	-0.328444000	-1.868054000
C	3.444948000	2.034878000	0.229148000
C	-2.093250000	4.037703000	0.874207000
C	5.733632000	-2.656892000	1.109577000
H	-1.756014000	-4.392164000	-1.818394000
H	-2.049768000	4.959660000	1.461764000
H	6.015577000	-3.710457000	1.186857000
H	-1.601370000	3.258498000	1.449049000
H	5.511958000	-2.452176000	0.065054000
C	0.104942000	-2.436676000	-2.795534000
C	3.270901000	4.293743000	-0.479126000
H	0.189914000	-3.101900000	-3.646819000
H	3.260108000	5.355726000	-0.259551000
C	-1.877107000	2.842411000	-2.516194000
C	4.121822000	-0.068438000	2.985924000
H	-2.453081000	3.611046000	-2.994307000
H	4.271677000	-0.397013000	3.996667000
C	-2.250221000	5.291158000	-1.250037000
C	4.932040000	-2.692985000	3.463243000
H	-1.793633000	5.561664000	-2.207193000
H	4.098286000	-2.555422000	4.157701000

5.2 Coordinates of all optimised structures

H	-2.311450000	6.202166000	-0.649458000
H	5.230317000	-3.742743000	3.512367000
H	-3.268213000	4.925834000	-1.410458000
H	5.785979000	-2.092750000	3.792124000
C	-0.410542000	-1.163369000	-2.969085000
C	3.439904000	3.383937000	0.550790000
H	-0.734602000	-0.816965000	-3.939418000
H	3.541007000	3.709109000	1.576398000
Pt	-3.713154000	-0.211290000	-0.159865000
N	-3.318747000	0.373359000	1.828901000
N	-2.295589000	-1.685060000	1.827065000
N	-4.727388000	2.693313000	-0.877187000
N	-2.804885000	-3.265398000	0.451897000
N	-3.790334000	-0.957275000	-3.182305000
C	-2.956065000	-1.942051000	0.649444000
C	-4.376167000	1.602715000	-0.676157000
C	-3.824894000	-0.714485000	-2.045364000
C	-4.962209000	-3.639834000	-0.693114000
H	-5.044538000	-2.630259000	-1.087759000
H	-5.492758000	-4.308743000	-1.376055000
H	-5.455486000	-3.679747000	0.283223000
C	-3.656284000	1.539908000	2.398045000
H	-4.314469000	2.168326000	1.813374000
C	-3.169932000	1.914940000	3.636567000
H	-3.452769000	2.872332000	4.056176000
C	-3.508488000	-4.105561000	-0.581838000
C	-1.676652000	-2.822456000	2.314665000
H	-1.036878000	-2.816167000	3.180531000
C	-2.504362000	-0.463570000	2.490425000
C	-2.773182000	-4.004378000	-1.914157000
H	-3.136386000	3.770973000	0.705744000
H	-3.301303000	-4.602728000	-2.662242000
H	-2.734324000	-2.978227000	-2.274121000
C	-2.299383000	1.058095000	4.299512000
H	-1.870157000	1.337797000	5.254980000
C	-1.993296000	-3.804805000	1.451827000
H	-1.703301000	-4.839271000	1.467050000
C	-3.506364000	-5.564506000	-0.112585000
H	-3.954762000	-5.676559000	0.879225000
H	-4.103229000	-6.146355000	-0.818341000
H	-2.503975000	-6.001971000	-0.107353000
C	-1.966774000	-0.161375000	3.729644000

5.2 Coordinates of all optimised structures

H	-1.264811000	-0.830684000	4.205219000
H	6.586540000	-2.045145000	1.421985000
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Pt-4 trimer T_1			
Pt	-0.506016000	-0.494791000	-0.010726000
Pt	-2.866546000	1.022652000	-0.680297000
N	0.343649000	-0.136275000	-1.897952000
N	-3.825416000	0.613714000	1.107330000
N	-0.906040000	-1.979903000	-2.428107000
N	-2.513726000	2.341782000	1.835698000
N	1.071198000	1.936035000	1.273465000
N	-4.296870000	-1.436502000	-2.088088000
N	-1.879122000	-3.283813000	-1.020252000
N	-1.486655000	3.737729000	0.516175000
N	-1.435087000	-1.058934000	2.917495000
N	-1.744229000	1.760914000	-3.511007000
C	-1.220186000	-2.112113000	-1.101750000
C	-2.185319000	2.557180000	0.511663000
C	0.436833000	1.068454000	0.828434000
C	-3.742420000	-0.530904000	-1.613996000
C	-1.143419000	-0.881691000	1.806879000
C	-2.126275000	1.506343000	-2.443329000
C	-3.457870000	-3.113266000	0.853893000
C	0.049235000	3.814474000	-1.410464000
H	-3.085043000	-2.125697000	1.105792000
H	-0.290957000	2.849930000	-1.771023000
H	-3.801454000	-3.583074000	1.780238000
H	0.357642000	4.401924000	-2.280854000
H	-4.298855000	-3.006118000	0.165970000
H	0.903943000	3.669807000	-0.745071000
C	1.212508000	0.841814000	-2.194332000
C	-4.826128000	-0.290759000	1.316940000
H	1.531916000	1.447967000	-1.360867000
H	-5.153567000	-0.824305000	0.435780000
C	1.675425000	1.042512000	-3.475371000
C	-5.373574000	-0.511291000	2.547647000
H	2.385888000	1.835277000	-3.669470000
H	-6.167190000	-1.241407000	2.651505000
C	-2.370290000	-3.968566000	0.217806000
C	-1.069550000	4.540350000	-0.670879000
C	-1.390270000	-3.039414000	-3.164516000

5.2 Coordinates of all optimised structures

C	-1.962569000	3.322539000	2.644520000
H	-1.271447000	-3.124757000	-4.229900000
H	-2.058479000	3.322065000	3.716014000
C	-0.059106000	-0.964159000	-2.869884000
C	-3.406349000	1.351092000	2.182392000
C	-1.177664000	-4.187232000	1.147200000
C	-2.294409000	4.775099000	-1.559718000
H	3.588226000	3.043287000	-0.980994000
H	-1.497295000	-4.779912000	2.010119000
H	-2.008225000	5.388273000	-2.418998000
H	-0.800225000	-3.239429000	1.518931000
H	-2.704824000	3.843838000	-1.943416000
C	1.238849000	0.194259000	-4.484658000
C	-4.898942000	0.221125000	3.662657000
H	1.589189000	0.321861000	-5.502288000
H	-5.306931000	0.052860000	4.652415000
C	-2.000620000	-3.846580000	-2.283754000
C	-1.330281000	4.174877000	1.817171000
H	-2.517413000	-4.769911000	-2.460930000
H	-0.776239000	5.060271000	2.067172000
C	-2.961977000	-5.332279000	-0.146499000
C	-0.541753000	5.903212000	-0.211950000
H	-3.829398000	-5.242068000	-0.806370000
H	0.362867000	5.810379000	0.396388000
H	-3.304467000	-5.802462000	0.778354000
H	-0.278492000	6.478504000	-1.102689000
H	-2.221319000	-5.996751000	-0.601364000
H	-1.293925000	6.473849000	0.341129000
C	0.362945000	-0.833037000	-4.181442000
C	-3.911623000	1.158954000	3.465666000
H	0.015716000	-1.514852000	-4.945141000
H	-3.528946000	1.748292000	4.289832000
Pt	3.168273000	-1.229122000	-0.008044000
N	2.394408000	-1.632842000	1.913093000
N	3.397087000	0.379860000	2.361020000
N	1.528366000	-3.665355000	-1.159647000
N	4.580393000	1.539491000	0.992394000
N	4.394569000	-0.784840000	-2.839979000
C	3.878478000	0.389956000	1.074791000
C	2.202199000	-2.787596000	-0.799278000
C	3.943158000	-0.933036000	-1.779129000
C	6.387720000	0.992389000	-0.584917000

H	5.937072000	0.034337000	-0.830725000
H	6.934351000	1.334749000	-1.467731000
H	7.100918000	0.855243000	0.234518000
C	1.722591000	-2.738243000	2.270776000
H	1.585736000	-3.471686000	1.487979000
C	1.217357000	-2.905265000	3.545013000
H	0.657581000	-3.800019000	3.785214000
C	5.341176000	2.039078000	-0.200258000
C	3.765211000	1.516689000	3.049533000
H	3.460842000	1.724388000	4.060246000
C	2.606764000	-0.676330000	2.825465000
C	4.345761000	2.330291000	-1.322836000
H	-0.377153000	-4.712915000	0.619271000
H	4.877435000	2.762550000	-2.175530000
H	3.862922000	1.420357000	-1.664309000
C	1.395574000	-1.887259000	4.472254000
H	0.974756000	-1.968739000	5.467856000
C	4.507038000	2.237759000	2.193717000
H	4.978283000	3.190853000	2.343199000
C	6.063653000	3.339960000	0.160867000
H	6.772820000	3.206342000	0.983354000
H	6.634454000	3.657366000	-0.714611000
H	5.367624000	4.147446000	0.407394000
C	2.110582000	-0.754342000	4.116455000
H	2.266916000	0.050760000	4.821507000
H	-3.073145000	5.302038000	-0.998815000

5.2.5 Pt-5

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Pt-5 monomer S_0

Pt	0.241909000	2.988581000	7.194736000
F	-0.215790000	5.443331000	2.444480000
F	2.274656000	7.592148000	5.756237000
O	0.056337000	1.584254000	8.755976000
O	-0.882638000	1.825280000	5.979980000
N	1.377419000	4.264115000	8.274830000
C	1.735051000	4.026501000	9.544208000
H	1.370615000	3.093592000	9.958442000
C	2.512832000	4.915706000	10.261486000
H	2.782963000	4.690823000	11.286280000
C	2.927941000	6.085640000	9.633697000

5.2 Coordinates of all optimised structures

C	2.558359000	6.331284000	8.321769000
C	1.771565000	5.402612000	7.638565000
C	1.288136000	5.489416000	6.263326000
C	0.502278000	4.391424000	5.828621000
C	-0.004306000	4.383650000	4.531017000
H	-0.607201000	3.556440000	4.175505000
C	0.271710000	5.450486000	3.693679000
C	1.036252000	6.540815000	4.084441000
C	1.530731000	6.533336000	5.372938000
C	-0.592609000	0.495374000	8.661729000
C	-1.285701000	0.041781000	7.530319000
H	-1.789373000	-0.912388000	7.615636000
C	-1.392178000	0.698275000	6.301298000
C	-0.584856000	-0.350061000	9.910280000
H	-1.149750000	-1.276814000	9.797406000
H	0.449773000	-0.589474000	10.173925000
H	-1.006131000	0.229324000	10.737400000
H	3.539691000	6.807450000	10.165270000
H	2.868889000	7.232233000	7.814700000
C	-2.181261000	0.062540000	5.186521000
H	-1.528187000	-0.076541000	4.319913000
H	-2.611830000	-0.898684000	5.471239000
H	-2.983174000	0.742003000	4.883007000
H	1.238528000	7.363415000	3.411535000

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Pt-5 monomer T_1

Pt	-0.635852000	0.042588000	0.284600000
F	2.798035000	-4.075672000	-0.007132000
F	4.561854000	0.233428000	-0.333490000
O	-2.402722000	1.160759000	0.428498000
O	-1.703633000	-1.649589000	0.456451000
N	0.566062000	1.666240000	0.119814000
C	0.100287000	2.921808000	0.157562000
H	-0.972327000	3.010909000	0.287569000
C	0.940822000	4.013352000	0.039010000
H	0.531363000	5.015730000	0.073966000
C	2.302682000	3.782933000	-0.121595000
C	2.783601000	2.483603000	-0.158182000
C	1.896043000	1.414835000	-0.034192000
C	2.215505000	-0.012152000	-0.043956000
C	1.106918000	-0.883125000	0.110712000

5.2 Coordinates of all optimised structures

C	1.311422000	-2.260029000	0.123847000
H	0.479695000	-2.943353000	0.249179000
C	2.599116000	-2.750370000	-0.018601000
C	3.706105000	-1.929408000	-0.174905000
C	3.485498000	-0.566056000	-0.183232000
C	-3.538199000	0.719659000	-0.049690000
C	-3.783336000	-0.665948000	-0.233441000
H	-4.792880000	-0.921989000	-0.545969000
C	-2.920958000	-1.777620000	-0.026718000
C	-4.592220000	1.750271000	-0.323285000
H	-5.517678000	1.304820000	-0.698331000
H	-4.827338000	2.313638000	0.588379000
H	-4.238106000	2.476247000	-1.065568000
H	2.992910000	4.614907000	-0.217684000
H	3.837159000	2.282742000	-0.280502000
C	-3.391169000	-3.188684000	-0.204440000
H	-3.374358000	-3.729025000	0.750748000
H	-4.407610000	-3.233577000	-0.604861000
H	-2.728558000	-3.730440000	-0.889504000
H	4.702982000	-2.335238000	-0.284662000

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Pt-5 dimer S_0

Pt	1.874209000	0.642829000	-0.969030000
Pt	-1.874236000	-0.642854000	0.969132000
F	0.237403000	5.554266000	0.432848000
F	-0.237469000	-5.554171000	-0.433203000
F	-2.871968000	2.741508000	-1.625751000
F	2.871990000	-2.741537000	1.625433000
O	3.410475000	1.600800000	-0.049482000
O	-3.410561000	-1.600768000	0.049624000
O	3.041116000	-1.113872000	-1.133369000
O	-3.041069000	1.113882000	1.133495000
N	0.245335000	-0.167321000	-1.848245000
N	-0.245312000	0.167257000	1.848290000
C	0.213872000	-1.424788000	-2.304660000
C	-0.213819000	1.424700000	2.304766000
H	1.129896000	-1.988787000	-2.174550000
H	-1.129838000	1.988718000	2.174707000
C	-0.921581000	-1.962111000	-2.882177000
C	0.921657000	1.961980000	2.882278000
H	-0.912334000	-2.987867000	-3.230109000

5.2 Coordinates of all optimised structures

H	0.912427000	2.987716000	3.230269000
C	-2.054643000	-1.164695000	-2.977955000
C	2.054710000	1.164544000	2.977993000
H	-2.966263000	-1.555417000	-3.418511000
H	2.966351000	1.555236000	3.418534000
C	-2.026376000	0.133631000	-2.494944000
C	2.026410000	-0.133760000	2.494927000
H	-2.902972000	0.761944000	-2.536480000
H	2.902997000	-0.762088000	2.536418000
C	-0.858871000	0.627182000	-1.916822000
C	0.858885000	-0.627265000	1.916803000
C	-0.648649000	1.950470000	-1.331275000
C	0.648635000	-1.950518000	1.331187000
C	0.657311000	2.191300000	-0.836148000
C	-0.657355000	-2.191328000	0.836125000
C	0.953013000	3.421849000	-0.252291000
C	-0.953079000	-3.421839000	0.252201000
H	1.943895000	3.625103000	0.136207000
H	-1.943987000	-3.625082000	-0.136235000
C	-0.043128000	4.375980000	-0.147846000
C	0.043079000	-4.375936000	0.147588000
C	-1.337345000	4.168067000	-0.602554000
C	1.337326000	-4.168032000	0.602209000
H	-2.101459000	4.928206000	-0.507344000
H	2.101453000	-4.928141000	0.506865000
C	-1.607046000	2.948278000	-1.191305000
C	1.607044000	-2.948292000	1.191057000
C	4.532283000	1.068238000	0.254876000
C	-4.532297000	-1.068116000	-0.254843000
C	4.947066000	-0.239131000	-0.000651000
C	-4.947014000	0.239278000	0.000667000
H	5.940889000	-0.507597000	0.334264000
H	-5.940798000	0.507815000	-0.334308000
C	4.215813000	-1.236433000	-0.669545000
C	-4.215729000	1.236530000	0.669596000
C	5.462777000	2.013890000	0.970518000
C	-5.462889000	-2.013757000	-0.970374000
H	6.408036000	1.545628000	1.249321000
H	-6.407979000	-1.545344000	-1.249493000
H	4.966894000	2.392524000	1.869638000
H	-4.966925000	-2.392800000	-1.869271000
H	5.663392000	2.875301000	0.326603000

5.2 Coordinates of all optimised structures

H	-5.663860000	-2.874919000	-0.326230000
C	-4.833469000	2.598229000	0.855377000
H	-5.909463000	2.599735000	0.671944000
H	-4.631773000	2.953260000	1.868840000
H	-4.355355000	3.288123000	0.154543000
C	4.833720000	-2.598035000	-0.855478000
H	5.909753000	-2.599359000	-0.672272000
H	4.355895000	-3.288075000	-0.154587000
H	4.631885000	-2.953061000	-1.868918000

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Pt-5 dimer T_1

Pt	-1.648588000	-0.196088000	1.228080000
Pt	1.692171000	-0.103932000	-1.264727000
F	0.563301000	4.671636000	1.654176000
F	-2.521096000	-3.281993000	-2.257481000
F	3.294563000	0.974156000	2.484723000
F	-3.262616000	1.334148000	-2.364703000
O	-3.080385000	1.180474000	0.804911000
O	2.321186000	-2.039946000	-1.113402000
O	-3.011505000	-1.759901000	0.829827000
O	3.589555000	0.580003000	-0.622195000
N	-0.121287000	-1.444189000	1.663996000
N	0.955321000	1.742123000	-1.457727000
C	-0.234895000	-2.776754000	1.606942000
C	1.652776000	2.859161000	-1.284892000
H	-1.207439000	-3.145019000	1.302065000
H	2.698027000	2.718520000	-1.034377000
C	0.821383000	-3.611405000	1.922161000
C	1.086069000	4.122461000	-1.391348000
H	0.692189000	-4.686036000	1.870801000
H	1.701557000	4.996682000	-1.220917000
C	2.028531000	-3.034684000	2.301207000
C	-0.301148000	4.238973000	-1.683372000
H	2.880289000	-3.657359000	2.555772000
H	-0.762579000	5.217746000	-1.750071000
C	2.150280000	-1.655752000	2.341729000
C	-1.040355000	3.112149000	-1.870770000
H	3.083926000	-1.187836000	2.612049000
H	-2.095469000	3.164890000	-2.095593000
C	1.056576000	-0.856700000	2.010994000
C	-0.432069000	1.814691000	-1.777111000

5.2 Coordinates of all optimised structures

C	1.000638000	0.602697000	1.979602000
C	-1.020016000	0.576124000	-1.932491000
C	-0.260289000	1.151372000	1.632373000
C	-0.127159000	-0.602201000	-1.765768000
C	-0.406805000	2.533370000	1.548551000
C	-0.646372000	-1.880522000	-1.900029000
H	-1.355516000	2.975475000	1.269554000
H	-0.008340000	-2.745102000	-1.757043000
C	0.692308000	3.340308000	1.779577000
C	-1.989062000	-2.046700000	-2.188508000
C	1.945624000	2.839762000	2.102385000
C	-2.879725000	-0.959130000	-2.368918000
H	2.793952000	3.491575000	2.264011000
H	-3.928145000	-1.133670000	-2.573164000
C	2.068149000	1.467867000	2.194338000
C	-2.403023000	0.298378000	-2.237355000
C	-4.285586000	0.915632000	0.470565000
C	3.477589000	-2.405087000	-0.715739000
C	-4.859962000	-0.348561000	0.311013000
C	4.523649000	-1.586462000	-0.279896000
H	-5.897632000	-0.373449000	0.003425000
H	5.424503000	-2.086573000	0.052332000
C	-4.214577000	-1.585376000	0.462032000
C	4.529518000	-0.182640000	-0.240121000
C	-5.109852000	2.143019000	0.186110000
C	3.669416000	-3.899890000	-0.735344000
H	-6.172289000	1.918262000	0.078451000
H	4.627290000	-4.208423000	-0.312837000
H	-4.745842000	2.590370000	-0.743539000
H	2.853807000	-4.370939000	-0.180104000
H	-4.966976000	2.872165000	0.987426000
H	3.605447000	-4.252584000	-1.769346000
C	5.730233000	0.536110000	0.318024000
H	6.561276000	-0.134599000	0.543161000
H	6.058839000	1.299361000	-0.392672000
H	5.419830000	1.047975000	1.233844000
C	-4.952334000	-2.854627000	0.123487000
H	-6.003141000	-2.684899000	-0.117793000
H	-4.451459000	-3.317672000	-0.732917000
H	-4.879012000	-3.552924000	0.961904000

Pt-5 trimer S_0

Pt	3.203826000	1.310510000	0.234327000
F	3.292540000	-1.274413000	4.931569000
F	3.286529000	-3.854066000	1.038438000
O	3.109726000	2.680748000	1.730191000
O	2.952147000	2.840775000	-1.208258000
N	3.302752000	-0.177412000	-1.128403000
C	3.258685000	0.038872000	-2.447971000
H	3.168806000	1.077010000	-2.745042000
C	3.305837000	-1.000009000	-3.358914000
H	3.258094000	-0.786168000	-4.419762000
C	3.396833000	-2.299058000	-2.875381000
H	3.431393000	-3.139642000	-3.561114000
C	3.430646000	-2.524596000	-1.509019000
H	3.477818000	-3.526581000	-1.110288000
C	3.371547000	-1.443816000	-0.631610000
C	3.366739000	-1.486533000	0.829523000
C	3.351387000	-0.222277000	1.469847000
C	3.341227000	-0.159441000	2.862203000
H	3.324121000	0.796442000	3.372148000
C	3.319954000	-1.335527000	3.590352000
C	3.304464000	-2.590055000	2.997341000
H	3.279377000	-3.497060000	3.586831000
C	3.327272000	-2.632259000	1.617021000
C	2.886878000	3.928880000	1.571628000
C	2.701469000	4.610930000	0.368080000
H	2.521482000	5.676373000	0.436230000
C	2.749616000	4.060849000	-0.924768000
C	2.823699000	4.690157000	2.871137000
H	2.613762000	5.751476000	2.728926000
H	3.775426000	4.578533000	3.398901000
H	2.049625000	4.248864000	3.506430000
Pt	-3.372298000	0.799630000	0.327693000
Pt	0.104921000	-1.532601000	-0.729659000
F	-2.769000000	-1.589205000	5.088915000
F	-0.234270000	0.881695000	-5.508752000
F	-2.551151000	-4.276232000	1.274107000
F	-0.356915000	3.586809000	-1.699114000
O	-3.425364000	2.218869000	1.778935000
O	0.187605000	-2.954132000	-2.182949000
O	-3.453993000	2.298782000	-1.166432000
O	0.281680000	-3.014877000	0.762634000

5.2 Coordinates of all optimised structures

N	-3.293365000	-0.732832000	-0.986633000
N	0.012948000	-0.004236000	0.585120000
C	-3.355135000	-0.560273000	-2.311909000
C	0.068113000	-0.178828000	1.907806000
H	-3.458088000	0.466750000	-2.641563000
H	0.164794000	-1.204984000	2.240854000
C	-3.272508000	-1.624639000	-3.190397000
C	0.005727000	0.887977000	2.786041000
H	-3.317212000	-1.444385000	-4.257612000
H	0.053083000	0.705129000	3.852489000
C	-3.116295000	-2.902171000	-2.667754000
C	-0.116890000	2.166262000	2.263963000
H	-3.042626000	-3.760900000	-3.327399000
H	-0.168688000	3.027075000	2.923057000
C	-3.040920000	-3.080480000	-1.296095000
C	-0.173193000	2.349243000	0.890827000
H	-2.897998000	-4.061271000	-0.868483000
H	-0.267697000	3.336138000	0.465677000
C	-3.120890000	-1.974058000	-0.452902000
C	-0.106587000	1.243072000	0.050790000
C	-3.031962000	-1.962261000	1.006083000
C	-0.148138000	1.234282000	-1.411370000
C	-3.196535000	-0.690733000	1.610176000
C	-0.058484000	-0.044454000	-2.011964000
C	-3.123614000	-0.576337000	2.997114000
C	-0.088854000	-0.154844000	-3.401477000
H	-3.240840000	0.386962000	3.479090000
H	-0.020914000	-1.125943000	-3.877472000
C	-2.861211000	-1.704214000	3.754016000
C	-0.205796000	0.989750000	-4.168316000
C	-2.664963000	-2.959113000	3.195504000
C	-0.296001000	2.259064000	-3.615776000
H	-2.449875000	-3.825316000	3.807150000
H	-0.387308000	3.142637000	-4.233784000
C	-2.758325000	-3.055370000	1.821166000
C	-0.264843000	2.343375000	-2.237555000
C	-3.417380000	3.480379000	1.575349000
C	0.326413000	-4.207976000	-1.971564000
C	-3.412900000	4.140658000	0.345948000
C	0.442464000	-4.854212000	-0.742820000
H	-3.404997000	5.222915000	0.375497000
H	0.560742000	-5.930201000	-0.767348000

5.2 Coordinates of all optimised structures

C	-3.439140000	3.544643000	-0.927012000
C	0.413715000	-4.252826000	0.530536000
C	-3.404065000	4.286560000	2.848950000
C	0.365450000	-5.020268000	-3.241471000
H	-3.389427000	5.362452000	2.667534000
H	0.479891000	-6.089600000	-3.057052000
H	-2.525852000	4.006464000	3.438867000
H	-0.555918000	-4.847427000	-3.806140000
H	-4.286193000	4.032626000	3.443927000
H	1.193818000	-4.670526000	-3.865434000
C	0.509528000	-5.121315000	1.755868000
H	-0.500187000	-5.251527000	2.156811000
H	0.934278000	-6.103608000	1.541100000
H	1.113056000	-4.612114000	2.509354000
C	2.514957000	4.961339000	-2.110659000
H	2.645600000	6.017203000	-1.865814000
H	3.194340000	4.682721000	-2.919414000
H	1.490319000	4.806795000	-2.460494000
C	-3.416896000	4.429361000	-2.147277000
H	-3.722726000	5.453731000	-1.925766000
H	-2.395665000	4.446534000	-2.538581000
H	-4.067497000	4.006845000	-2.916166000

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Pt-5 trimer T_1

Pt	2.960151000	-1.494601000	-0.955650000
F	2.248840000	3.028819000	-3.754602000
F	4.050421000	3.444764000	0.540775000
O	2.174186000	-1.999577000	-2.770887000
O	2.753738000	-3.495859000	-0.292723000
N	3.747325000	-0.871444000	0.771588000
C	4.045999000	-1.661957000	1.797553000
H	3.846634000	-2.716218000	1.642542000
C	4.555369000	-1.178210000	2.994351000
H	4.763942000	-1.869326000	3.801304000
C	4.761268000	0.220789000	3.145447000
H	5.146764000	0.616557000	4.078386000
C	4.464133000	1.054689000	2.111234000
H	4.608472000	2.122059000	2.192547000
C	3.950967000	0.533681000	0.877348000
C	3.581458000	1.224506000	-0.260516000
C	3.076180000	0.402859000	-1.394427000

5.2 Coordinates of all optimised structures

C	2.663478000	1.025873000	-2.562783000
H	2.265120000	0.437513000	-3.381376000
C	2.724749000	2.403515000	-2.661088000
C	3.217231000	3.230598000	-1.619869000
H	3.230011000	4.307101000	-1.732504000
C	3.624326000	2.651904000	-0.469071000
C	1.760349000	-3.162459000	-3.092751000
C	1.727807000	-4.305209000	-2.286992000
H	1.303026000	-5.197706000	-2.728650000
C	2.189609000	-4.412833000	-0.965818000
C	1.249172000	-3.242292000	-4.508143000
H	0.844864000	-4.225173000	-4.756502000
H	2.067304000	-3.007309000	-5.195696000
H	0.476536000	-2.481526000	-4.649291000
Pt	-3.435918000	-0.578192000	0.642765000
Pt	0.366261000	1.488444000	0.225942000
F	-4.672645000	1.829117000	-3.985328000
F	1.854043000	-1.061605000	4.702332000
F	-2.724402000	4.440725000	-0.638994000
F	-0.086570000	-3.611973000	1.299162000
O	-4.187540000	-1.968633000	-0.633374000
O	1.132177000	2.861151000	1.515169000
O	-3.013966000	-2.088234000	2.067036000
O	-0.008899000	3.001774000	-1.193191000
N	-2.710415000	0.924434000	1.781740000
N	-0.358036000	0.012885000	-0.942323000
C	-2.233136000	0.737263000	3.017546000
C	-0.822048000	0.228735000	-2.176439000
H	-2.264633000	-0.284215000	3.377388000
H	-0.780536000	1.256349000	-2.517105000
C	-1.718856000	1.779875000	3.765864000
C	-1.340445000	-0.796089000	-2.947358000
H	-1.331138000	1.587283000	4.758793000
H	-1.723817000	-0.580398000	-3.937429000
C	-1.698644000	3.049767000	3.203827000
C	-1.374366000	-2.075057000	-2.408879000
H	-1.294217000	3.890472000	3.758365000
H	-1.780856000	-2.902840000	-2.981263000
C	-2.182904000	3.242681000	1.920161000
C	-0.887158000	-2.298911000	-1.131449000
H	-2.153360000	4.215809000	1.454272000
H	-0.910058000	-3.284130000	-0.693490000

5.2 Coordinates of all optimised structures

C	-2.683578000	2.157769000	1.203785000
C	-0.375895000	-1.233576000	-0.396299000
C	-3.204872000	2.160881000	-0.162073000
C	0.170233000	-1.271004000	0.959212000
C	-3.691475000	0.912989000	-0.624956000
C	0.612799000	-0.025402000	1.466781000
C	-4.202888000	0.813219000	-1.917637000
C	1.165166000	0.041526000	2.742754000
H	-4.574659000	-0.132725000	-2.293167000
H	1.522479000	0.982958000	3.141920000
C	-4.199492000	1.931214000	-2.732224000
C	1.287522000	-1.119024000	3.483806000
C	-3.707353000	3.162112000	-2.322323000
C	0.869903000	-2.358195000	3.020296000
H	-3.709369000	4.021994000	-2.979168000
H	0.983890000	-3.255397000	3.614358000
C	-3.218959000	3.245117000	-1.032979000
C	0.317029000	-2.398294000	1.755374000
C	-4.195222000	-3.229815000	-0.426159000
C	1.181239000	4.120792000	1.303145000
C	-3.736160000	-3.905902000	0.704764000
C	0.756976000	4.804155000	0.162171000
H	-3.824946000	-4.984910000	0.695475000
H	0.891975000	5.878392000	0.162127000
C	-3.192615000	-3.327838000	1.865857000
C	0.229521000	4.233447000	-1.009516000
C	-4.772225000	-4.016349000	-1.575468000
C	1.810001000	4.890510000	2.434874000
H	-4.761110000	-5.092934000	-1.398044000
H	1.700714000	5.970401000	2.321272000
H	-4.203303000	-3.792801000	-2.483269000
H	1.366569000	4.572610000	3.382414000
H	-5.801487000	-3.690574000	-1.752170000
H	2.874892000	4.642116000	2.467256000
C	-0.057239000	5.107072000	-2.201017000
H	-1.096900000	4.960983000	-2.502899000
H	0.118688000	6.166126000	-2.004371000
H	0.581477000	4.775265000	-3.025731000
C	1.998811000	-5.708183000	-0.219666000
H	1.621327000	-6.512663000	-0.853405000
H	2.947699000	-6.011563000	0.230904000
H	1.289268000	-5.525563000	0.593255000

C	-2.738766000	-4.229085000	2.985492000
H	-3.186606000	-5.223159000	2.928794000
H	-1.651615000	-4.331295000	2.922134000
H	-2.980432000	-3.768188000	3.945741000

5.2.6 Pt-6

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C	1.170726000	-2.776117000	-0.135069000
C	2.143028000	-3.726486000	-0.168778000
C	3.501991000	-3.347796000	-0.085014000
C	3.816063000	-1.966478000	0.019369000
H	4.289223000	-5.354764000	-0.174175000
H	0.112958000	-3.013680000	-0.162532000
H	1.869700000	-4.773059000	-0.242836000
C	4.546537000	-4.303869000	-0.085639000
C	6.165991000	-2.537894000	0.170388000
C	5.850730000	-3.907915000	0.032746000
H	7.200658000	-2.233834000	0.288513000
H	6.646939000	-4.645385000	0.034095000
C	2.873104000	0.424275000	0.005451000
C	3.888016000	1.378980000	-0.047881000
N	1.689345000	1.098378000	0.046509000
C	3.199902000	2.587695000	-0.022746000
H	4.955154000	1.263999000	-0.122640000
N	1.876517000	2.403787000	0.033559000
C	3.771773000	3.959477000	-0.046072000
F	5.111870000	3.903994000	-0.164673000
F	3.302757000	4.688116000	-1.071717000
F	3.494612000	4.645073000	1.075902000
C	-1.170654000	2.776069000	0.135182000
C	-2.142930000	3.726464000	0.168913000
C	-3.501903000	3.347812000	0.085127000
C	-3.816013000	1.966506000	-0.019303000
H	-4.289081000	5.354799000	0.174347000
H	-0.112878000	3.013598000	0.162664000
H	-1.869575000	4.773027000	0.243007000
C	-4.546422000	4.303913000	0.085774000
C	-6.165923000	2.537991000	-0.170325000
C	-5.850625000	3.907999000	-0.032636000
H	-7.200597000	2.233964000	-0.288471000

5.2 Coordinates of all optimised structures

H	-6.646814000	4.645491000	-0.033968000
C	-2.873113000	-0.424274000	-0.005462000
C	-3.888051000	-1.378955000	0.047827000
N	-1.689369000	-1.098403000	-0.046537000
C	-3.199967000	-2.587686000	0.022652000
H	-4.955187000	-1.263950000	0.122583000
N	-1.876577000	-2.403807000	-0.033635000
C	-3.771873000	-3.959455000	0.045914000
F	-5.111965000	-3.903945000	0.164562000
F	-3.494768000	-4.644989000	-1.076112000
F	-3.302840000	-4.688168000	1.071498000
Pt	0.000001000	-0.000030000	0.000019000
N	-1.468562000	1.447122000	0.060718000
C	-2.742913000	1.024849000	0.009992000
C	2.742938000	-1.024852000	-0.009947000
N	1.468596000	-1.447159000	-0.060646000
C	5.176411000	-1.591939000	0.164678000
H	5.437655000	-0.554461000	0.302104000
C	-5.176370000	1.592009000	-0.164638000
H	-5.437641000	0.554542000	-0.302101000

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C	1.241606000	2.774016000	0.039361000
C	2.247620000	3.684922000	-0.019028000
C	3.600016000	3.261869000	-0.155076000
C	3.862229000	1.865899000	-0.203583000
H	4.444433000	5.238994000	-0.213775000
H	0.200707000	3.062637000	0.106535000
H	2.010904000	4.742259000	0.020083000
C	4.664472000	4.176695000	-0.261451000
C	6.216418000	2.356895000	-0.520367000
C	5.956292000	3.735126000	-0.432524000
H	7.231338000	2.009205000	-0.683869000
H	6.771212000	4.446877000	-0.514262000
C	2.843215000	-0.462405000	0.023245000
C	3.808646000	-1.441718000	0.164948000
N	1.609533000	-1.118206000	-0.014964000
C	3.071745000	-2.639349000	0.192680000
H	4.873651000	-1.350208000	0.286870000
N	1.767918000	-2.445680000	0.081894000
C	3.618563000	-4.025154000	0.294619000

5.2 Coordinates of all optimised structures

F	2.937396000	-4.765615000	1.176664000
F	3.571719000	-4.661644000	-0.885735000
F	4.904633000	-3.989097000	0.683311000
C	-1.241534000	-2.774021000	0.038724000
C	-2.247551000	-3.684910000	-0.019768000
C	-3.599985000	-3.261815000	-0.155414000
C	-3.862204000	-1.865830000	-0.203457000
H	-4.444414000	-5.238919000	-0.214532000
H	-0.200622000	-3.062648000	0.105625000
H	-2.010827000	-4.742259000	0.018952000
C	-4.664462000	-4.176606000	-0.261848000
C	-6.216461000	-2.356730000	-0.519912000
C	-5.956318000	-3.734987000	-0.432532000
H	-7.231415000	-2.008994000	-0.683104000
H	-6.771254000	-4.446713000	-0.514317000
C	-2.843135000	0.462423000	0.023672000
C	-3.808479000	1.441725000	0.165846000
N	-1.609437000	1.118180000	-0.014661000
C	-3.071502000	2.639361000	0.193650000
H	-4.873436000	1.350181000	0.288249000
N	-1.767743000	2.445669000	0.082491000
C	-3.618655000	4.025105000	0.294408000
F	-2.929283000	4.770678000	1.165565000
F	-3.584744000	4.655607000	-0.889690000
F	-4.900723000	3.989701000	0.696194000
Pt	0.000038000	-0.000012000	0.003746000
N	-1.476890000	-1.429815000	0.027635000
C	-2.762767000	-0.965706000	-0.052854000
C	2.762820000	0.965727000	-0.053021000
N	1.476957000	1.429816000	0.027799000
C	5.195289000	1.441634000	-0.411850000
H	5.416785000	0.390339000	-0.523230000
C	-5.195308000	-1.441503000	-0.411330000
H	-5.416825000	-0.390175000	-0.522353000

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C	-0.369829000	3.120656000	1.260016000
C	-1.036303000	4.291092000	1.064064000
C	-2.444368000	4.320803000	1.160712000
C	-3.133600000	3.109137000	1.435470000
H	-2.642942000	6.431942000	0.761780000

5.2 Coordinates of all optimised structures

H	0.710543000	3.056699000	1.234080000
H	-0.472707000	5.186825000	0.833079000
C	-3.183249000	5.516794000	0.983175000
C	-5.231195000	4.320863000	1.417896000
C	-4.546860000	5.515738000	1.099479000
H	-6.309388000	4.333871000	1.538281000
H	-5.106335000	6.436102000	0.965125000
C	-2.907445000	0.557031000	1.617166000
C	-4.151177000	-0.072026000	1.579058000
N	-1.963526000	-0.424822000	1.676589000
C	-3.832837000	-1.427736000	1.639591000
H	-5.137352000	0.345347000	1.468067000
N	-2.511489000	-1.623234000	1.700894000
C	-4.778958000	-2.573366000	1.617396000
F	-5.722072000	-2.388495000	0.656164000
F	-4.168208000	-3.734768000	1.359780000
F	-5.449339000	-2.713291000	2.773453000
C	0.307168000	-2.839930000	1.486764000
C	0.973564000	-4.020393000	1.364216000
C	2.382829000	-4.038159000	1.417801000
C	3.075211000	-2.809231000	1.592202000
H	2.573453000	-6.169768000	1.147077000
H	-0.774076000	-2.779740000	1.466679000
H	0.409563000	-4.931692000	1.209497000
C	3.119120000	-5.242203000	1.289574000
C	5.176420000	-4.015922000	1.555783000
C	4.485626000	-5.231656000	1.350813000
H	6.259482000	-4.015755000	1.617665000
H	5.043651000	-6.157616000	1.253711000
C	2.840286000	-0.251620000	1.689742000
C	4.082084000	0.382177000	1.674137000
N	1.892802000	0.727864000	1.660322000
C	3.757944000	1.736516000	1.639871000
H	5.075126000	-0.030608000	1.643371000
N	2.434926000	1.928831000	1.637180000
C	4.701513000	2.881063000	1.561547000
F	5.700695000	2.606529000	0.678764000
F	4.105604000	4.003988000	1.151265000
F	5.304620000	3.142957000	2.732840000
Pt	-0.033576000	0.148622000	1.623585000
N	0.965975000	-1.655375000	1.625455000
C	2.308960000	-1.607739000	1.653526000

5.2 Coordinates of all optimised structures

C	-2.370788000	1.907697000	1.529952000
N	-1.028878000	1.949215000	1.486848000
C	-4.543475000	3.148459000	1.581862000
H	-5.081005000	2.252523000	1.851640000
C	4.491099000	-2.837360000	1.673156000
H	5.040776000	-1.924780000	1.839381000
C	-1.959878000	2.099095000	-1.854317000
C	-3.184646000	2.689087000	-1.846876000
C	-4.351302000	1.891270000	-1.801149000
C	-4.207684000	0.479444000	-1.784363000
H	-5.735480000	3.543480000	-1.748005000
H	-1.033751000	2.662808000	-1.865268000
H	-3.262146000	3.770421000	-1.852589000
C	-5.645770000	2.461953000	-1.754872000
C	-6.618107000	0.256218000	-1.725170000
C	-6.755447000	1.661930000	-1.708969000
H	-7.502144000	-0.372120000	-1.705409000
H	-7.745786000	2.104507000	-1.669482000
C	-2.546344000	-1.473184000	-1.638517000
C	-3.194989000	-2.675387000	-1.362456000
N	-1.209686000	-1.737045000	-1.683498000
C	-2.152449000	-3.588256000	-1.251556000
H	-4.233620000	-2.882089000	-1.178976000
N	-0.961381000	-3.010420000	-1.449934000
C	-2.229222000	-4.997435000	-0.796240000
F	-3.482286000	-5.466407000	-0.882371000
F	-1.426519000	-5.812568000	-1.498932000
F	-1.852310000	-5.120574000	0.500850000
C	2.031967000	-2.411592000	-1.856522000
C	3.256268000	-3.002049000	-1.885225000
C	4.420755000	-2.211814000	-1.749308000
C	4.276001000	-0.807615000	-1.599532000
H	5.805183000	-3.862878000	-1.836654000
H	1.105455000	-2.973326000	-1.885926000
H	3.333404000	-4.080038000	-1.969423000
C	5.713696000	-2.788052000	-1.716337000
C	6.673965000	-0.614345000	-1.317538000
C	6.817777000	-2.006128000	-1.513185000
H	7.549304000	-0.004015000	-1.121627000
H	7.806101000	-2.453991000	-1.483790000
C	2.619979000	1.161192000	-1.620417000
C	3.267789000	2.391561000	-1.501415000

5.2 Coordinates of all optimised structures

N	1.282358000	1.418100000	-1.685528000
C	2.222835000	3.308426000	-1.480355000
H	4.311769000	2.628733000	-1.401037000
N	1.032588000	2.707343000	-1.596304000
C	2.287727000	4.769949000	-1.233759000
F	3.549026000	5.217404000	-1.311321000
F	1.542442000	5.471370000	-2.103741000
F	1.827127000	5.089670000	0.000153000
Pt	0.036986000	-0.158472000	-1.749028000
N	1.889843000	-1.058789000	-1.753456000
C	2.960565000	-0.252330000	-1.658030000
C	-2.887390000	-0.065460000	-1.757537000
N	-1.816521000	0.743468000	-1.798273000
C	-5.377144000	-0.321358000	-1.765394000
H	-5.296008000	-1.395658000	-1.793650000
C	5.436954000	-0.028261000	-1.361468000
H	5.349012000	1.025598000	-1.153989000

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C	0.210734000	-2.615661000	1.583150000
C	0.885949000	-3.796866000	1.583233000
C	2.291726000	-3.799175000	1.702289000
C	2.969039000	-2.554870000	1.817244000
H	2.503090000	-5.942887000	1.596809000
H	-0.867785000	-2.566028000	1.503793000
H	0.334377000	-4.721544000	1.467954000
C	3.037991000	-5.003331000	1.694845000
C	5.076067000	-3.744983000	1.954042000
C	4.400739000	-4.977970000	1.813195000
H	6.155952000	-3.730740000	2.055826000
H	4.966713000	-5.904187000	1.808348000
C	2.714276000	0.001642000	1.741705000
C	3.951227000	0.644791000	1.761227000
N	1.765290000	0.969002000	1.589764000
C	3.623217000	1.989803000	1.611935000
H	4.946246000	0.241153000	1.827153000
N	2.301623000	2.170628000	1.515065000
C	4.569242000	3.128999000	1.499708000
F	5.595057000	2.806870000	0.663993000
F	3.987601000	4.226979000	1.011871000
F	5.138222000	3.452825000	2.673050000

5.2 Coordinates of all optimised structures

C	-0.513213000	3.309650000	0.991283000
C	-1.198415000	4.491568000	0.809971000
C	-2.608041000	4.535977000	0.953385000
C	-3.297110000	3.313642000	1.221198000
H	-2.796457000	6.649542000	0.613860000
H	0.569470000	3.271203000	0.959142000
H	-0.633761000	5.388286000	0.583186000
C	-3.336000000	5.733008000	0.832274000
C	-5.377033000	4.558809000	1.311172000
C	-4.708473000	5.746337000	0.998971000
H	-6.450028000	4.569451000	1.474611000
H	-5.261080000	6.675178000	0.906072000
C	-3.034518000	0.773439000	1.376113000
C	-4.283629000	0.119308000	1.381503000
N	-2.075546000	-0.210631000	1.485715000
C	-3.951037000	-1.221388000	1.494535000
H	-5.270016000	0.532040000	1.255471000
N	-2.617265000	-1.401750000	1.557138000
C	-4.867582000	-2.392839000	1.557126000
F	-5.747432000	-2.380870000	0.524995000
F	-4.205130000	-3.553025000	1.500476000
F	-5.607655000	-2.394280000	2.678106000
Pt	-0.152057000	0.373729000	1.485062000
N	-1.139244000	2.145647000	1.218461000
C	-2.532442000	2.098728000	1.242156000
C	2.194317000	-1.357813000	1.763182000
N	0.854485000	-1.417676000	1.667951000
C	4.380736000	-2.566234000	1.955379000
H	4.920460000	-1.639868000	2.067899000
C	-4.687097000	3.360696000	1.422047000
H	-5.225165000	2.466855000	1.699263000
C	2.222636000	-2.615498000	-1.691333000
C	3.461269000	-3.174626000	-1.639206000
C	4.597603000	-2.349663000	-1.471295000
C	4.410830000	-0.945082000	-1.384759000
H	6.027404000	-3.963643000	-1.419248000
H	1.312607000	-3.201921000	-1.740875000
H	3.568947000	-4.252492000	-1.678683000
C	5.900383000	-2.888488000	-1.340591000
C	6.777829000	-0.677657000	-0.949807000
C	6.969122000	-2.070125000	-1.094859000
H	7.622849000	-0.039340000	-0.713872000

5.2 Coordinates of all optimised structures

H	7.964727000	-2.489592000	-0.989664000
C	2.722669000	0.978014000	-1.619304000
C	3.345558000	2.228029000	-1.594679000
N	1.382849000	1.200378000	-1.724567000
C	2.282304000	3.121429000	-1.662317000
H	4.384995000	2.490272000	-1.508761000
N	1.106563000	2.487095000	-1.742632000
C	2.306983000	4.602039000	-1.559540000
F	3.564052000	5.066360000	-1.585713000
F	1.625290000	5.195824000	-2.553490000
F	1.742309000	5.033725000	-0.406418000
C	-1.837545000	1.798153000	-1.739676000
C	-3.091490000	2.382084000	-1.605174000
C	-4.256682000	1.584674000	-1.623316000
C	-4.098625000	0.171188000	-1.736111000
H	-5.638523000	3.217816000	-1.415959000
H	-0.932568000	2.395886000	-1.779622000
H	-3.168468000	3.461448000	-1.569343000
C	-5.544781000	2.141884000	-1.517255000
C	-6.513509000	-0.046123000	-1.740989000
C	-6.666155000	1.331984000	-1.565753000
H	-7.389436000	-0.683211000	-1.806188000
H	-7.657431000	1.765815000	-1.488278000
C	-2.405729000	-1.734490000	-1.585783000
C	-3.051115000	-2.951544000	-1.300451000
N	-1.056824000	-1.996960000	-1.615495000
C	-2.007009000	-3.848856000	-1.167154000
H	-4.093134000	-3.148938000	-1.122391000
N	-0.809411000	-3.265065000	-1.362422000
C	-2.081897000	-5.249293000	-0.683780000
F	-3.315941000	-5.749628000	-0.840089000
F	-1.216423000	-6.058901000	-1.310769000
F	-1.792532000	-5.327845000	0.638697000
Pt	0.173394000	-0.404318000	-1.720869000
N	-1.670961000	0.480997000	-1.768297000
C	-2.769132000	-0.365712000	-1.722182000
C	3.090762000	-0.427089000	-1.551503000
N	2.043179000	-1.263863000	-1.656383000
C	5.532246000	-0.126188000	-1.093249000
H	5.401020000	0.930264000	-0.919262000
C	-5.255184000	-0.619045000	-1.830706000
H	-5.171290000	-1.683311000	-1.989419000

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C	-0.024018000	2.696263000	1.342977000
C	0.491452000	3.818143000	1.916066000
C	1.889869000	3.980721000	2.000883000
C	2.730164000	2.952363000	1.494507000
H	1.817416000	5.913983000	2.955497000
H	-1.089500000	2.539893000	1.236466000
H	-0.184911000	4.581456000	2.278983000
C	2.474294000	5.140117000	2.570905000
C	4.672168000	4.267146000	2.104215000
C	3.834063000	5.278001000	2.628315000
H	5.749533000	4.394079000	2.125125000
H	4.274133000	6.168446000	3.066242000
C	2.803190000	0.604994000	0.455789000
C	4.107073000	0.119037000	0.357975000
N	1.982108000	-0.349919000	-0.067671000
C	3.948465000	-1.123665000	-0.253123000
H	5.035409000	0.551851000	0.688562000
N	2.661049000	-1.390852000	-0.499722000
C	5.012338000	-2.079809000	-0.649152000
F	5.757979000	-2.475810000	0.412263000
F	4.524690000	-3.173141000	-1.233045000
F	5.899507000	-1.514521000	-1.508797000
C	0.023946000	-2.696415000	-1.343109000
C	-0.491493000	-3.818337000	-1.916142000
C	-1.889904000	-3.980863000	-2.001145000
C	-2.730224000	-2.952482000	-1.494859000
H	-1.817412000	-5.914122000	-2.955763000
H	1.089420000	-2.540089000	-1.236460000
H	0.184909000	-4.581755000	-2.278761000
C	-2.474307000	-5.140237000	-2.571237000
C	-4.672205000	-4.267224000	-2.104729000
C	-3.834073000	-5.278079000	-2.628791000
H	-5.749572000	-4.394133000	-2.125752000
H	-4.274125000	-6.168496000	-3.066794000
C	-2.803306000	-0.605131000	-0.456114000
C	-4.107216000	-0.119277000	-0.358159000
N	-1.982246000	0.349807000	0.067332000
C	-3.948633000	1.123434000	0.252929000
H	-5.035539000	-0.552126000	-0.688744000

5.2 Coordinates of all optimised structures

N	-2.661218000	1.390683000	0.499468000
C	-5.012551000	2.079449000	0.649159000
F	-5.900002000	1.513684000	1.508196000
F	-4.524993000	3.172416000	1.233810000
F	-5.757871000	2.476107000	-0.412225000
Pt	-0.000070000	-0.000076000	-0.000081000
N	-0.775799000	-1.700423000	-0.871747000
C	-2.113686000	-1.788055000	-0.952156000
C	2.113596000	1.787943000	0.951813000
N	0.775707000	1.700333000	0.871442000
C	4.135721000	3.136289000	1.550683000
H	4.795314000	2.398770000	1.121717000
C	-4.135781000	-3.136391000	-1.551125000
H	-4.795386000	-2.398856000	-1.122201000
C	1.529576000	0.372366000	3.888206000
C	2.703026000	0.987296000	4.195080000
C	3.928210000	0.314602000	3.978843000
C	3.893609000	-1.007764000	3.464749000
H	5.186899000	1.946611000	4.613342000
H	0.563051000	0.845287000	4.024075000
H	2.694500000	1.996940000	4.590020000
C	5.176663000	0.925122000	4.246423000
C	6.309257000	-1.097701000	3.580266000
C	6.342862000	0.237722000	4.039033000
H	7.236108000	-1.645118000	3.446177000
H	7.298114000	0.711437000	4.242706000
C	2.412270000	-2.816503000	2.406189000
C	3.175976000	-3.760062000	1.720354000
N	1.102878000	-3.134480000	2.205437000
C	2.222247000	-4.587794000	1.138636000
H	4.239010000	-3.819245000	1.572749000
N	0.976386000	-4.200205000	1.439013000
C	2.453174000	-5.678259000	0.159296000
F	3.719910000	-6.120248000	0.224421000
F	1.635587000	-6.725451000	0.354031000
F	2.248531000	-5.261079000	-1.109611000
C	-2.068380000	-4.017775000	1.870016000
C	-3.239376000	-4.644742000	1.580721000
C	-4.458695000	-3.935421000	1.682809000
C	-4.425050000	-2.583336000	2.112647000
H	-5.703049000	-5.556696000	0.994226000
H	-1.099703000	-4.483420000	1.729005000

5.2 Coordinates of all optimised structures

H	-3.229407000	-5.668521000	1.224299000
C	-5.694468000	-4.518851000	1.312205000
C	-6.806661000	-2.416984000	1.703887000
C	-6.845431000	-3.778788000	1.329498000
H	-7.715317000	-1.824656000	1.678002000
H	-7.788711000	-4.229624000	1.037360000
C	-2.945715000	-0.702794000	3.054069000
C	-3.696773000	0.418666000	3.407250000
N	-1.636205000	-0.391728000	3.271348000
C	-2.735461000	1.349502000	3.782071000
H	-4.756914000	0.589916000	3.377019000
N	-1.497465000	0.845421000	3.699243000
C	-2.940697000	2.780965000	4.117437000
F	-4.251000000	3.060449000	4.214138000
F	-2.357007000	3.129565000	5.276775000
F	-2.427608000	3.595078000	3.171578000
Pt	-0.268884000	-1.785470000	2.792297000
N	-2.035924000	-2.733082000	2.328266000
C	-3.165605000	-2.025828000	2.495696000
C	2.627241000	-1.558359000	3.100726000
N	1.496628000	-0.873177000	3.333709000
C	5.114597000	-1.707528000	3.303677000
H	5.105007000	-2.734639000	2.974605000
C	-5.628749000	-1.833343000	2.089335000
H	-5.613582000	-0.778639000	2.312770000
C	2.068947000	4.017943000	-1.870271000
C	3.240083000	4.644718000	-1.581109000
C	4.459260000	3.935152000	-1.683163000
C	4.425329000	2.583014000	-2.112801000
H	5.703954000	5.556288000	-0.994882000
H	1.100373000	4.483810000	-1.729300000
H	3.230328000	5.668534000	-1.224787000
C	5.695163000	4.518396000	-1.312701000
C	6.806909000	2.416234000	-1.704051000
C	6.845975000	3.778095000	-1.329896000
H	7.715438000	1.823714000	-1.678085000
H	7.789357000	4.228782000	-1.037858000
C	2.945631000	0.702700000	-3.054074000
C	3.696503000	-0.418845000	-3.407371000
N	1.636062000	0.391810000	-3.271223000
C	2.735021000	-1.349529000	-3.782165000
H	4.756632000	-0.590205000	-3.377296000

5.2 Coordinates of all optimised structures

N	1.497097000	-0.845298000	-3.699158000
C	2.940029000	-2.781013000	-4.117575000
F	4.250274000	-3.060571000	-4.214888000
F	2.427347000	-3.595058000	-3.171436000
F	2.355756000	-3.129629000	-5.276610000
C	-1.529486000	-0.371979000	-3.888102000
C	-2.702941000	-0.986900000	-4.194975000
C	-3.928122000	-0.314223000	-3.978666000
C	-3.893515000	1.008128000	-3.464528000
H	-5.186820000	-1.946229000	-4.613151000
H	-0.562960000	-0.844894000	-4.023990000
H	-2.694420000	-1.996522000	-4.589973000
C	-5.176581000	-0.924750000	-4.246207000
C	-6.309166000	1.098043000	-3.579935000
C	-6.342778000	-0.237369000	-4.038740000
H	-7.236018000	1.645444000	-3.445784000
H	-7.298034000	-0.711090000	-4.242375000
C	-2.412145000	2.816833000	-2.405960000
C	-3.175851000	3.760339000	-1.720064000
N	-1.102744000	3.134818000	-2.205272000
C	-2.222116000	4.588055000	-1.138331000
H	-4.238889000	3.819482000	-1.572460000
N	-0.976262000	4.200458000	-1.438728000
C	-2.452991000	5.678314000	-0.158759000
F	-3.719500000	6.120913000	-0.224258000
F	-2.249074000	5.260565000	1.110077000
F	-1.634819000	6.725175000	-0.352781000
Pt	0.268990000	1.785755000	-2.792125000
N	-1.496540000	0.873537000	-3.333546000
C	-2.627140000	1.558715000	-3.100530000
C	3.165765000	2.025714000	-2.495756000
N	2.036222000	2.733200000	-2.328369000
C	5.628869000	1.832776000	-2.089397000
H	5.613480000	0.778035000	-2.312653000
C	-5.114502000	1.707877000	-3.303386000
H	-5.104907000	2.734980000	-2.974287000

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C	-0.100231000	2.667210000	1.099613000
C	0.395194000	3.832263000	1.600027000
C	1.790043000	4.027941000	1.665265000

5.2 Coordinates of all optimised structures

C	2.648531000	2.988473000	1.216644000
H	1.681026000	6.012310000	2.504337000
H	-1.162670000	2.481122000	1.013207000
H	-0.292328000	4.602231000	1.923733000
C	2.352474000	5.231093000	2.162112000
C	4.565417000	4.378399000	1.731918000
C	3.709311000	5.400422000	2.202708000
H	5.639927000	4.529088000	1.736285000
H	4.132886000	6.324041000	2.584640000
C	2.766353000	0.581928000	0.334637000
C	4.080775000	0.118889000	0.270175000
N	1.967399000	-0.422885000	-0.124166000
C	3.950413000	-1.163675000	-0.257841000
H	4.998916000	0.590805000	0.574358000
N	2.669257000	-1.475978000	-0.487159000
C	5.043278000	-2.112702000	-0.583795000
F	5.860150000	-2.312638000	0.480746000
F	4.591809000	-3.301793000	-0.979595000
F	5.853331000	-1.635598000	-1.563982000
C	0.038875000	-2.907508000	-1.106987000
C	-0.486075000	-4.145269000	-1.545040000
C	-1.888444000	-4.322910000	-1.718462000
C	-2.750895000	-3.222410000	-1.421040000
H	-1.747493000	-6.350030000	-2.386394000
H	1.111400000	-2.771170000	-1.016884000
H	0.209900000	-4.945577000	-1.757812000
C	-2.422618000	-5.526148000	-2.175562000
C	-4.632987000	-4.603696000	-2.112402000
C	-3.802982000	-5.675553000	-2.366835000
H	-5.704246000	-4.690580000	-2.266333000
H	-4.205063000	-6.618962000	-2.720148000
C	-2.817598000	-0.867773000	-0.421463000
C	-4.150242000	-0.440204000	-0.218472000
N	-2.011577000	0.178720000	-0.006885000
C	-4.014060000	0.838241000	0.295428000
H	-5.070687000	-0.976425000	-0.372537000
N	-2.722837000	1.199223000	0.416748000
C	-5.102748000	1.762061000	0.706284000
F	-6.018424000	1.119473000	1.471421000
F	-4.653234000	2.808781000	1.398876000
F	-5.795056000	2.247278000	-0.352763000
Pt	-0.021566000	-0.116010000	-0.071129000

5.2 Coordinates of all optimised structures

N	-0.718374000	-1.891521000	-0.793538000
C	-2.157073000	-2.013394000	-0.889935000
C	2.052679000	1.779184000	0.754982000
N	0.716131000	1.658920000	0.686384000
C	4.050111000	3.205877000	1.249743000
H	4.723191000	2.459602000	0.858544000
C	-4.111446000	-3.381343000	-1.648700000
H	-4.792667000	-2.559957000	-1.489194000
C	1.659394000	0.740353000	3.901399000
C	2.830629000	1.387469000	4.142639000
C	4.059507000	0.715477000	3.947386000
C	4.032186000	-0.637529000	3.519603000
H	5.307489000	2.399248000	4.454181000
H	0.689851000	1.210746000	4.024524000
H	2.817433000	2.422007000	4.466889000
C	5.304640000	1.356933000	4.151384000
C	6.451515000	-0.688104000	3.587723000
C	6.475963000	0.673074000	3.964150000
H	7.382972000	-1.230822000	3.467054000
H	7.428363000	1.170321000	4.119051000
C	2.554610000	-2.518230000	2.587988000
C	3.325788000	-3.496609000	1.960963000
N	1.247432000	-2.835960000	2.373368000
C	2.379727000	-4.338440000	1.389332000
H	4.390826000	-3.571372000	1.838293000
N	1.130344000	-3.929593000	1.645922000
C	2.621029000	-5.458384000	0.447015000
F	3.890123000	-5.886331000	0.521879000
F	1.810678000	-6.505540000	0.671521000
F	2.408418000	-5.082059000	-0.836836000
C	-1.920433000	-3.706815000	1.980927000
C	-3.085667000	-4.317831000	1.638000000
C	-4.316908000	-3.666287000	1.876979000
C	-4.301078000	-2.389620000	2.497062000
H	-5.543170000	-5.208573000	1.001882000
H	-0.948249000	-4.150651000	1.798606000
H	-3.064142000	-5.288347000	1.155344000
C	-5.552775000	-4.242464000	1.496442000
C	-6.719875000	-2.333985000	2.395011000
C	-6.728828000	-3.586134000	1.741234000
H	-7.656562000	-1.828459000	2.604481000
H	-7.673659000	-4.030325000	1.444129000

5.2 Coordinates of all optimised structures

C	-2.818547000	-0.440187000	3.271899000
C	-3.571154000	0.711010000	3.505130000
N	-1.508379000	-0.103268000	3.437842000
C	-2.611389000	1.676342000	3.785588000
H	-4.628305000	0.884045000	3.417683000
N	-1.372394000	1.171430000	3.742406000
C	-2.820108000	3.135599000	3.958256000
F	-4.111436000	3.406487000	4.208445000
F	-2.085029000	3.645198000	4.959936000
F	-2.481578000	3.824765000	2.846089000
Pt	-0.132724000	-1.486951000	2.948277000
N	-1.897881000	-2.459665000	2.531659000
C	-3.035143000	-1.791530000	2.782401000
C	2.765701000	-1.224691000	3.217413000
N	1.631385000	-0.539368000	3.429822000
C	5.260264000	-1.328896000	3.373702000
H	5.260501000	-2.373979000	3.107872000
C	-5.537449000	-1.751306000	2.766358000
H	-5.553739000	-0.802938000	3.278430000
C	1.955009000	3.918681000	-2.176968000
C	3.126561000	4.568326000	-1.944969000
C	4.347513000	3.857533000	-2.008849000
C	4.315251000	2.478858000	-2.344149000
H	5.591944000	5.526388000	-1.445185000
H	0.985721000	4.389574000	-2.058984000
H	3.116118000	5.614653000	-1.661556000
C	5.584322000	4.468922000	-1.690202000
C	6.700528000	2.347996000	-1.943923000
C	6.737579000	3.732749000	-1.665574000
H	7.611457000	1.761611000	-1.884255000
H	7.681634000	4.205463000	-1.413248000
C	2.835742000	0.535592000	-3.146008000
C	3.590717000	-0.601812000	-3.431740000
N	1.525902000	0.202725000	-3.324504000
C	2.631561000	-1.563013000	-3.726962000
H	4.651957000	-0.764472000	-3.399113000
N	1.391209000	-1.062690000	-3.663528000
C	2.848069000	-3.005711000	-4.002655000
F	4.132221000	-3.337265000	-3.791851000
F	2.089109000	-3.784749000	-3.204743000
F	2.543746000	-3.348523000	-5.267375000
C	-1.635143000	-0.616308000	-3.843235000

C	-2.805040000	-1.258095000	-4.107928000
C	-4.034554000	-0.602413000	-3.874142000
C	-4.010925000	0.728024000	-3.379145000
H	-5.277919000	-2.261207000	-4.467978000
H	-0.664798000	-1.077452000	-3.989134000
H	-2.789118000	-2.276327000	-4.479210000
C	-5.278363000	-1.236851000	-4.108748000
C	-6.430444000	0.772105000	-3.436107000
C	-6.451407000	-0.567997000	-3.882113000
H	-7.363460000	1.304410000	-3.285071000
H	-7.402650000	-1.059512000	-4.060834000
C	-2.528316000	2.612680000	-2.458568000
C	-3.282051000	3.592442000	-1.813151000
N	-1.219895000	2.980411000	-2.361542000
C	-2.323720000	4.498494000	-1.370675000
H	-4.336510000	3.633668000	-1.606270000
N	-1.084992000	4.117515000	-1.706881000
C	-2.536532000	5.701101000	-0.527095000
F	-3.826565000	6.076090000	-0.548982000
F	-2.216398000	5.476262000	0.765943000
F	-1.793307000	6.744709000	-0.928217000
Pt	0.155459000	1.613664000	-2.903004000
N	-1.609644000	0.644817000	-3.328406000
C	-2.745210000	1.314646000	-3.075475000
C	3.054623000	1.893148000	-2.676989000
N	1.923362000	2.605233000	-2.544381000
C	5.521771000	1.735429000	-2.278472000
H	5.509066000	0.667500000	-2.428063000
C	-5.241068000	1.406663000	-3.196120000
H	-5.243238000	2.437287000	-2.879481000

5.2.7 Pt-7

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C	12.583433000	6.350592000	10.665762000
C	10.517941000	7.932120000	7.097606000
C	10.110208000	7.564501000	5.822659000
H	9.591795000	8.272896000	5.188259000
C	10.373996000	6.277589000	5.367981000
H	10.060288000	5.978543000	4.373474000
C	11.039102000	5.386474000	6.197024000

5.2 Coordinates of all optimised structures

C	11.421268000	5.813670000	7.462098000
N	11.167614000	7.049135000	7.897351000
Pt	11.685375000	7.883394000	9.822561000
C	11.842509000	9.210761000	11.305968000
C	12.421452000	9.080863000	12.568174000
H	12.872642000	8.134176000	12.844008000
C	12.424965000	10.144392000	13.466982000
H	12.882487000	10.017273000	14.444018000
C	11.850036000	11.367825000	13.129927000
H	11.857485000	12.191039000	13.836935000
C	11.266104000	11.529001000	11.882276000
H	10.818048000	12.483614000	11.620399000
C	11.257654000	10.468844000	10.974645000
C	10.656274000	10.572978000	9.637765000
C	10.019613000	11.665871000	9.044997000
H	9.918927000	12.597910000	9.586955000
C	9.520017000	11.541611000	7.757632000
H	9.024286000	12.386375000	7.290848000
C	9.645348000	10.345132000	7.052437000
H	9.252967000	10.254776000	6.047556000
C	10.284150000	9.283336000	7.676200000
N	10.757179000	9.434054000	8.922987000
H	11.263358000	4.375072000	5.879404000
H	11.943985000	5.172016000	8.163714000
N	13.096615000	5.390083000	11.077479000

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C	-0.122007000	-2.742529000	0.201063000
C	2.344404000	0.906649000	-0.015462000
C	3.718046000	1.241798000	-0.049818000
H	4.007866000	2.283242000	0.033339000
C	4.663553000	0.264492000	-0.192021000
H	5.715832000	0.526646000	-0.223602000
C	4.266104000	-1.093604000	-0.299735000
C	2.933657000	-1.393825000	-0.239660000
N	1.980407000	-0.441370000	-0.082836000
Pt	-0.049310000	-0.759050000	0.206761000
C	-1.962397000	-0.372582000	-0.103394000
C	-2.996824000	-1.296253000	-0.335456000
H	-2.751936000	-2.343233000	-0.471484000
C	-4.314746000	-0.870237000	-0.322836000

5.2 Coordinates of all optimised structures

H	-5.116104000	-1.590886000	-0.450800000
C	-4.619891000	0.483707000	-0.145204000
H	-5.656475000	0.805506000	-0.146383000
C	-3.610654000	1.426824000	0.012209000
H	-3.863397000	2.476038000	0.127541000
C	-2.280676000	1.022387000	0.005169000
C	-1.130170000	1.933057000	0.076723000
C	-1.113162000	3.308133000	0.018753000
H	-2.033217000	3.875398000	-0.043288000
C	0.144951000	3.961827000	0.011939000
H	0.179118000	5.045158000	-0.031631000
C	1.315776000	3.246306000	0.018140000
H	2.270851000	3.755315000	-0.039346000
C	1.271361000	1.831073000	0.064829000
N	0.035710000	1.248299000	0.157314000
H	4.993408000	-1.886622000	-0.420489000
H	2.562394000	-2.410491000	-0.299024000
N	-0.134165000	-3.904560000	0.170543000

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C	-0.697698000	-3.121375000	0.812408000
C	2.984203000	0.181191000	-0.848841000
C	4.216764000	0.653286000	-0.399713000
H	4.315646000	1.703321000	-0.145682000
C	5.308409000	-0.202196000	-0.263305000
H	6.258950000	0.191975000	0.086232000
C	5.192453000	-1.555804000	-0.566255000
H	6.043858000	-2.219573000	-0.453424000
C	3.981175000	-2.053197000	-1.031131000
H	3.893970000	-3.107311000	-1.278294000
C	2.889342000	-1.200193000	-1.184756000
C	1.583894000	-1.658049000	-1.695256000
C	1.193270000	-2.943792000	-2.058079000
H	1.882146000	-3.773492000	-1.967193000
C	-0.107035000	-3.158011000	-2.489794000
H	-0.429055000	-4.162802000	-2.736803000
C	-1.014495000	-2.105784000	-2.566509000
H	-2.038260000	-2.282734000	-2.868808000
C	-0.585927000	-0.843211000	-2.189327000
C	1.105900000	0.641054000	2.266730000
C	2.309699000	1.182802000	2.688834000

5.2 Coordinates of all optimised structures

H	2.395612000	2.246656000	2.867032000
C	3.414691000	0.351469000	2.822982000
H	4.367520000	0.764960000	3.134959000
C	3.292928000	-0.998305000	2.531959000
C	2.064041000	-1.475138000	2.099179000
N	0.681360000	-0.663702000	-1.789027000
N	1.000190000	-0.680253000	1.975482000
Pt	-0.939152000	-1.210237000	1.215860000
C	1.790231000	2.871304000	-0.320408000
C	-2.841325000	-1.016690000	0.626024000
C	-3.698368000	-1.945118000	0.031980000
H	-3.340216000	-2.956138000	-0.132811000
C	-4.995508000	-1.595482000	-0.338491000
H	-5.642688000	-2.339661000	-0.794994000
C	-5.476403000	-0.307333000	-0.115351000
H	-6.491910000	-0.043951000	-0.394192000
C	-4.649062000	0.638724000	0.475800000
H	-5.023029000	1.644531000	0.646559000
C	-3.345809000	0.299978000	0.836411000
C	-2.395184000	1.276056000	1.398895000
C	-2.586235000	2.631307000	1.660878000
C	-1.516146000	3.385020000	2.126086000
H	-1.645421000	4.446038000	2.311997000
C	-0.269951000	2.803452000	2.341483000
H	0.573525000	3.405711000	2.647983000
C	-0.130650000	1.445767000	2.091962000
C	-1.413049000	0.389014000	-2.153490000
C	-2.737924000	0.428218000	-2.563118000
H	-3.230312000	-0.472345000	-2.905166000
C	-3.436594000	1.625945000	-2.493520000
H	-4.476944000	1.662808000	-2.796910000
C	-2.794198000	2.761658000	-2.021765000
C	-1.469855000	2.656278000	-1.620932000
N	-1.180796000	0.746191000	1.636868000
N	-0.799094000	1.504569000	-1.682830000
Pt	1.254176000	1.148834000	-1.112199000
H	-0.911725000	3.499462000	-1.229588000
H	-3.303737000	3.715754000	-1.953833000
H	1.904544000	-2.513712000	1.832743000
H	4.137694000	-1.672266000	2.600328000
N	2.037207000	3.862091000	0.241299000
N	-0.489469000	-4.239800000	0.562118000

5.2 Coordinates of all optimised structures

H	-3.551324000	3.091445000	1.487530000
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C	0.002366000	-3.570456000	-0.105408000
C	2.341398000	0.222698000	-1.290272000
C	3.721504000	0.133922000	-1.055257000
H	4.227924000	0.974912000	-0.595203000
C	4.424410000	-1.011725000	-1.385113000
H	5.492394000	-1.062084000	-1.192025000
C	3.773412000	-2.123553000	-1.943363000
H	4.334146000	-3.024163000	-2.171034000
C	2.417529000	-2.072506000	-2.206036000
H	1.913164000	-2.940632000	-2.615457000
C	1.698965000	-0.909166000	-1.909328000
C	0.271601000	-0.762881000	-2.184518000
C	-0.602456000	-1.693354000	-2.737696000
H	-0.246412000	-2.672243000	-3.029088000
C	-1.954304000	-1.362581000	-2.849886000
H	-2.648391000	-2.082155000	-3.268956000
C	-2.429629000	-0.154095000	-2.368939000
H	-3.488366000	0.070114000	-2.402650000
C	-1.523297000	0.760132000	-1.811964000
C	1.527016000	-0.031856000	2.065472000
C	2.726769000	0.506249000	2.542879000
H	2.760555000	1.535659000	2.874254000
C	3.869159000	-0.266070000	2.530270000
H	4.803777000	0.149861000	2.891244000
C	3.817813000	-1.576776000	2.041372000
C	2.621447000	-2.048361000	1.545705000
N	-0.210889000	0.441152000	-1.793723000
N	1.503381000	-1.305042000	1.551020000
Pt	-0.386350000	-1.825720000	0.749807000
C	2.262619000	2.834427000	0.200566000
C	-2.345872000	-1.812425000	0.490065000
C	-3.178119000	-2.788902000	-0.089126000
H	-2.732135000	-3.718254000	-0.425806000
C	-4.532973000	-2.559147000	-0.256104000
H	-5.155941000	-3.315846000	-0.723648000
C	-5.110524000	-1.357694000	0.174638000
H	-6.175260000	-1.191591000	0.044158000
C	-4.329413000	-0.384272000	0.781798000

5.2 Coordinates of all optimised structures

H	-4.785988000	0.539002000	1.124710000
C	-2.964386000	-0.600174000	0.960081000
C	-2.070939000	0.363956000	1.616139000
C	-2.383164000	1.579104000	2.197331000
C	-1.332989000	2.358151000	2.731140000
H	-1.556454000	3.317331000	3.184169000
C	-0.028531000	1.911415000	2.687206000
H	0.779343000	2.518819000	3.075214000
C	0.247912000	0.660111000	2.108758000
C	-1.835604000	2.037783000	-1.191671000
C	-3.130197000	2.538633000	-1.039415000
H	-3.973013000	1.974090000	-1.419999000
C	-3.330340000	3.746255000	-0.396058000
H	-4.334757000	4.139603000	-0.278720000
C	-2.227913000	4.456785000	0.090253000
C	-0.969008000	3.910572000	-0.069010000
N	-0.787048000	-0.055047000	1.602415000
N	-0.765277000	2.736127000	-0.680318000
Pt	1.060026000	1.663138000	-0.841508000
H	-0.074824000	4.398118000	0.303324000
H	-2.343832000	5.411070000	0.590170000
H	2.520845000	-3.035041000	1.108919000
H	4.698558000	-2.206720000	2.013151000
N	2.880955000	3.509776000	0.920883000
N	0.261396000	-4.560695000	-0.658970000
H	-3.405236000	1.932456000	2.229795000

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C	0.002366000	-3.570456000	-0.105408000
C	2.341398000	0.222698000	-1.290272000
C	3.721504000	0.133922000	-1.055257000
H	4.227924000	0.974912000	-0.595203000
C	4.424410000	-1.011725000	-1.385113000
H	5.492394000	-1.062084000	-1.192025000
C	3.773412000	-2.123553000	-1.943363000
H	4.334146000	-3.024163000	-2.171034000
C	2.417529000	-2.072506000	-2.206036000
H	1.913164000	-2.940632000	-2.615457000
C	1.698965000	-0.909166000	-1.909328000
C	0.271601000	-0.762881000	-2.184518000
C	-0.602456000	-1.693354000	-2.737696000

5.2 Coordinates of all optimised structures

H	-0.246412000	-2.672243000	-3.029088000
C	-1.954304000	-1.362581000	-2.849886000
H	-2.648391000	-2.082155000	-3.268956000
C	-2.429629000	-0.154095000	-2.368939000
H	-3.488366000	0.070114000	-2.402650000
C	-1.523297000	0.760132000	-1.811964000
C	1.527016000	-0.031856000	2.065472000
C	2.726769000	0.506249000	2.542879000
H	2.760555000	1.535659000	2.874254000
C	3.869159000	-0.266070000	2.530270000
H	4.803777000	0.149861000	2.891244000
C	3.817813000	-1.576776000	2.041372000
C	2.621447000	-2.048361000	1.545705000
N	-0.210889000	0.441152000	-1.793723000
N	1.503381000	-1.305042000	1.551020000
Pt	-0.386350000	-1.825720000	0.749807000
C	2.262619000	2.834427000	0.200566000
C	-2.345872000	-1.812425000	0.490065000
C	-3.178119000	-2.788902000	-0.089126000
H	-2.732135000	-3.718254000	-0.425806000
C	-4.532973000	-2.559147000	-0.256104000
H	-5.155941000	-3.315846000	-0.723648000
C	-5.110524000	-1.357694000	0.174638000
H	-6.175260000	-1.191591000	0.044158000
C	-4.329413000	-0.384272000	0.781798000
H	-4.785988000	0.539002000	1.124710000
C	-2.964386000	-0.600174000	0.960081000
C	-2.070939000	0.363956000	1.616139000
C	-2.383164000	1.579104000	2.197331000
C	-1.332989000	2.358151000	2.731140000
H	-1.556454000	3.317331000	3.184169000
C	-0.028531000	1.911415000	2.687206000
H	0.779343000	2.518819000	3.075214000
C	0.247912000	0.660111000	2.108758000
C	-1.835604000	2.037783000	-1.191671000
C	-3.130197000	2.538633000	-1.039415000
H	-3.973013000	1.974090000	-1.419999000
C	-3.330340000	3.746255000	-0.396058000
H	-4.334757000	4.139603000	-0.278720000
C	-2.227913000	4.456785000	0.090253000
C	-0.969008000	3.910572000	-0.069010000
N	-0.787048000	-0.055047000	1.602415000

5.2 Coordinates of all optimised structures

N	-0.765277000	2.736127000	-0.680318000
Pt	1.060026000	1.663138000	-0.841508000
H	-0.074824000	4.398118000	0.303324000
H	-2.343832000	5.411070000	0.590170000
H	2.520845000	-3.035041000	1.108919000
H	4.698558000	-2.206720000	2.013151000
N	2.880955000	3.509776000	0.920883000
N	0.261396000	-4.560695000	-0.658970000
H	-3.405236000	1.932456000	2.229795000

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C	0.176025000	-1.061400000	1.749784000
C	-3.174894000	-1.946132000	0.458484000
C	-3.361798000	-3.123473000	-0.261480000
H	-3.504478000	-3.068819000	-1.335290000
C	-3.348399000	-4.361180000	0.378761000
C	-3.141163000	-4.448194000	1.752638000
H	-3.115441000	-5.415459000	2.243798000
C	-2.968928000	-3.287903000	2.496852000
H	-2.799228000	-3.356762000	3.566611000
C	-2.998507000	-2.046226000	1.866753000
C	-2.849573000	-0.776930000	2.595232000
C	-2.665554000	-0.569195000	3.961811000
H	-2.579859000	-1.412971000	4.633376000
C	-2.555320000	0.727403000	4.436046000
H	-2.396234000	0.898484000	5.495381000
H	-2.542631000	2.829340000	3.945703000
C	-2.815932000	1.568802000	2.219691000
C	-0.420469000	-1.534023000	-2.660553000
C	-0.660523000	-2.471208000	-3.650789000
H	-0.812256000	-2.155879000	-4.673986000
C	-0.699099000	-3.817290000	-3.312912000
H	-0.879638000	-4.562623000	-4.080024000
C	-0.506910000	-4.194536000	-1.991989000
C	-0.287048000	-3.206900000	-1.044104000
N	-2.908593000	0.299720000	1.792013000
N	-0.242063000	-1.916813000	-1.372568000
Pt	0.081207000	-0.249382000	-0.048398000
C	-3.398286000	-0.375002000	-2.104104000
C	0.240131000	1.646731000	0.587637000
C	0.444131000	2.134418000	1.874393000

5.2 Coordinates of all optimised structures

H	0.547979000	1.434021000	2.695312000
C	0.530711000	3.505702000	2.109377000
H	0.702606000	3.865092000	3.120626000
C	0.427906000	4.412256000	1.060271000
H	0.512211000	5.478758000	1.244497000
C	0.231173000	3.946910000	-0.235474000
H	0.168659000	4.655371000	-1.055526000
C	0.135619000	2.580725000	-0.479647000
C	-0.066731000	2.016024000	-1.826172000
C	-0.210031000	2.682998000	-3.036162000
H	-0.154868000	3.763926000	-3.075139000
C	-0.419927000	1.937742000	-4.193825000
H	-0.532338000	2.446093000	-5.145506000
C	-0.496548000	0.551742000	-4.148236000
H	-0.678191000	-0.021435000	-5.046387000
C	-0.346251000	-0.077477000	-2.921498000
C	-2.946226000	2.585108000	1.143108000
C	-2.947443000	3.952392000	1.377807000
H	-2.811559000	4.333141000	2.381741000
C	-3.118230000	4.826764000	0.311855000
H	-3.119668000	5.897680000	0.485070000
C	-3.280624000	4.317833000	-0.967911000
H	3.355469000	4.318115000	-2.825070000
C	-3.262392000	2.940802000	-1.139981000
H	2.932174000	1.862939000	-2.792433000
N	2.513173000	-1.168201000	-3.598199000
N	-0.127214000	0.669651000	-1.831420000
N	-3.100068000	2.102762000	-0.115835000
Pt	-3.121446000	-0.052520000	-0.179476000
C	2.893553000	-2.265519000	0.246302000
C	2.747032000	-3.503242000	-0.375772000
H	2.578012000	-3.540527000	-1.446807000
C	2.809426000	-4.683485000	0.362214000
C	3.022173000	-4.643365000	1.737573000
H	3.060496000	-5.563127000	2.312853000
C	3.194029000	-3.420575000	2.374505000
C	3.141166000	-2.236176000	1.645054000
C	3.348498000	-0.904948000	2.245484000
C	3.623735000	-0.584970000	3.554772000
H	3.669703000	-1.355486000	4.313301000
C	3.843106000	0.769806000	3.888912000
H	4.053627000	1.034458000	4.920222000

C	3.811088000	1.754841000	2.928871000
H	3.999708000	2.788430000	3.194594000
C	3.530290000	1.408812000	1.592038000
H	-0.533050000	-5.233513000	-1.685843000
H	-0.142261000	-3.433477000	0.004359000
N	0.177650000	-1.491572000	2.829853000
N	3.275354000	0.091546000	1.324653000
C	2.637013000	-0.927760000	-2.465715000
C	3.487346000	2.273937000	0.451713000
C	3.732360000	3.661912000	0.485912000
H	3.956335000	4.135740000	1.434713000
C	3.685505000	4.404486000	-0.666096000
H	3.876028000	5.472375000	-0.634361000
C	3.387299000	3.767609000	-1.892233000
C	3.157811000	2.412863000	-1.884714000
N	3.187957000	1.670697000	-0.763457000
Pt	2.871753000	-0.421744000	-0.562709000
N	-3.542239000	-0.490675000	-3.253904000
C	-2.635289000	1.818564000	3.569641000
H	-3.493333000	-5.267282000	-0.203200000
H	-3.378382000	2.472933000	-2.111482000
H	-3.419146000	4.967029000	-1.824534000
H	3.361523000	-3.392555000	3.446679000
H	2.692028000	-5.639860000	-0.140476000

5.2.8 Pt-8

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C	16.991638000	16.658783000	10.293071000
C	17.421339000	13.817644000	10.967443000
C	18.341252000	14.237971000	11.929207000
H	18.526641000	15.299248000	12.049474000
C	19.014185000	13.315634000	12.725191000
H	19.725381000	13.669080000	13.466439000
C	18.788574000	11.947714000	12.584431000
H	19.318440000	11.236434000	13.209802000
C	17.880550000	11.499218000	11.637962000
H	17.704667000	10.432649000	11.528175000
C	17.199955000	12.415992000	10.834223000
C	16.225926000	12.006195000	9.815665000
C	15.811649000	10.715865000	9.472386000

5.2 Coordinates of all optimised structures

H	16.226448000	9.857670000	9.986077000
C	14.867041000	10.546857000	8.471539000
H	14.543169000	9.546731000	8.202696000
C	14.327117000	11.647216000	7.806258000
H	13.587491000	11.527310000	7.023361000
C	14.768767000	12.905495000	8.180834000
C	14.337218000	14.190532000	7.623269000
C	13.445376000	14.574911000	6.656055000
C	12.733005000	16.873536000	5.855350000
H	13.269871000	17.821570000	5.923013000
H	12.738324000	16.549612000	4.812081000
C	11.327253000	16.981170000	6.393815000
C	10.234730000	16.663327000	5.593093000
H	10.391268000	16.341834000	4.566580000
C	8.941846000	16.762675000	6.099614000
H	8.094128000	16.516495000	5.468181000
C	8.740702000	17.173614000	7.411463000
H	7.733533000	17.249612000	7.808710000
C	9.832782000	17.489659000	8.216863000
H	9.679066000	17.813154000	9.241203000
C	11.121723000	17.396588000	7.710391000
H	11.975143000	17.644168000	8.336100000
N	17.385723000	17.692772000	10.652512000
N	15.685403000	13.047575000	9.151522000
N	14.897200000	15.341767000	8.121366000
N	14.408068000	16.377856000	7.521663000
N	13.533625000	15.924088000	6.627349000
Pt	16.330858000	14.905507000	9.703277000
H	12.772803000	14.025758000	6.017066000

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C	16.971576000	16.650961000	10.288811000
C	17.401851000	13.846213000	10.948947000
C	18.329151000	14.281649000	11.920241000
H	18.494454000	15.348161000	12.022182000
C	19.003666000	13.388379000	12.713832000
H	19.714218000	13.733243000	13.456849000
C	18.773007000	11.976978000	12.566566000
H	19.319590000	11.290465000	13.207011000
C	17.892730000	11.477749000	11.651303000
H	17.743343000	10.406286000	11.567570000

5.2 Coordinates of all optimised structures

C	17.171564000	12.365856000	10.807128000
C	16.240587000	11.969000000	9.829854000
C	15.811488000	10.668590000	9.463908000
H	16.227836000	9.807411000	9.974790000
C	14.878761000	10.499715000	8.474174000
H	14.551205000	9.504908000	8.195134000
C	14.331225000	11.632911000	7.804049000
H	13.591673000	11.514060000	7.020801000
C	14.763926000	12.885614000	8.175823000
C	14.328073000	14.167338000	7.618866000
C	13.440959000	14.567007000	6.652962000
C	12.742846000	16.874223000	5.868029000
H	13.284342000	17.819201000	5.941140000
H	12.748967000	16.554594000	4.823459000
C	11.336021000	16.987575000	6.402703000
C	10.243900000	16.685906000	5.595254000
H	10.401743000	16.371413000	4.566797000
C	8.949961000	16.791517000	6.097755000
H	8.102705000	16.557430000	5.461103000
C	8.747146000	17.192602000	7.412378000
H	7.739128000	17.273171000	7.806604000
C	9.838781000	17.492368000	8.224538000
H	9.683843000	17.807730000	9.251253000
C	11.128811000	17.393034000	7.722062000
H	11.982079000	17.627370000	8.352998000
N	17.362053000	17.685824000	10.648403000
N	15.682283000	13.048372000	9.147767000
N	14.891049000	15.314457000	8.127521000
N	14.407415000	16.361660000	7.534722000
N	13.535840000	15.916743000	6.637394000
Pt	16.322062000	14.876839000	9.705187000
H	12.768024000	14.026969000	6.006900000

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C	2.553105000	0.934131000	-2.078184000
C	-2.552816000	0.934832000	2.077996000
C	2.081473000	-2.001512000	-2.060447000
C	-2.081480000	-2.000931000	2.060863000
C	3.456733000	-2.185095000	-2.217993000
C	-3.456747000	-2.184390000	2.218481000
H	4.094774000	-1.313434000	-2.318113000

5.2 Coordinates of all optimised structures

H	-4.094716000	-1.312669000	2.318548000
C	4.015073000	-3.460811000	-2.247249000
C	-4.015186000	-3.460061000	2.247869000
H	5.088678000	-3.573602000	-2.371016000
H	-5.088795000	-3.572759000	2.371686000
C	3.211515000	-4.591880000	-2.126550000
C	-3.211725000	-4.591204000	2.127227000
H	3.650673000	-5.584121000	-2.155248000
H	-3.650965000	-5.583406000	2.156020000
C	1.839093000	-4.442245000	-1.979542000
C	-1.839296000	-4.441693000	1.980146000
H	1.211718000	-5.324472000	-1.886886000
H	-1.211994000	-5.323978000	1.887533000
C	1.272953000	-3.168610000	-1.944698000
C	-1.273060000	-3.168107000	1.945177000
C	-0.168696000	-2.945119000	-1.741270000
C	0.168595000	-2.944738000	1.741628000
C	-1.180861000	-3.886367000	-1.567022000
C	1.180674000	-3.886072000	1.567316000
H	-0.952772000	-4.944647000	-1.591692000
H	0.952489000	-4.944332000	1.591926000
C	-2.480857000	-3.452121000	-1.337477000
C	2.480703000	-3.451934000	1.337771000
H	-3.267955000	-4.178698000	-1.169555000
H	3.267735000	-4.178576000	1.169823000
C	-2.778916000	-2.094699000	-1.283871000
C	2.778871000	-2.094534000	1.284123000
H	-3.780785000	-1.743381000	-1.071854000
C	-1.739755000	-1.195398000	-1.466002000
C	1.739778000	-1.195149000	1.466196000
C	-1.812494000	0.261069000	-1.378366000
C	1.812563000	0.261297000	1.378256000
C	-2.779390000	1.154240000	-0.999951000
H	-3.804839000	1.044165000	-0.691910000
C	-2.673994000	3.626355000	-0.486822000
H	-2.621911000	3.578430000	0.602684000
H	-1.981155000	4.385352000	-0.852349000
C	-4.085069000	3.865625000	-0.955203000
C	-4.326691000	4.394993000	-2.222995000
H	-3.489470000	4.656779000	-2.864978000
C	-5.629504000	4.589751000	-2.663511000
H	-5.811298000	5.006036000	-3.649429000

5.2 Coordinates of all optimised structures

C	-6.699201000	4.254670000	-1.837295000
H	-7.717776000	4.409197000	-2.180054000
C	-6.461779000	3.725082000	-0.573676000
C	-5.157348000	3.529245000	-0.129058000
H	-4.957835000	3.102911000	0.850573000
N	3.457898000	1.667913000	-2.104240000
N	-3.457470000	1.668792000	2.103777000
N	-0.492366000	-1.637991000	-1.692440000
N	0.492368000	-1.637649000	1.692736000
N	-0.663001000	0.983847000	-1.571491000
N	0.663043000	0.984150000	1.571062000
N	-0.873071000	2.240094000	-1.333221000
N	0.873142000	2.240317000	1.332446000
N	-2.151856000	2.347346000	-0.986661000
Pt	1.034175000	-0.304061000	-1.904083000
Pt	-1.034047000	-0.303593000	1.904132000
C	2.779499000	1.154350000	0.999688000
N	2.151946000	2.347461000	0.985970000
H	3.804982000	1.044215000	0.691784000
C	2.674142000	3.626262000	0.485703000
H	1.981117000	4.385386000	0.850618000
H	2.622465000	3.577820000	-0.603806000
C	4.085016000	3.865856000	0.954529000
C	4.326060000	4.395569000	2.222288000
C	5.157665000	3.529443000	0.128892000
C	5.628667000	4.590643000	2.663275000
C	6.461891000	3.725616000	0.573970000
C	6.698740000	4.255546000	1.837553000
H	3.488541000	4.657367000	2.863880000
H	4.958661000	3.102856000	-0.850726000
H	5.809995000	5.007180000	3.649171000
H	7.294271000	3.464746000	-0.072209000
H	7.717161000	4.410331000	2.180652000
H	3.780763000	-1.743308000	1.072059000
H	-7.293861000	3.464214000	0.072886000

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C	-1.381658000	-1.858756000	-1.352207000
C	1.381156000	-1.859428000	1.351567000
C	-1.763319000	1.052026000	-1.383591000
C	1.763681000	1.051249000	1.383501000

5.2 Coordinates of all optimised structures

C	-3.130298000	0.783654000	-1.345198000
C	3.130575000	0.782474000	1.345115000
H	-3.469287000	-0.243592000	-1.280487000
H	3.469260000	-0.244860000	1.280296000
C	-4.061459000	1.817533000	-1.386294000
C	4.062062000	1.816058000	1.386335000
H	-5.121952000	1.581072000	-1.362359000
H	5.122479000	1.579249000	1.362381000
C	-3.640914000	3.143916000	-1.473924000
C	3.641924000	3.142561000	1.474115000
H	-4.369189000	3.948419000	-1.507215000
H	4.370441000	3.946841000	1.507476000
C	-2.286396000	3.436751000	-1.522421000
C	2.287496000	3.435798000	1.522658000
H	-1.963827000	4.471053000	-1.597158000
H	1.965246000	4.470190000	1.597522000
C	-1.338246000	2.410239000	-1.484600000
C	1.339020000	2.409579000	1.484717000
C	0.101841000	2.632854000	-1.575429000
C	-0.100977000	2.632605000	1.575590000
C	0.798770000	3.834583000	-1.684919000
C	-0.797508000	3.834550000	1.685463000
H	0.257973000	4.773475000	-1.658772000
H	-0.256387000	4.773261000	1.659567000
C	2.179008000	3.823007000	-1.826163000
C	-2.177721000	3.823406000	1.826799000
H	2.723627000	4.757093000	-1.905474000
H	-2.722033000	4.757645000	1.906413000
C	2.876372000	2.603862000	-1.878926000
C	-2.875491000	2.604458000	1.879289000
H	3.953533000	2.577965000	-1.991057000
C	2.161351000	1.436715000	-1.759813000
C	-2.160876000	1.437108000	1.759835000
C	2.682077000	0.075871000	-1.759188000
C	-2.682060000	0.076442000	1.759129000
C	3.928253000	-0.493547000	-1.732442000
H	4.922753000	-0.080752000	-1.703324000
C	4.674181000	-2.904117000	-1.490809000
H	4.093719000	-3.760484000	-1.145358000
H	5.106675000	-3.137837000	-2.467367000
C	5.732728000	-2.495391000	-0.498191000
C	7.011725000	-2.150314000	-0.926922000

5.2 Coordinates of all optimised structures

H	7.268650000	-2.230096000	-1.980420000
C	7.962608000	-1.707027000	-0.011372000
H	8.959212000	-1.443103000	-0.351297000
C	7.631248000	-1.603294000	1.334500000
H	8.369954000	-1.255116000	2.049935000
C	6.352676000	-1.951955000	1.765583000
C	5.403197000	-2.400568000	0.856165000
H	4.400730000	-2.667450000	1.185160000
N	-2.134737000	-2.744443000	-1.381911000
N	2.133760000	-2.745539000	1.380838000
N	0.811002000	1.470326000	-1.602179000
N	-0.810522000	1.470285000	1.602080000
N	1.784634000	-0.962746000	-1.688894000
N	-1.784976000	-0.962444000	1.688438000
N	2.399874000	-2.102102000	-1.639783000
N	-2.400588000	-2.101607000	1.639587000
N	3.694733000	-1.824728000	-1.657728000
Pt	-0.237679000	-0.245696000	-1.391283000
Pt	0.237653000	-0.246025000	1.390900000
C	-3.928434000	-0.492590000	1.732941000
N	-3.695380000	-1.823834000	1.658155000
H	-4.922828000	-0.079489000	1.704455000
C	-4.675226000	-2.902950000	1.491961000
H	-5.107786000	-3.135808000	2.468696000
H	-4.095068000	-3.759798000	1.147191000
C	-5.733633000	-2.494688000	0.498989000
C	-7.012772000	-2.149623000	0.927265000
C	-5.403778000	-2.400441000	-0.855334000
C	-7.963521000	-1.706954000	0.011264000
C	-6.353113000	-1.952440000	-1.765191000
C	-7.631866000	-1.603828000	-1.334575000
H	-7.269940000	-2.228954000	1.980738000
H	-4.401124000	-2.667134000	-1.183925000
H	-8.960245000	-1.443026000	0.350834000
H	-6.092257000	-1.878358000	-2.816251000
H	-8.370461000	-1.256133000	-2.050360000
H	-3.952647000	2.578887000	1.991543000
H	6.092059000	-1.877448000	2.816674000

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C	-2.623644000	3.115691000	2.462939000
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5.2 Coordinates of all optimised structures

C	-3.841631000	3.222399000	-0.227814000
C	-5.087053000	3.372909000	0.386529000
H	-5.134336000	3.427148000	1.468596000
C	-6.255142000	3.470609000	-0.367877000
H	-7.208429000	3.601071000	0.136736000
C	-6.213746000	3.403891000	-1.758189000
H	-7.126508000	3.476775000	-2.340263000
C	-4.992542000	3.236116000	-2.398085000
H	-4.958771000	3.187635000	-3.482994000
C	-3.817040000	3.148040000	-1.651364000
C	-2.486991000	3.009031000	-2.271610000
C	-2.169492000	2.778103000	-3.608875000
H	-2.955389000	2.688237000	-4.348948000
C	-0.837137000	2.630104000	-3.974321000
H	-0.584371000	2.412244000	-5.006404000
C	0.179361000	2.737771000	-3.029434000
H	-2.751872000	0.071579000	3.020933000
C	-0.188987000	2.991261000	-1.717809000
C	0.705121000	3.136934000	-0.570719000
C	-2.889582000	-0.319113000	-0.027147000
H	-3.835530000	-0.448703000	0.467847000
C	-3.791739000	-0.452682000	-2.410960000
H	-3.385886000	-1.154985000	-3.138727000
H	-3.907078000	0.534220000	-2.865014000
C	-5.097778000	-0.942545000	-1.843445000
C	-5.897276000	-0.083293000	-1.087973000
H	-5.582880000	0.941388000	-0.924264000
C	-7.086407000	-0.538996000	-0.532699000
H	-7.696609000	0.137723000	0.057480000
C	-7.492558000	-1.854225000	-0.742534000
H	7.267525000	5.750447000	-1.396325000
C	5.587643000	6.051728000	-0.086311000
H	5.612394000	7.133327000	-0.172418000
C	4.626704000	5.443093000	0.710799000
H	3.897655000	6.048098000	1.243324000
N	-2.996579000	2.982944000	3.558174000
N	-1.483576000	3.102305000	-1.378674000
N	0.160146000	3.210267000	0.684615000
N	1.095500000	3.319191000	1.576791000
N	-2.756880000	-0.316417000	-1.369386000
Pt	-2.018869000	3.184412000	0.592751000
C	-1.871765000	-3.468677000	-2.027092000

5.2 Coordinates of all optimised structures

C	2.246743000	0.182845000	-1.767552000
C	-2.224149000	-3.522371000	0.906059000
C	2.875716000	-0.050288000	1.118660000
C	-3.603527000	-3.528489000	0.690185000
C	4.230337000	-0.132963000	0.789687000
H	-3.977271000	-3.556686000	-0.325430000
H	4.515912000	-0.183354000	-0.255047000
C	-4.501532000	-3.470938000	1.751775000
C	5.220140000	-0.152620000	1.772035000
H	-5.567921000	-3.452291000	1.544240000
H	6.263992000	-0.226094000	1.477713000
C	-4.044562000	-3.425849000	3.067915000
C	4.877976000	-0.068735000	3.119283000
H	-4.747730000	-3.378447000	3.893195000
H	5.647831000	-0.071767000	3.884230000
C	-2.679832000	-3.442239000	3.317461000
C	3.537385000	0.014496000	3.480241000
H	-2.323225000	-3.404846000	4.343078000
H	3.269524000	0.069729000	4.531573000
C	-1.773461000	-3.488262000	2.256581000
C	2.544014000	0.012787000	2.502362000
C	-0.315849000	-3.455711000	2.451950000
C	1.103129000	0.035529000	2.821999000
C	0.403164000	-3.416366000	3.647210000
C	0.487265000	0.154660000	4.063071000
H	-0.117277000	-3.427823000	4.596550000
H	1.082035000	0.271508000	4.960712000
C	1.789461000	-3.348706000	3.602789000
C	-0.901950000	0.158252000	4.131785000
H	2.354845000	-3.305878000	4.528021000
H	-1.396150000	0.291995000	5.087413000
C	2.464852000	-3.312632000	2.385774000
C	-1.672092000	0.029736000	2.982323000
H	3.543086000	-3.219047000	2.339262000
H	1.218063000	2.574953000	-3.289404000
C	1.708047000	-3.358362000	1.225571000
C	-1.012380000	-0.082067000	1.769699000
C	2.202073000	-3.272213000	-0.146887000
C	-1.615070000	-0.161339000	0.445360000
C	3.424112000	-3.012906000	-0.709399000
C	2.065193000	3.209281000	-0.418180000
H	4.398427000	-2.841789000	-0.286609000

5.2 Coordinates of all optimised structures

H	2.879684000	3.154219000	-1.120588000
C	4.098570000	-2.612069000	-3.137889000
C	3.515733000	3.391793000	1.654887000
H	3.647641000	-1.773391000	-3.669099000
H	3.294459000	3.950441000	2.565694000
H	4.128197000	-3.485126000	-3.794154000
H	3.795709000	2.374238000	1.929985000
C	5.468732000	-2.259278000	-2.621008000
C	4.588213000	4.053810000	0.831071000
C	6.372235000	-3.263624000	-2.271094000
C	5.522171000	3.280651000	0.143784000
H	6.097906000	-4.306012000	-2.413067000
H	5.490785000	2.200013000	0.237626000
C	7.615492000	-2.939309000	-1.740350000
C	6.483808000	3.889774000	-0.656096000
H	8.311462000	-3.727531000	-1.471164000
H	7.207014000	3.280283000	-1.189446000
C	7.967714000	-1.604104000	-1.562820000
C	6.517430000	5.274663000	-0.772505000
H	8.939882000	-1.349387000	-1.152042000
H	-8.424402000	-2.210622000	-0.313652000
C	7.076039000	-0.599020000	-1.923841000
C	-6.705777000	-2.708275000	-1.509045000
H	7.350911000	0.444340000	-1.798066000
H	-7.020281000	-3.733360000	-1.679349000
C	5.829460000	-0.922274000	-2.451126000
C	-5.508545000	-2.257267000	-2.057862000
H	5.118606000	-0.146983000	-2.720248000
H	-4.873677000	-2.923148000	-2.634302000
N	-2.572671000	-3.433167000	-2.956659000
N	2.849104000	0.421468000	-2.737091000
N	0.369101000	-3.438633000	1.291346000
N	0.330525000	-0.081532000	1.726647000
N	1.298590000	-3.332293000	-1.176162000
N	-0.797239000	-0.078047000	-0.648698000
N	1.891359000	-3.128584000	-2.308946000
N	-1.489763000	-0.164918000	-1.741405000
N	3.177337000	-2.932946000	-2.034239000
N	2.249609000	3.326511000	0.913253000
Pt	-0.735074000	-3.467489000	-0.424504000
Pt	1.268831000	-0.041748000	-0.075727000

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C	-3.749810000	2.174695000	2.489297000
C	-4.846076000	2.407442000	-0.233621000
C	-6.104081000	2.134405000	0.308257000
H	-6.199692000	2.024815000	1.383027000
C	-7.226263000	2.001920000	-0.507833000
H	-8.192613000	1.790289000	-0.058493000
C	-7.124339000	2.148931000	-1.889452000
H	-8.002939000	2.053683000	-2.519273000
C	-5.886044000	2.416179000	-2.458022000
H	-5.803921000	2.521455000	-3.536084000
C	-4.755236000	2.534118000	-1.649788000
C	-3.401637000	2.724673000	-2.198050000
C	-3.001087000	2.721142000	-3.532966000
H	-3.734834000	2.614540000	-4.322336000
C	-1.649549000	2.812222000	-3.836281000
H	-1.326055000	2.775745000	-4.870915000
C	-0.697522000	2.919200000	-2.826013000
H	-3.000281000	-0.720026000	3.450760000
C	-1.150289000	2.937688000	-1.517278000
C	-0.327606000	3.020658000	-0.310496000
C	-3.495398000	-0.739102000	0.427817000
H	-4.377323000	-0.942395000	1.011392000
C	-4.666274000	-0.823347000	-1.801412000
H	-4.302830000	-0.587275000	-2.802222000
H	-5.446669000	-0.111217000	-1.530493000
C	-5.138587000	-2.249391000	-1.679461000
C	-6.343392000	-2.534918000	-1.043477000
H	-6.969089000	-1.720322000	-0.686623000
C	-6.743134000	-3.856338000	-0.863133000
H	-7.683692000	-4.074072000	-0.366648000
C	-5.933427000	-4.892196000	-1.315013000
H	5.433560000	7.183293000	-0.089043000
C	3.690923000	6.762464000	1.100973000
H	3.433577000	7.807761000	1.238736000
C	2.899353000	5.774219000	1.671331000
H	2.020801000	6.046212000	2.250508000
N	-4.150853000	1.792549000	3.513807000
N	-2.462170000	2.849240000	-1.242236000
N	-0.937272000	2.914867000	0.914558000
N	-0.061854000	3.023989000	1.865517000

5.2 Coordinates of all optimised structures

N	-3.522864000	-0.601107000	-0.914069000
Pt	-3.085014000	2.611476000	0.689006000
C	-0.282379000	-2.826383000	-2.135759000
C	1.405257000	0.394751000	-1.791631000
C	-0.379124000	-3.455060000	0.753919000
C	2.337544000	-0.007177000	0.952646000
C	-1.743418000	-3.669346000	0.569447000
C	3.609496000	0.299191000	0.475634000
H	-2.179205000	-3.516465000	-0.410661000
H	3.757118000	0.450286000	-0.586803000
C	-2.551217000	-4.065964000	1.630732000
C	4.695115000	0.406330000	1.343483000
H	-3.612066000	-4.228474000	1.460602000
H	5.676190000	0.646556000	0.941045000
C	-2.003542000	-4.259225000	2.899214000
C	4.524790000	0.217886000	2.713574000
H	-2.636452000	-4.564229000	3.726868000
H	5.370235000	0.301717000	3.388927000
C	-0.646059000	-4.065169000	3.104120000
C	3.265579000	-0.086346000	3.214811000
H	-0.223835000	-4.226371000	4.091722000
H	3.136451000	-0.237808000	4.281918000
C	0.181359000	-3.671167000	2.047455000
C	2.170759000	-0.197146000	2.356132000
C	1.623877000	-3.481344000	2.167827000
C	0.803694000	-0.456634000	2.815904000
C	2.434209000	-3.625465000	3.282731000
C	0.336104000	-0.601784000	4.121163000
H	1.989005000	-3.873565000	4.239695000
H	1.034028000	-0.597634000	4.949764000
C	3.818177000	-3.467374000	3.170810000
C	-1.026365000	-0.719006000	4.347876000
H	4.451967000	-3.584199000	4.042236000
H	-1.400227000	-0.802204000	5.362229000
C	4.387680000	-3.169715000	1.922661000
C	-1.932033000	-0.698446000	3.283088000
H	5.459238000	-3.044731000	1.813560000
H	0.362257000	2.923099000	-3.044635000
C	3.561646000	-3.014054000	0.834725000
C	-1.425491000	-0.590822000	2.006576000
C	3.940259000	-2.652097000	-0.517281000
C	-2.180989000	-0.563391000	0.764297000

5.2 Coordinates of all optimised structures

C	5.104722000	-2.280714000	-1.142874000
C	1.010718000	3.199107000	-0.071225000
H	6.117266000	-2.165090000	-0.793560000
H	1.859896000	3.299074000	-0.726231000
C	5.551308000	-1.335582000	-3.443042000
C	2.333480000	3.357395000	2.080956000
H	4.881810000	-1.201054000	-4.293518000
H	1.983881000	3.607701000	3.083659000
H	6.345027000	-2.032079000	-3.724994000
H	2.840586000	2.393624000	2.118872000
C	6.112657000	-0.026281000	-2.943452000
C	3.222433000	4.427460000	1.502627000
C	7.455478000	0.080006000	-2.590885000
C	4.346228000	4.079882000	0.755683000
H	8.121244000	-0.767130000	-2.736581000
H	4.598866000	3.032519000	0.622380000
C	7.949757000	1.265696000	-2.054520000
C	5.140023000	5.070894000	0.185537000
H	8.998408000	1.342278000	-1.785020000
H	6.016534000	4.792521000	-0.390738000
C	7.097428000	2.347848000	-1.867137000
C	4.813785000	6.411195000	0.355864000
H	7.484870000	3.272903000	-1.450578000
H	-6.240236000	-5.923587000	-1.170335000
C	5.754149000	2.245804000	-2.223287000
C	-4.728830000	-4.606475000	-1.955111000
H	5.086271000	3.089502000	-2.078616000
H	-4.093014000	-5.411805000	-2.309206000
C	5.259600000	1.064622000	-2.763760000
C	-4.329589000	-3.289136000	-2.142679000
H	4.205688000	0.984461000	-3.022447000
H	-3.379242000	-3.071350000	-2.627052000
N	-1.066207000	-2.862739000	-2.994152000
N	1.917947000	0.892242000	-2.710467000
N	2.205325000	-3.157735000	0.969279000
N	-0.092595000	-0.476904000	1.804941000
N	2.944167000	-2.525356000	-1.460448000
N	-1.506294000	-0.335099000	-0.406849000
N	3.428890000	-2.108515000	-2.592762000
N	-2.321064000	-0.352039000	-1.416942000
N	4.732100000	-1.959224000	-2.403273000
N	1.116997000	3.202722000	1.274638000

Pt	0.979037000	-2.891450000	-0.606737000
Pt	0.623372000	-0.180510000	-0.070076000

5.2.9 Pt-9

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Pt-9 monomer S_0

C	8.858828000	1.792909000	11.158629000
C	8.269786000	1.964167000	12.411468000
H	8.874834000	2.339903000	13.228964000
C	6.927374000	1.659406000	12.617290000
H	6.492086000	1.801986000	13.602312000
C	6.135476000	1.174344000	11.578129000
H	5.089756000	0.939797000	11.748618000
C	6.691869000	0.992383000	10.321642000
H	6.073640000	0.614467000	9.512129000
C	8.037530000	1.295550000	10.103861000
C	8.683089000	1.123450000	8.796392000
C	8.136196000	0.641262000	7.608537000
H	7.098130000	0.338070000	7.565613000
C	8.948373000	0.546931000	6.488419000
H	8.538108000	0.162799000	5.560298000
N	9.984282000	1.491156000	8.797850000
C	11.447549000	2.751131000	12.290970000
C	10.287660000	0.929663000	6.521800000
H	10.907241000	0.830897000	5.645904000
C	10.776788000	1.416996000	7.725943000
C	13.673154000	2.610217000	9.265839000
C	14.240004000	2.482367000	7.966377000
C	15.512694000	2.736377000	7.441365000
H	16.306938000	3.103152000	8.082566000
C	15.720205000	2.511321000	6.097930000
H	16.694007000	2.697998000	5.658874000
C	14.672552000	2.044622000	5.282450000
H	14.859127000	1.883929000	4.225616000
C	13.408915000	1.786089000	5.778669000
H	12.631970000	1.443419000	5.111712000
C	13.198341000	2.004673000	7.145893000
N	11.911478000	3.121993000	13.291669000
N	12.420764000	2.248782000	9.251996000
N	12.091746000	1.861240000	7.964437000
Pt	10.731625000	2.135651000	10.567134000

5.2 Coordinates of all optimised structures

H	14.115210000	2.948782000	10.192378000
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Pt-9 monomer T_1

C	8.890947000	1.809420000	11.159620000
C	8.300272000	1.985621000	12.425959000
H	8.922691000	2.364131000	13.229024000
C	6.977586000	1.687056000	12.645219000
H	6.531781000	1.824726000	13.623970000
C	6.165181000	1.183319000	11.569221000
H	5.122026000	0.955139000	11.768959000
C	6.661807000	0.985566000	10.314765000
H	6.019119000	0.605178000	9.527804000
C	8.026804000	1.282647000	10.040700000
C	8.645254000	1.117721000	8.789383000
C	8.111838000	0.626731000	7.570667000
H	7.071472000	0.327312000	7.521041000
C	8.918189000	0.526059000	6.469595000
H	8.521270000	0.142541000	5.536621000
N	9.988471000	1.496772000	8.795307000
C	11.441383000	2.747298000	12.282988000
C	10.288200000	0.913840000	6.520651000
H	10.916338000	0.800058000	5.652742000
C	10.770054000	1.406917000	7.717352000
C	13.665484000	2.594961000	9.275490000
C	14.237651000	2.475711000	7.981136000
C	15.513523000	2.734170000	7.460969000
H	16.305894000	3.095608000	8.107567000
C	15.724637000	2.521069000	6.117528000
H	16.699786000	2.711449000	5.682928000
C	14.677970000	2.063129000	5.292545000
H	14.868408000	1.915021000	4.234517000
C	13.413852000	1.800152000	5.781167000
H	12.634727000	1.468719000	5.110974000
C	13.199144000	2.003882000	7.151231000
N	11.902565000	3.117482000	13.284728000
N	12.410228000	2.231314000	9.248252000
N	12.090595000	1.850752000	7.958454000
Pt	10.712150000	2.127217000	10.553683000
H	14.100030000	2.929191000	10.206918000

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Pt-9 dimer S_0

C	0.533656000	-3.546219000	0.122322000
C	-2.554135000	0.673971000	1.563649000
C	-3.881626000	1.060116000	1.384485000
H	-4.095976000	1.976257000	0.846040000
C	-4.926898000	0.277527000	1.868601000
H	-5.952369000	0.598551000	1.710807000
C	-4.671418000	-0.916771000	2.536432000
H	-5.490232000	-1.526110000	2.905746000
C	-3.358729000	-1.323482000	2.737508000
H	-3.159116000	-2.250843000	3.266535000
C	-2.305324000	-0.538362000	2.269781000
C	-0.892944000	-0.908047000	2.465874000
C	-0.366766000	-2.057181000	3.038661000
H	-1.017003000	-2.837075000	3.411623000
C	1.011331000	-2.226751000	3.054617000
H	1.428829000	-3.150207000	3.437460000
C	-0.665763000	1.645286000	-2.960528000
H	-1.584171000	2.137700000	-3.230396000
C	-0.649893000	0.467576000	-2.224738000
C	-2.737087000	-1.979029000	-0.888689000
H	-2.787226000	-2.942394000	-0.402270000
C	-3.778227000	-1.096480000	-1.285727000
C	-5.174302000	-1.150247000	-1.196418000
H	-5.664075000	-2.022064000	-0.776932000
C	-5.893175000	-0.059243000	-1.631480000
H	-6.976359000	-0.064081000	-1.574142000
C	-5.232588000	1.085571000	-2.118639000
H	-5.820638000	1.950841000	-2.406563000
C	-3.857127000	1.162145000	-2.218943000
H	-3.385357000	2.089178000	-2.507901000
C	-3.130673000	0.034328000	-1.819755000
N	0.536741000	-4.519572000	0.761562000
N	-0.038969000	0.020901000	1.981425000
N	-1.571650000	-1.464699000	-1.171519000
N	-1.775033000	-0.235848000	-1.773620000
Pt	0.504822000	-1.852981000	-0.878854000
C	-1.699071000	2.975190000	-0.123901000
C	2.481995000	-1.585673000	-0.983564000
C	3.522825000	-2.366328000	-0.476902000
H	3.279222000	-3.276165000	0.061662000
C	4.853560000	-2.001519000	-0.666544000

5.2 Coordinates of all optimised structures

H	5.644272000	-2.631097000	-0.267393000
C	5.181431000	-0.841606000	-1.363929000
H	6.219559000	-0.557469000	-1.501755000
C	4.170182000	-0.043235000	-1.878379000
H	4.427344000	0.865977000	-2.413777000
C	2.834381000	-0.403793000	-1.698616000
C	1.717521000	0.407504000	-2.213318000
C	1.761565000	1.591347000	-2.939761000
H	2.710846000	2.032713000	-3.215837000
C	0.562471000	2.193714000	-3.307096000
H	0.576795000	3.119485000	-3.872376000
C	1.867151000	-1.262811000	2.534526000
H	2.928017000	-1.442444000	2.480321000
C	1.286416000	-0.125998000	1.994534000
C	2.049257000	2.793385000	0.240216000
H	1.648428000	3.634582000	-0.306349000
C	3.395156000	2.441126000	0.531026000
C	4.634039000	3.023715000	0.233228000
H	4.685369000	3.939612000	-0.346081000
C	5.772036000	2.407086000	0.703286000
H	6.747576000	2.831321000	0.492081000
C	5.682410000	1.229598000	1.471093000
H	6.594215000	0.769753000	1.837827000
C	4.474199000	0.635497000	1.774174000
H	4.448111000	-0.262293000	2.372544000
C	3.316754000	1.249707000	1.281022000
N	-2.160901000	3.754817000	-0.856218000
N	0.510000000	-0.106756000	-1.896115000
N	1.230226000	1.912317000	0.747656000
N	1.975559000	0.943464000	1.389279000
Pt	-0.868200000	1.562651000	0.966974000

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Pt-9 dimer T_1

C	1.423450000	-0.504530000	-2.026800000
C	-1.514176000	-0.545452000	1.715762000
C	-2.498985000	0.258192000	2.293055000
H	-2.247324000	1.269347000	2.592907000
C	-3.784087000	-0.231758000	2.493415000
H	-4.535945000	0.404607000	2.951466000
C	-4.111855000	-1.536879000	2.119457000
H	-5.118376000	-1.912675000	2.271055000

5.2 Coordinates of all optimised structures

C	-3.153616000	-2.351464000	1.540905000
H	-3.418318000	-3.362055000	1.245170000
C	-1.854901000	-1.875342000	1.327587000
C	-0.787904000	-2.678542000	0.737122000
C	-0.830709000	-3.982593000	0.257824000
H	-1.766887000	-4.527985000	0.251452000
C	0.340778000	-4.579983000	-0.189832000
H	0.320114000	-5.598675000	-0.560549000
C	-3.503931000	2.633692000	-0.139737000
H	-4.555029000	2.396015000	-0.120979000
C	-2.555309000	1.718560000	-0.578536000
C	-2.123255000	-1.514648000	-1.822389000
H	-1.415105000	-2.237618000	-2.197412000
C	-3.523125000	-1.611043000	-1.632358000
C	-4.452738000	-2.644634000	-1.810142000
H	-4.133189000	-3.606520000	-2.197415000
C	-5.771636000	-2.406024000	-1.484003000
H	-6.512011000	-3.188304000	-1.613668000
C	-6.170913000	-1.154184000	-0.984464000
H	-7.213735000	-0.991596000	-0.732715000
C	-5.269409000	-0.120713000	-0.794367000
H	-5.610346000	0.819082000	-0.386289000
C	-3.933919000	-0.359943000	-1.121581000
N	2.144083000	-1.274030000	-2.519336000
N	0.411170000	-2.021096000	0.714836000
N	-1.702781000	-0.312447000	-1.479126000
N	-2.793909000	0.426290000	-1.040842000
Pt	0.114347000	0.741201000	-1.227663000
C	0.379450000	1.648888000	2.258261000
C	1.347439000	2.283551000	-0.901818000
C	2.722601000	2.372142000	-1.108616000
H	3.256461000	1.515608000	-1.505549000
C	3.406680000	3.547476000	-0.812083000
H	4.478267000	3.602629000	-0.983112000
C	2.728406000	4.653342000	-0.302331000
H	3.268443000	5.563635000	-0.063155000
C	1.357885000	4.589360000	-0.099227000
H	0.835144000	5.449440000	0.306867000
C	0.658263000	3.421109000	-0.397937000
C	-0.791997000	3.287719000	-0.216973000
C	-1.702575000	4.220993000	0.244711000
H	-1.368608000	5.195375000	0.575790000

5.2 Coordinates of all optimised structures

C	-3.054502000	3.880606000	0.280772000
H	-3.778258000	4.603976000	0.640305000
C	1.564016000	-3.894940000	-0.156318000
H	2.469923000	-4.382291000	-0.476328000
C	1.562653000	-2.595782000	0.304605000
C	3.631930000	0.124911000	1.007565000
H	3.678594000	1.131196000	1.396076000
C	4.639699000	-0.683093000	0.423123000
C	6.004066000	-0.488245000	0.164330000
H	6.490881000	0.435515000	0.458633000
C	6.694704000	-1.491467000	-0.476614000
H	7.750290000	-1.371380000	-0.695266000
C	6.037689000	-2.674232000	-0.870845000
H	6.599807000	-3.438260000	-1.397834000
C	4.696545000	-2.889143000	-0.624746000
H	4.220796000	-3.790240000	-0.980601000
C	3.995944000	-1.879454000	0.044407000
N	0.326336000	2.687184000	2.779711000
N	-1.254327000	2.064306000	-0.589475000
N	2.486476000	-0.510611000	0.998831000
N	2.678713000	-1.759403000	0.440638000
Pt	0.416655000	-0.135546000	1.408655000

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Pt-9 trimer S_0

C	-0.834953000	-0.759064000	2.952273000
C	4.190127000	-0.108473000	0.928188000
C	5.087959000	0.955784000	0.856502000
H	5.403136000	1.313822000	-0.117170000
C	5.561164000	1.573257000	2.011405000
H	6.255534000	2.404204000	1.927008000
C	5.141989000	1.147795000	3.269116000
H	5.510269000	1.636452000	4.165702000
C	4.254276000	0.084621000	3.373232000
H	3.933854000	-0.252916000	4.354793000
C	3.785635000	-0.548501000	2.222070000
C	2.845648000	-1.681606000	2.267624000
C	2.233194000	-2.260146000	3.371343000
H	2.421381000	-1.884247000	4.368216000
C	1.324881000	-3.290672000	3.168406000
H	0.801892000	-3.714476000	4.017980000
C	0.807105000	1.030152000	-2.692834000

5.2 Coordinates of all optimised structures

H	1.428801000	1.835174000	-3.044596000
C	0.655747000	0.758427000	-1.340507000
C	1.470775000	1.962310000	1.825166000
H	1.301164000	1.863326000	2.886835000
C	2.295761000	2.866634000	1.107423000
C	3.144342000	3.912676000	1.492058000
H	3.248786000	4.178518000	2.538479000
C	3.855619000	4.562331000	0.508949000
H	4.526740000	5.373991000	0.769172000
C	3.751157000	4.157239000	-0.837337000
H	4.358658000	4.654938000	-1.585931000
C	2.918577000	3.133903000	-1.241409000
H	2.922675000	2.803739000	-2.268276000
C	2.160128000	2.505072000	-0.247673000
N	-1.088323000	-0.863727000	4.085159000
N	2.554086000	-2.167193000	1.040682000
N	0.863130000	1.151456000	1.001409000
N	1.247254000	1.470443000	-0.285916000
Pt	-0.450460000	-0.514216000	1.036928000
C	-1.279343000	3.633975000	-1.431946000
C	-0.754168000	4.180307000	-2.603861000
H	-1.066408000	3.770137000	-3.558286000
C	0.152425000	5.236653000	-2.560699000
H	0.546378000	5.642789000	-3.488245000
C	0.561326000	5.775762000	-1.343400000
H	1.277992000	6.589797000	-1.315564000
C	0.057478000	5.255530000	-0.160571000
C	-0.853182000	4.198568000	-0.194027000
C	-1.400132000	3.585978000	1.027084000
C	-1.161863000	3.922378000	2.355453000
H	-0.510967000	4.750982000	2.603798000
C	-1.772130000	3.171667000	3.353922000
H	-1.595503000	3.418650000	4.395530000
N	-2.222725000	2.547576000	0.766794000
C	3.962373000	-0.074189000	-2.048617000
C	-1.603152000	-1.998033000	0.349539000
C	-2.336676000	-2.961728000	1.041738000
H	-2.319720000	-2.955189000	2.126670000
C	-3.113118000	-3.900438000	0.364733000
H	-3.686292000	-4.629842000	0.930250000
C	-3.178642000	-3.894575000	-1.024909000
H	-3.786666000	-4.624063000	-1.550595000

5.2 Coordinates of all optimised structures

C	-2.448012000	-2.956023000	-1.743752000
H	-2.487213000	-2.962143000	-2.828720000
C	-1.659919000	-2.021628000	-1.074404000
C	-0.843711000	-1.016003000	-1.781885000
C	-0.730328000	-0.791204000	-3.143285000
H	-1.311028000	-1.367341000	-3.851039000
C	0.095832000	0.239271000	-3.582664000
H	0.165484000	0.451146000	-4.643211000
C	1.029697000	-3.759073000	1.893562000
H	0.268348000	-4.506552000	1.746265000
C	1.680057000	-3.152569000	0.829109000
C	0.897438000	-4.167434000	-2.566553000
C	0.255659000	-4.971121000	-3.516983000
H	0.377589000	-4.772117000	-4.576421000
C	-0.521886000	-6.015226000	-3.066602000
H	-1.032948000	-6.657885000	-3.775130000
C	-0.653982000	-6.264445000	-1.687214000
H	-1.266746000	-7.097628000	-1.359036000
C	-0.034869000	-5.483177000	-0.732166000
H	-0.161218000	-5.710169000	0.315218000
C	0.741290000	-4.411041000	-1.186710000
N	4.249883000	0.594017000	-2.958249000
N	-0.136184000	-0.235603000	-0.936161000
N	2.102473000	-2.635415000	-1.465825000
N	1.485157000	-3.447916000	-0.533177000
Pt	3.315513000	-1.150286000	-0.532811000
C	-2.882125000	1.721236000	-3.079010000
C	-2.603634000	2.098220000	3.055569000
H	-3.053854000	1.514099000	3.840297000
C	-2.801822000	1.805018000	1.713196000
C	-4.625075000	-0.262225000	-0.416263000
C	-5.004408000	-0.916925000	0.787486000
C	-5.824472000	-2.015413000	1.071187000
H	-6.359492000	-2.520290000	0.274326000
C	-5.906278000	-2.443036000	2.377831000
H	-6.529992000	-3.292941000	2.633659000
C	-5.158871000	-1.805816000	3.388007000
H	-5.203685000	-2.192775000	4.400811000
C	-4.347641000	-0.717197000	3.134381000
H	-3.722717000	-0.312466000	3.916115000
C	-4.300014000	-0.257057000	1.813041000
N	-3.050641000	1.418268000	-4.190730000

5.2 Coordinates of all optimised structures

N	-3.799147000	0.714821000	-0.160649000
N	-3.600026000	0.768700000	1.206440000
Pt	-2.567884000	2.128803000	-1.180278000
C	1.765074000	-3.044361000	-2.657738000
H	2.148296000	-2.524282000	-3.523664000
H	-4.896984000	-0.471853000	-1.440576000
H	0.390724000	5.665682000	0.788004000

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C	0.855059000	0.799939000	2.959965000
C	-4.171312000	0.121637000	0.919229000
C	-5.069166000	-0.942053000	0.841046000
H	-5.381545000	-1.296449000	-0.134895000
C	-5.546190000	-1.563401000	1.992364000
H	-6.240654000	-2.393797000	1.902990000
C	-5.130709000	-1.142479000	3.252747000
H	-5.501738000	-1.634134000	4.146549000
C	-4.243200000	-0.079691000	3.363257000
H	-3.925644000	0.254273000	4.346934000
C	-3.771082000	0.557435000	2.215848000
C	-2.831994000	1.691214000	2.268320000
C	-2.224959000	2.267329000	3.376053000
H	-2.415914000	1.887944000	4.371058000
C	-1.317676000	3.300105000	3.179781000
H	-0.798292000	3.721721000	4.032561000
C	-0.776772000	-0.961328000	-2.699633000
H	-1.408121000	-1.755573000	-3.058632000
C	-0.616303000	-0.706825000	-1.345005000
C	-1.435436000	-1.927253000	1.814904000
H	-1.267139000	-1.833151000	2.877015000
C	-2.257144000	-2.830570000	1.091166000
C	-3.108930000	-3.875753000	1.470579000
H	-3.218515000	-4.141812000	2.516388000
C	-3.817020000	-4.523776000	0.483964000
H	-4.491553000	-5.333701000	0.740813000
C	-3.704602000	-4.118650000	-0.861529000
H	-4.310657000	-4.613299000	-1.613454000
C	-2.868756000	-3.095202000	-1.260830000
H	-2.868481000	-2.764896000	-2.287550000
C	-2.115060000	-2.467646000	-0.262850000
N	1.091787000	0.916572000	4.095159000

5.2 Coordinates of all optimised structures

N	-2.536010000	2.180361000	1.043831000
N	-0.824960000	-1.114927000	0.995292000
N	-1.199700000	-1.433596000	-0.294722000
Pt	0.486678000	0.552237000	1.042235000
C	1.214421000	-3.658686000	-1.434407000
C	0.658198000	-4.200119000	-2.598142000
H	0.970240000	-3.789526000	-3.552475000
C	-0.259505000	-5.231822000	-2.549122000
H	-0.678992000	-5.642371000	-3.461159000
C	-0.662344000	-5.783644000	-1.281142000
H	-1.389681000	-6.589771000	-1.271207000
C	-0.167566000	-5.317427000	-0.106321000
C	0.774771000	-4.234882000	-0.109686000
C	1.307197000	-3.647002000	1.037226000
C	1.067452000	-3.945973000	2.409575000
H	0.401673000	-4.759498000	2.672567000
C	1.677370000	-3.197825000	3.379514000
H	1.501568000	-3.414528000	4.427218000
N	2.178475000	-2.591778000	0.758141000
C	-3.934810000	0.097938000	-2.056873000
C	1.642525000	2.037493000	0.365022000
C	2.377759000	2.995044000	1.063932000
H	2.358457000	2.982346000	2.148676000
C	3.159590000	3.933641000	0.393464000
H	3.734766000	4.657617000	0.963908000
C	3.228068000	3.935279000	-0.996222000
H	3.840417000	4.665095000	-1.516423000
C	2.496334000	3.002976000	-1.721495000
H	2.537920000	3.015014000	-2.806388000
C	1.703772000	2.067513000	-1.058595000
C	0.887253000	1.067295000	-1.773132000
C	0.770137000	0.854976000	-3.136498000
H	1.348781000	1.438107000	-3.840361000
C	-0.064200000	-0.165357000	-3.583872000
H	-0.140103000	-0.365050000	-4.646300000
C	-1.018329000	3.772703000	1.907546000
H	-0.258260000	4.522542000	1.766007000
C	-1.662385000	3.167458000	0.838594000
C	-0.871436000	4.195043000	-2.551651000
C	-0.226841000	5.001696000	-3.497727000
H	-0.349160000	4.808619000	-4.558228000
C	0.554057000	6.040764000	-3.041712000

H	1.067455000	6.685470000	-3.746685000
C	0.687419000	6.281604000	-1.660920000
H	1.304130000	7.109992000	-1.328092000
C	0.065369000	5.497570000	-0.710145000
H	0.194686000	5.717251000	0.338373000
C	-0.715247000	4.431080000	-1.170450000
N	-4.217899000	-0.568417000	-2.969305000
N	0.179303000	0.280715000	-0.933095000
N	-2.079609000	2.659552000	-1.459347000
N	-1.461995000	3.466572000	-0.522242000
Pt	-3.292961000	1.169224000	-0.535459000
C	2.810705000	-1.802168000	-3.086873000
C	2.545485000	-2.123207000	3.048789000
H	3.001628000	-1.531534000	3.823835000
C	2.751829000	-1.854262000	1.702866000
C	4.584779000	0.176680000	-0.458463000
C	4.979101000	0.840328000	0.733029000
C	5.813988000	1.933684000	0.998863000
H	6.344868000	2.426469000	0.191728000
C	5.915832000	2.370309000	2.300166000
H	6.551088000	3.215882000	2.541744000
C	5.173985000	1.748461000	3.325321000
H	5.235501000	2.143156000	4.334284000
C	4.349436000	0.666754000	3.090711000
H	3.732673000	0.271124000	3.883362000
C	4.280489000	0.195546000	1.773389000
N	2.974582000	-1.505472000	-4.200657000
N	3.753644000	-0.793021000	-0.181420000
N	3.567751000	-0.830552000	1.187700000
Pt	2.502509000	-2.207058000	-1.177005000
C	-1.740982000	3.074115000	-2.649018000
H	-2.124459000	2.559002000	-3.517774000
H	4.848029000	0.372105000	-1.487740000
H	-0.502706000	-5.739776000	0.834373000

5.2.10 Pt-10

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Pt-10 monomer S_0

C	1.686317000	1.749614000	7.127950000
C	1.067581000	2.878366000	9.808879000
C	0.788875000	1.586115000	10.255118000

5.2 Coordinates of all optimised structures

H	0.885702000	0.759011000	9.560969000
C	0.392329000	1.353937000	11.568739000
H	0.181293000	0.338124000	11.890647000
C	0.262272000	2.404468000	12.475796000
H	-0.047631000	2.211942000	13.497752000
C	0.531728000	3.699757000	12.063920000
H	0.430597000	4.518993000	12.770395000
C	0.930432000	3.944597000	10.747782000
C	1.229376000	5.291884000	10.252412000
C	1.184594000	6.512794000	10.927203000
H	0.896153000	6.549975000	11.969861000
C	1.513909000	7.676229000	10.245676000
H	1.480796000	8.628044000	10.765230000
C	1.888196000	7.651334000	8.902459000
H	2.145003000	8.557892000	8.370362000
C	1.912950000	6.409926000	8.290575000
C	2.612588000	4.977435000	5.194804000
H	2.669958000	4.072142000	4.608048000
C	2.873152000	6.316008000	4.833056000
H	3.187710000	6.688410000	3.870803000
C	2.641127000	7.047717000	5.968299000
H	2.713986000	8.107220000	6.156997000
N	1.717539000	0.722570000	6.581976000
N	1.595868000	5.300321000	8.951252000
N	2.248026000	4.900217000	6.459549000
N	2.263971000	6.177954000	6.942956000
Pt	1.647581000	3.505024000	8.008254000

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C	1.682099000	1.755631000	7.137122000
C	1.077163000	2.877750000	9.778783000
C	0.797077000	1.568800000	10.224590000
H	0.899829000	0.757352000	9.513018000
C	0.406287000	1.323174000	11.517089000
H	0.192995000	0.313818000	11.850673000
C	0.275531000	2.411192000	12.446460000
H	-0.035093000	2.191369000	13.463980000
C	0.528304000	3.706132000	12.092441000
H	0.418671000	4.501541000	12.822130000
C	0.935146000	4.007762000	10.765944000
C	1.222022000	5.300891000	10.289005000

5.2 Coordinates of all optimised structures

C	1.185220000	6.554017000	10.951832000
H	0.898703000	6.598470000	11.996320000
C	1.510098000	7.699808000	10.274679000
H	1.482330000	8.657947000	10.780380000
C	1.889248000	7.656443000	8.899198000
H	2.146093000	8.559014000	8.360694000
C	1.911722000	6.419812000	8.295761000
C	2.602322000	4.954810000	5.205302000
H	2.654505000	4.041324000	4.631132000
C	2.865748000	6.284350000	4.828403000
H	3.179228000	6.644703000	3.861272000
C	2.638468000	7.032377000	5.957975000
H	2.715244000	8.093737000	6.134279000
N	1.712148000	0.727982000	6.593203000
N	1.597965000	5.301775000	8.945492000
N	2.240001000	4.897730000	6.475493000
N	2.261622000	6.181188000	6.942892000
Pt	1.641279000	3.517123000	8.032175000

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Pt-10 dimer S_0

C	1.943209000	3.027195000	-0.362679000
C	-1.940562000	-3.028070000	0.362420000
C	2.983638000	0.368737000	0.469359000
C	-2.983728000	-0.370338000	-0.468597000
C	4.172902000	0.656100000	-0.203633000
C	-4.172539000	-0.658926000	0.204669000
H	4.279910000	1.620354000	-0.689417000
H	-4.278572000	-1.623409000	0.690210000
C	5.218344000	-0.264297000	-0.242359000
C	-5.218802000	0.260525000	0.243898000
H	6.136680000	-0.010284000	-0.764722000
H	-6.136810000	0.005512000	0.766352000
C	5.103478000	-1.499024000	0.390588000
C	-5.105204000	1.495535000	-0.388733000
H	5.924161000	-2.208862000	0.364138000
H	-5.926518000	2.204627000	-0.361880000
C	3.932190000	-1.815642000	1.065409000
C	-3.934282000	1.813466000	-1.063558000
H	3.843148000	-2.777786000	1.562088000
H	-3.846096000	2.775952000	-1.559732000
C	2.879841000	-0.901875000	1.108869000

5.2 Coordinates of all optimised structures

C	-2.881146000	0.900633000	-1.107582000
C	1.609987000	-1.184958000	1.799591000
C	-1.611692000	1.185024000	-1.798500000
C	1.196836000	-2.347327000	2.442929000
C	-1.199200000	2.348342000	-2.440563000
H	1.848091000	-3.210994000	2.488045000
H	-1.850777000	3.211836000	-2.484316000
C	-0.074939000	-2.396932000	3.001435000
C	0.072443000	2.399159000	-2.999245000
H	-0.426628000	-3.312540000	3.461160000
H	0.423892000	3.315587000	-3.457521000
C	-0.932148000	-1.302306000	2.942830000
C	0.930112000	1.304812000	-2.942268000
H	-1.937155000	-1.357116000	3.337729000
H	1.935022000	1.360624000	-3.337257000
C	-0.465438000	-0.182879000	2.282168000
C	0.464137000	0.184475000	-2.282650000
C	-1.526456000	2.998077000	1.349184000
C	1.527963000	-2.995916000	-1.350989000
H	-1.283844000	3.922038000	0.845094000
H	1.286317000	-3.920122000	-0.846891000
C	-2.705651000	2.604271000	2.009984000
C	2.706753000	-2.600838000	-2.011774000
H	-3.619060000	3.165722000	2.120606000
H	3.620675000	-3.161408000	-2.122554000
C	-2.463295000	1.328073000	2.450026000
C	2.463131000	-1.324809000	-2.451559000
H	-3.091356000	0.627197000	2.975214000
H	3.090495000	-0.623217000	-2.976622000
N	2.257080000	3.908483000	-1.056154000
N	-2.252808000	-3.909603000	1.056318000
N	0.753962000	-0.143696000	1.750488000
N	-0.755125000	0.144162000	-1.750702000
N	-0.626681000	2.032411000	1.387475000
N	0.627252000	-2.031126000	-1.389020000
N	-1.200774000	1.002244000	2.075677000
N	1.200291000	-1.000273000	-2.077125000
Pt	1.346963000	1.489638000	0.709424000
Pt	-1.346364000	-1.489941000	-0.709942000

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5.2 Coordinates of all optimised structures

C	2.850988000	2.198985000	-0.307764000
C	-0.845047000	-3.419061000	0.134315000
C	2.293656000	-0.260171000	1.211826000
C	-2.597511000	-1.115266000	-0.509569000
C	3.627402000	-0.645797000	1.003001000
C	-3.647257000	-1.809123000	0.124492000
H	4.314095000	0.069088000	0.564943000
H	-3.457518000	-2.813088000	0.487257000
C	4.057005000	-1.917202000	1.332399000
C	-4.886916000	-1.223832000	0.302126000
H	5.093486000	-2.196547000	1.167065000
H	-5.680761000	-1.774208000	0.797947000
C	3.158510000	-2.870912000	1.853574000
C	-5.129350000	0.079891000	-0.160252000
H	3.504974000	-3.875600000	2.073530000
H	-6.108166000	0.529121000	-0.022533000
C	1.844396000	-2.533809000	2.093820000
C	-4.131162000	0.792082000	-0.803762000
H	1.151650000	-3.277371000	2.470999000
H	-4.333577000	1.795722000	-1.166588000
C	1.398509000	-1.231564000	1.813212000
C	-2.872207000	0.216556000	-1.004395000
C	0.060276000	-0.767346000	2.112784000
C	-1.773676000	0.889259000	-1.678713000
C	-0.995314000	-1.446582000	2.720279000
C	-1.712220000	2.159518000	-2.230006000
H	-0.872133000	-2.480407000	3.014684000
H	-2.588315000	2.796424000	-2.225416000
C	-2.220093000	-0.811250000	2.871398000
C	-0.505957000	2.627124000	-2.751300000
H	-3.053425000	-1.337597000	3.320034000
H	-0.444966000	3.625139000	-3.168881000
C	-2.416997000	0.481456000	2.362174000
C	0.643365000	1.822015000	-2.724017000
H	-3.392897000	0.948640000	2.387202000
H	1.601808000	2.192580000	-3.061268000
C	-1.326812000	1.123167000	1.807326000
C	0.515129000	0.551702000	-2.203856000
C	-0.478828000	4.090804000	0.196939000
C	2.355125000	-2.359805000	-1.687758000
H	0.296875000	4.669504000	-0.281286000
H	2.358879000	-3.369639000	-1.306231000

5.2 Coordinates of all optimised structures

C	-1.834938000	4.392112000	0.416806000
C	3.385017000	-1.598836000	-2.261915000
H	-2.363210000	5.289885000	0.135760000
H	4.406239000	-1.899349000	-2.434671000
C	-2.353021000	3.296428000	1.064358000
C	2.833017000	-0.366768000	-2.526535000
H	-3.348662000	3.082432000	1.418843000
H	3.269383000	0.545121000	-2.902309000
N	3.651278000	2.574690000	-1.066584000
N	-0.886107000	-4.399086000	0.760720000
N	-0.124022000	0.543660000	1.750309000
N	-0.653463000	0.098476000	-1.727441000
N	-0.184874000	2.894643000	0.684924000
N	1.243051000	-1.643515000	-1.608652000
N	-1.342598000	2.404129000	1.228467000
N	1.536734000	-0.415217000	-2.138104000
Pt	1.390894000	1.436656000	0.782274000
Pt	-0.734538000	-1.680079000	-0.806383000

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C	0.326575000	-1.709686000	2.530696000
C	3.298766000	2.185734000	-1.911019000
C	-0.695049000	-2.227048000	-0.209181000
C	4.237510000	0.953510000	0.617693000
C	-0.854565000	-3.570783000	0.127594000
C	4.777894000	2.185588000	0.985411000
H	-0.503348000	-3.914545000	1.094688000
H	4.774421000	2.996252000	0.265328000
C	-1.478608000	-4.462806000	-0.744461000
C	5.296093000	2.390299000	2.261887000
H	-1.596282000	-5.504008000	-0.454776000
H	5.710533000	3.360379000	2.522621000
C	-1.981206000	-4.024283000	-1.966911000
C	5.283756000	1.368621000	3.208340000
H	-2.496471000	-4.712562000	-2.629310000
H	5.682446000	1.536227000	4.203726000
C	-1.826351000	-2.692975000	-2.336395000
C	4.770872000	0.124471000	2.866076000
H	-2.240617000	-2.342149000	-3.275431000
H	4.771135000	-0.676766000	3.599243000
C	-1.166555000	-1.808203000	-1.486749000

5.2 Coordinates of all optimised structures

C	4.262645000	-0.092730000	1.585186000
C	-0.896010000	-0.407685000	-1.855017000
C	3.709343000	-1.388302000	1.162534000
C	-1.204646000	0.265709000	-3.030880000
C	3.542716000	-2.554305000	1.901523000
H	-1.781719000	-0.222372000	-3.804515000
H	3.836347000	-2.592135000	2.942023000
C	-0.810776000	1.592008000	-3.165647000
C	2.944332000	-3.654696000	1.301610000
H	-1.048139000	2.129303000	-4.077190000
H	2.787292000	-4.557453000	1.881126000
C	-0.138470000	2.260730000	-2.147074000
C	2.501974000	-3.608683000	-0.016856000
H	0.177051000	3.288567000	-2.252190000
H	1.988350000	-4.444371000	-0.471380000
C	0.105147000	1.541483000	-0.992689000
C	2.688463000	-2.416350000	-0.692008000
C	1.475336000	1.960507000	2.177125000
C	1.934787000	-0.948391000	-3.757754000
H	1.725555000	1.507349000	3.124696000
H	1.971937000	-0.060098000	-4.370621000
C	1.722330000	3.261612000	1.701119000
C	1.397626000	-2.221190000	-4.033321000
H	0.905052000	-2.548154000	-4.935324000
C	1.233675000	3.278957000	0.418169000
C	1.606067000	-2.955511000	-2.893264000
H	1.264865000	4.036340000	-0.347991000
H	1.320670000	-3.963412000	-2.636675000
N	0.356486000	-2.262090000	3.556857000
N	3.115624000	3.257687000	-2.329133000
N	-0.238591000	0.260927000	-0.886401000
N	3.293994000	-1.379084000	-0.122342000
N	0.863459000	1.238905000	1.257274000
N	2.438075000	-0.910026000	-2.537964000
N	0.710895000	2.054020000	0.171096000
N	2.243762000	-2.153192000	-2.004858000
Pt	0.124299000	-0.730893000	0.836468000
Pt	3.376605000	0.397173000	-1.095373000
C	-4.323715000	-0.177676000	-1.944603000
C	-3.297981000	2.263267000	-0.603191000
C	-3.550381000	2.976806000	-1.776450000
H	-4.044197000	2.471563000	-2.599378000

5.2 Coordinates of all optimised structures

C	-3.161175000	4.306528000	-1.907674000
H	-3.366418000	4.836388000	-2.833819000
C	-2.505108000	4.964393000	-0.868581000
H	-2.197745000	5.999226000	-0.980607000
C	-2.258390000	4.290128000	0.318747000
H	-1.753536000	4.803009000	1.132597000
C	-2.655156000	2.959261000	0.462367000
C	-2.405472000	2.186898000	1.689909000
C	-1.786932000	2.585542000	2.870290000
H	-1.433613000	3.601807000	2.987604000
C	-1.599832000	1.650251000	3.883145000
H	-1.103020000	1.947419000	4.800761000
C	-2.010686000	0.329940000	3.738071000
H	-1.807373000	-0.415101000	4.494462000
C	-2.632993000	0.001918000	2.544396000
C	-4.017275000	-2.746721000	0.929186000
H	-4.497003000	-3.128818000	0.040555000
C	-3.603482000	-3.415411000	2.099474000
H	-3.700928000	-4.465221000	2.326025000
C	-3.007281000	-2.456131000	2.876122000
H	-2.489309000	-2.522361000	3.819618000
N	-4.603952000	-0.515005000	-3.023516000
N	-2.832942000	0.909582000	1.592872000
N	-3.705574000	-1.467573000	0.991192000
N	-3.091343000	-1.281714000	2.199123000
Pt	-3.660239000	0.348601000	-0.168381000
H	2.236063000	4.060323000	2.211419000

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C	0.354470000	-1.730827000	2.532153000
C	3.243434000	2.177837000	-1.961604000
C	-0.680065000	-2.233342000	-0.179329000
C	4.255347000	0.988811000	0.553087000
C	-0.781455000	-3.590025000	0.103879000
C	4.793521000	2.231377000	0.887790000
H	-0.389656000	-3.949994000	1.049526000
H	4.761043000	3.031491000	0.156760000
C	-1.400824000	-4.475840000	-0.774097000
C	5.346705000	2.459116000	2.145414000
H	-1.479577000	-5.529394000	-0.525205000
H	5.758679000	3.436819000	2.380291000

5.2 Coordinates of all optimised structures

C	-2.022043000	-3.989436000	-1.979217000
C	5.372559000	1.450931000	3.106062000
H	-2.573610000	-4.687395000	-2.602533000
H	5.798662000	1.636572000	4.086790000
C	-1.955931000	-2.683822000	-2.335370000
C	4.862197000	0.197410000	2.796515000
H	-2.478980000	-2.314619000	-3.209647000
H	4.891615000	-0.593091000	3.540722000
C	-1.209999000	-1.757514000	-1.509731000
C	4.318772000	-0.042960000	1.534225000
C	-0.925326000	-0.448888000	-1.860545000
C	3.766825000	-1.349789000	1.146169000
C	-1.244956000	0.271141000	-3.053551000
C	3.639421000	-2.508497000	1.904272000
H	-1.822570000	-0.215308000	-3.828510000
H	3.967596000	-2.529647000	2.934918000
C	-0.859798000	1.578912000	-3.177394000
C	3.041807000	-3.626000000	1.335687000
H	-1.102827000	2.132519000	-4.076781000
H	2.918742000	-4.524626000	1.929672000
C	-0.177653000	2.249532000	-2.132098000
C	2.559083000	-3.602694000	0.030964000
H	0.129005000	3.280508000	-2.227695000
H	2.048085000	-4.452730000	-0.399472000
C	0.081151000	1.521644000	-0.978648000
C	2.703742000	-2.414971000	-0.662730000
C	1.493896000	1.934656000	2.171911000
C	1.829555000	-0.996579000	-3.719913000
H	1.757886000	1.476521000	3.113288000
H	1.833253000	-0.115733000	-4.344287000
C	1.731091000	3.238448000	1.700203000
C	1.296810000	-2.278457000	-3.959951000
H	0.775140000	-2.621953000	-4.839115000
C	1.221685000	3.264687000	0.424875000
C	1.549721000	-2.994466000	-2.817525000
H	1.238538000	4.027662000	-0.336206000
H	1.288788000	-4.003009000	-2.538771000
N	0.409093000	-2.283172000	3.557089000
N	3.053236000	3.246443000	-2.385030000
N	-0.242067000	0.247922000	-0.862348000
N	3.311476000	-1.362440000	-0.125262000
N	0.868146000	1.218286000	1.256080000

N	2.373205000	-0.936527000	-2.518273000
N	0.696033000	2.041938000	0.177085000
N	2.208836000	-2.172718000	-1.961519000
Pt	0.119164000	-0.748215000	0.835713000
Pt	3.349460000	0.400735000	-1.125473000
C	-4.329956000	-0.177407000	-1.916820000
C	-3.301805000	2.268623000	-0.577993000
C	-3.562304000	2.983016000	-1.748899000
H	-4.054155000	2.476777000	-2.572038000
C	-3.182696000	4.315762000	-1.877482000
H	-3.393888000	4.846289000	-2.801843000
C	-2.528641000	4.975743000	-0.838444000
H	-2.229478000	6.013157000	-0.948666000
C	-2.271607000	4.299717000	0.345491000
H	-1.767224000	4.813777000	1.158886000
C	-2.657465000	2.965268000	0.486152000
C	-2.395053000	2.190614000	1.708824000
C	-1.767619000	2.588556000	2.885029000
H	-1.416037000	3.605530000	3.001135000
C	-1.568717000	1.652087000	3.894188000
H	-1.064536000	1.948815000	4.807901000
C	-1.977136000	0.330744000	3.749774000
H	-1.765686000	-0.415214000	4.503110000
C	-2.608885000	0.003766000	2.560974000
C	-3.975561000	-2.752934000	0.943815000
H	-4.457369000	-3.135616000	0.056424000
C	-3.546223000	-3.422177000	2.107635000
H	-3.628415000	-4.474287000	2.329422000
C	-2.959843000	-2.458338000	2.886602000
H	-2.436096000	-2.522926000	3.827005000
N	-4.619669000	-0.525902000	-2.989801000
N	-2.819337000	0.911970000	1.612316000
N	-3.680934000	-1.469527000	1.010983000
N	-3.064904000	-1.281672000	2.217145000
Pt	-3.651072000	0.350831000	-0.146580000
H	2.250811000	4.034897000	2.208040000

5.2.11 Pt-11

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H	3.837853000	-0.608182000	2.048444000
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5.2 Coordinates of all optimised structures

C	-3.644629000	-1.641079000	0.498473000
C	-4.311529000	-2.853570000	0.634468000
H	-5.369519000	-2.860492000	0.883085000
C	-3.633532000	-4.058168000	0.463999000
H	-4.153995000	-5.004845000	0.569882000
C	-2.277381000	-4.036332000	0.181615000
H	-1.742947000	-4.976922000	0.086351000
C	-1.606350000	-2.816792000	0.049813000
C	-0.154694000	-2.750902000	-0.172096000
C	0.652254000	-3.832112000	-0.489506000
H	0.225831000	-4.819180000	-0.607165000
C	2.005908000	-3.613344000	-0.689561000
H	2.657682000	-4.436642000	-0.964155000
C	2.541705000	-2.348518000	-0.548344000
H	3.595973000	-2.195224000	-0.710139000
C	1.694122000	1.281212000	0.200512000
C	2.541612000	2.348682000	0.548232000
H	3.595891000	2.195453000	0.710009000
C	2.005754000	3.613482000	0.689440000
H	2.657494000	4.436818000	0.964004000
C	0.652085000	3.832179000	0.489417000
H	0.225613000	4.819225000	0.607077000
C	-0.154814000	2.750923000	0.172042000
H	-1.743170000	4.976865000	-0.086396000
C	4.398921000	-0.343043000	1.158173000
C	5.789193000	-0.343197000	1.156045000
H	6.329215000	-0.610109000	2.058595000
C	6.484659000	0.000023000	0.000097000
Pt	-1.056153000	-0.000012000	-0.000011000
N	0.383485000	1.502622000	0.044967000
N	0.383546000	-1.502578000	-0.045011000
N	2.266213000	0.000060000	-0.000018000
C	-1.606480000	2.816742000	-0.049824000
C	-2.277569000	4.036251000	-0.181620000
C	-3.633733000	4.058024000	-0.463947000
H	-4.154241000	5.004676000	-0.569827000
C	-4.311686000	2.853394000	-0.634364000
H	-5.369687000	2.860265000	-0.882935000
C	-3.644727000	1.640934000	-0.498377000
H	-4.194323000	0.722257000	-0.664108000
C	-2.283917000	1.576867000	-0.178127000
C	-2.283836000	-1.576948000	0.178165000

5.2 Coordinates of all optimised structures

H	-4.194257000	-0.722427000	0.664243000
C	1.694167000	-1.281103000	-0.200584000
C	5.789264000	0.343253000	-1.155892000
H	6.329342000	0.610153000	-2.058412000
C	4.398993000	0.343124000	-1.158098000
H	3.837980000	0.608273000	-2.048401000
C	3.710670000	0.000054000	0.000020000
H	7.569881000	0.000013000	0.000127000

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H	3.845788000	0.462946000	-2.095366000
C	-3.676997000	1.613706000	-0.421035000
C	-4.358384000	2.820288000	-0.527932000
H	-5.424040000	2.819463000	-0.741292000
C	-3.684250000	4.029709000	-0.374789000
H	-4.215282000	4.972696000	-0.458351000
C	-2.319631000	4.017601000	-0.139633000
H	-1.791827000	4.962869000	-0.057561000
C	-1.632307000	2.803465000	-0.035481000
C	-0.173874000	2.752663000	0.137139000
C	0.632399000	3.852797000	0.386751000
H	0.200669000	4.838991000	0.489062000
C	1.995563000	3.655837000	0.528593000
H	2.649542000	4.495865000	0.740243000
C	2.541295000	2.392632000	0.408063000
H	3.604156000	2.260241000	0.523058000
C	1.699179000	-1.278218000	-0.147654000
C	2.568091000	-2.364888000	-0.382364000
H	3.627183000	-2.215303000	-0.503495000
C	2.044643000	-3.672054000	-0.460086000
H	2.726143000	-4.500088000	-0.623594000
C	0.706535000	-3.888015000	-0.324921000
H	0.294805000	-4.888161000	-0.368061000
C	-0.160202000	-2.775147000	-0.128723000
H	-1.822352000	-4.992737000	-0.319048000
C	4.405452000	0.275692000	-1.184743000
C	5.795929000	0.283436000	-1.178845000
H	6.337587000	0.478847000	-2.098604000
C	6.489194000	0.038751000	0.002952000
Pt	-1.055744000	-0.011788000	-0.010368000
N	0.389996000	-1.473809000	-0.046381000

5.2 Coordinates of all optimised structures

N	0.375216000	1.506355000	0.029046000
N	2.271112000	0.019026000	-0.009592000
C	-1.545379000	-2.833860000	-0.014621000
C	-2.306007000	-4.057527000	-0.060148000
C	-3.622032000	-4.041524000	0.271580000
H	-4.186365000	-4.970023000	0.269552000
C	-4.289208000	-2.825477000	0.642725000
H	-5.333954000	-2.859301000	0.933000000
C	-3.608630000	-1.623526000	0.593601000
H	-4.129952000	-0.709691000	0.852052000
C	-2.267690000	-1.542576000	0.196239000
C	-2.305423000	1.559599000	-0.145595000
H	-4.224037000	0.691355000	-0.575834000
C	1.695615000	1.300298000	0.143746000
C	5.791578000	-0.214058000	1.180915000
H	6.330094000	-0.405812000	2.103285000
C	4.401500000	-0.221653000	1.178773000
H	3.838495000	-0.419349000	2.085107000
C	3.715155000	0.023935000	-0.005024000
H	7.574443000	0.044283000	0.006095000

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H	2.761600000	2.299346000	0.146620000
C	-4.778485000	0.999392000	-0.893776000
C	-5.601099000	1.736371000	-1.738795000
H	-6.439234000	1.252067000	-2.233520000
C	-5.353344000	3.089243000	-1.960440000
H	-5.992613000	3.667742000	-2.620014000
C	-4.265675000	3.685982000	-1.342440000
H	-4.050871000	4.730484000	-1.546792000
C	-3.436322000	2.940647000	-0.499694000
C	-2.211010000	3.512390000	0.080490000
C	-1.878262000	4.854938000	0.059676000
H	-2.550289000	5.581066000	-0.377279000
C	-0.674702000	5.247839000	0.624474000
H	-0.388919000	6.294838000	0.630888000
C	0.173264000	4.314617000	1.181759000
H	1.108666000	4.632155000	1.611495000
C	0.563433000	0.641324000	2.024015000
C	1.706121000	-0.067269000	2.448743000
H	2.676690000	0.399801000	2.458457000

5.2 Coordinates of all optimised structures

C	1.579444000	-1.383115000	2.830371000
H	2.462618000	-1.932468000	3.136607000
C	0.340843000	-2.011541000	2.795055000
H	0.237798000	-3.048794000	3.085064000
C	-0.748166000	-1.295931000	2.333733000
H	-1.771065000	-3.618654000	3.368872000
C	2.974109000	2.647729000	1.147545000
C	4.228768000	3.131520000	1.499073000
H	5.011930000	3.163003000	0.749141000
C	4.473848000	3.542597000	2.806189000
H	-1.254484000	-8.203601000	-0.692544000
Pt	-2.264345000	0.737591000	0.919354000
N	-0.610115000	0.004231000	1.942476000
N	-1.376809000	2.598194000	0.654141000
N	0.689245000	2.017558000	1.747865000
C	-2.113837000	-1.828909000	2.202840000
C	-2.487959000	-3.041771000	2.790441000
C	-3.787622000	-3.508862000	2.666267000
H	-4.077732000	-4.449443000	3.124521000
C	-4.719472000	-2.736891000	1.977143000
H	-5.747987000	-3.078488000	1.894347000
C	-4.351977000	-1.517263000	1.418462000
H	-5.114910000	-0.920972000	0.933479000
C	-3.042842000	-1.024505000	1.493639000
C	-3.682945000	1.570021000	-0.234605000
H	-4.976836000	-0.058811000	-0.770820000
C	-0.201512000	2.958049000	1.183744000
C	3.465611000	3.466108000	3.764281000
H	3.655978000	3.786449000	4.783647000
C	2.212601000	2.971461000	3.419012000
H	1.416674000	2.892598000	4.152881000
C	1.978904000	2.564851000	2.110523000
H	0.985380000	-5.008595000	-2.500508000
C	4.389036000	1.366182000	-1.791227000
C	5.743564000	1.558557000	-1.540295000
H	6.267362000	2.384702000	-2.014519000
C	6.434249000	0.695454000	-0.691951000
H	7.488951000	0.848511000	-0.485958000
C	5.766773000	-0.387875000	-0.142874000
H	6.320053000	-1.085120000	0.479056000
C	4.409385000	-0.590470000	-0.411140000
C	3.697459000	-1.796175000	0.043123000

5.2 Coordinates of all optimised structures

C	4.239038000	-2.781823000	0.851025000
H	5.244646000	-2.685984000	1.238003000
C	3.465394000	-3.895292000	1.150236000
H	3.860184000	-4.679683000	1.788440000
C	2.188881000	-4.014778000	0.644980000
H	1.594592000	-4.881392000	0.884958000
C	-0.528968000	-2.239926000	-1.312417000
C	-1.816502000	-2.696267000	-1.636573000
H	-2.127170000	-3.702216000	-1.412476000
C	-2.703613000	-1.833107000	-2.246125000
H	-3.702410000	-2.182108000	-2.486756000
C	-2.328727000	-0.534678000	-2.540167000
H	-3.023228000	0.148665000	-3.005813000
C	-1.056782000	-0.117555000	-2.190597000
H	-2.378309000	2.074758000	-3.169707000
C	0.335469000	-5.385918000	-1.717370000
C	-0.087322000	-6.711067000	-1.709207000
H	0.233685000	-7.383325000	-2.498276000
C	-0.922392000	-7.170317000	-0.695373000
Pt	1.727927000	-0.191348000	-1.363863000
N	-0.185455000	-0.975882000	-1.586628000
N	2.425942000	-1.918632000	-0.440720000
N	0.381762000	-3.156235000	-0.719319000
C	-0.528719000	1.233645000	-2.427346000
C	-1.337349000	2.256585000	-2.926255000
C	-0.831466000	3.539726000	-3.069932000
H	-1.468545000	4.335211000	-3.443780000
C	0.483019000	3.797105000	-2.697514000
H	0.883071000	4.804443000	-2.778846000
C	1.291646000	2.771687000	-2.215377000
H	2.306574000	3.016150000	-1.926197000
C	0.829267000	1.458291000	-2.083745000
C	3.665249000	0.318720000	-1.206572000
H	3.883939000	2.043266000	-2.469821000
C	1.672026000	-2.991386000	-0.174898000
C	-1.337191000	-6.302382000	0.311474000
H	-1.998655000	-6.650781000	1.098243000
C	-0.912149000	-4.979500000	0.310759000
H	-1.247326000	-4.282820000	1.070276000
C	-0.076826000	-4.528623000	-0.705104000
H	5.453837000	3.919414000	3.081985000

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H	-3.981829000	0.777824000	-0.105367000
C	2.955975000	-3.022873000	1.013952000
C	3.256814000	-4.315069000	0.597138000
H	4.293720000	-4.604092000	0.443944000
C	2.238849000	-5.234351000	0.359630000
H	2.469008000	-6.242439000	0.028194000
C	0.920865000	-4.843496000	0.540901000
H	0.125962000	-5.550697000	0.325892000
C	0.621973000	-3.548543000	0.973053000
C	-0.766825000	-3.093365000	1.149325000
C	-1.874886000	-3.919135000	1.104166000
H	-1.766959000	-4.976309000	0.907646000
C	-3.123355000	-3.363242000	1.330686000
H	-4.011211000	-3.986597000	1.309027000
C	-3.252803000	-2.014297000	1.581321000
H	-4.230959000	-1.598631000	1.754340000
C	-1.339307000	1.244387000	1.915904000
C	-1.832021000	2.563780000	1.919980000
H	-2.879217000	2.765476000	1.767598000
C	-0.954539000	3.610169000	2.100299000
H	-1.332670000	4.627209000	2.092850000
C	0.400667000	3.370717000	2.273511000
H	1.094056000	4.189316000	2.407746000
C	0.851730000	2.065037000	2.230279000
H	3.041873000	3.623742000	2.813866000
C	-4.417549000	0.877850000	0.880942000
C	-5.733532000	1.290353000	1.050627000
H	-6.333945000	1.516793000	0.175435000
C	-6.266343000	1.417988000	2.330438000
H	7.338736000	2.653095000	-1.850736000
Pt	0.906556000	-0.795241000	1.740745000
N	-0.024362000	1.033820000	2.047457000
N	-0.902908000	-1.758791000	1.396425000
N	-2.264747000	0.182599000	1.827223000
C	2.252505000	1.649230000	2.416473000
C	3.255814000	2.561011000	2.755439000
C	4.538075000	2.117226000	3.043850000
H	5.314202000	2.828114000	3.309893000
C	4.803188000	0.750002000	3.023841000
H	5.791680000	0.385802000	3.291780000

5.2 Coordinates of all optimised structures

C	3.809305000	-0.154511000	2.661357000
H	4.042806000	-1.211932000	2.668358000
C	2.519034000	0.258930000	2.302981000
C	1.640981000	-2.596901000	1.233533000
H	3.770197000	-2.321165000	1.144539000
C	-2.103876000	-1.202447000	1.593811000
C	-5.480286000	1.133173000	3.443875000
H	-5.893161000	1.231038000	4.442756000
C	-4.161746000	0.722467000	3.279238000
H	-3.531511000	0.498393000	4.134050000
C	-3.639952000	0.598829000	1.997324000
H	3.514256000	1.986828000	-3.700907000
C	-3.735434000	1.157857000	-2.574160000
C	-4.727515000	2.120220000	-2.529440000
H	-5.708179000	1.928213000	-2.951956000
C	-4.470115000	3.377367000	-1.881530000
H	-5.279735000	4.096898000	-1.792786000
C	-3.241265000	3.690410000	-1.394999000
H	-3.068120000	4.652789000	-0.925155000
C	-2.155377000	2.755476000	-1.555060000
C	-0.814669000	3.064319000	-1.345175000
C	-0.297501000	4.353916000	-1.050018000
H	-0.967862000	5.202496000	-0.997208000
C	1.046979000	4.496848000	-0.856961000
H	1.471027000	5.467139000	-0.619063000
C	1.905571000	3.391376000	-0.965467000
H	2.958942000	3.518079000	-0.783777000
C	2.091524000	-0.311780000	-1.789685000
C	3.222844000	-1.119889000	-1.996902000
H	4.216641000	-0.709940000	-1.937120000
C	3.056712000	-2.461334000	-2.269862000
H	3.932369000	-3.084470000	-2.416987000
C	1.789844000	-3.014259000	-2.345428000
H	1.658545000	-4.066797000	-2.549238000
C	0.698932000	-2.193967000	-2.125355000
H	-0.267639000	-4.740914000	-2.463713000
C	4.167395000	1.954716000	-2.834566000
C	5.490914000	2.372358000	-2.915061000
H	5.885136000	2.735660000	-3.858710000
C	6.305897000	2.325092000	-1.786838000
Pt	-0.918374000	0.191406000	-1.773952000
N	0.872296000	-0.866656000	-1.853889000

N	0.068463000	1.973283000	-1.472524000
N	2.286470000	1.065941000	-1.546766000
C	-0.702425000	-2.643969000	-2.166696000
C	-1.040089000	-3.989385000	-2.338437000
C	-2.368586000	-4.385257000	-2.328148000
H	-2.626604000	-5.431028000	-2.464728000
C	-3.361334000	-3.431680000	-2.121180000
H	-4.404717000	-3.734720000	-2.085491000
C	-3.025484000	-2.093703000	-1.946974000
H	-3.818235000	-1.379781000	-1.754692000
C	-1.698943000	-1.651029000	-1.991996000
C	-2.470468000	1.367311000	-2.001549000
H	-3.948777000	0.194643000	-3.022897000
C	1.379157000	2.128594000	-1.320505000
C	5.796185000	1.858069000	-0.578941000
H	6.420326000	1.820564000	0.307845000
C	4.473481000	1.438401000	-0.493031000
H	4.062137000	1.066622000	0.435704000
C	3.668261000	1.490988000	-1.622907000
H	-7.294435000	1.740623000	2.461770000

5.2.12 Pt-12

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Pt	1.413866000	-0.462338000	0.157615000
P	2.087933000	1.039377000	-1.537007000
P	1.052748000	-2.201151000	-1.401898000
P	0.729634000	-1.960740000	1.851124000
P	1.836548000	1.256024000	1.723864000
O	2.430074000	0.478788000	-2.913300000
O	3.321264000	1.975372000	-1.091528000
H	3.276133000	2.116921000	-0.080977000
O	-0.552684000	-2.297971000	-1.790329000
O	1.748331000	-1.970514000	-2.833394000
H	2.015550000	-0.991316000	-2.946095000
O	1.431948000	-3.611728000	-0.950016000
O	1.241970000	-3.467407000	1.599809000
H	1.324391000	-3.621330000	0.593439000
O	1.052851000	-1.617813000	3.301463000
O	0.908721000	2.194915000	-1.717346000
O	3.047755000	2.147397000	1.448146000

5.2 Coordinates of all optimised structures

O	1.966966000	0.755338000	3.246566000
H	1.581305000	-0.185055000	3.346537000
Pt	-1.414044000	0.462237000	-0.157884000
P	-2.088424000	-1.039656000	1.536621000
O	-2.431433000	-0.478789000	2.912620000
O	-3.321217000	-1.976061000	1.090598000
H	-3.276602000	-2.116358000	0.079893000
O	-0.909003000	-2.194775000	1.717925000
P	-0.729881000	1.960956000	-1.851034000
P	-1.053356000	2.200820000	1.401964000
O	0.551477000	2.295982000	1.793305000
P	-1.836435000	-1.256077000	-1.724165000
O	-3.049080000	-2.145955000	-1.449658000
O	-1.963535000	-0.755989000	-3.247252000
H	-1.579695000	0.185251000	-3.346383000
O	-1.751427000	1.970532000	2.832328000
H	-2.018546000	0.991266000	2.944655000
O	-1.430665000	3.611793000	0.949699000
O	-1.242290000	3.467519000	-1.599457000
H	-1.324400000	3.621139000	-0.592956000
O	-1.053043000	1.618192000	-3.301454000

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Pt	-0.051874000	1.383930000	0.029934000
P	1.610604000	1.473538000	1.727352000
P	-1.756128000	1.378193000	1.683373000
P	-1.723941000	1.468748000	-1.643328000
P	1.691851000	1.588646000	-1.566695000
O	1.170302000	1.817993000	3.145109000
O	2.831449000	2.457089000	1.359577000
H	2.917406000	2.527307000	0.344404000
O	-1.935727000	-0.139953000	2.317796000
O	-1.339633000	2.179243000	3.016405000
H	-0.337714000	2.056531000	3.168112000
O	-3.139273000	1.882364000	1.283844000
O	-3.009598000	2.335670000	-1.213351000
H	-3.161004000	2.196010000	-0.212309000
O	-1.319889000	1.933466000	-3.038418000
O	2.422500000	0.028833000	1.773910000
O	2.836346000	2.531061000	-1.193386000
O	1.205970000	1.975102000	-3.045467000

5.2 Coordinates of all optimised structures

H	0.184742000	1.951554000	-3.116119000
Pt	0.039350000	-1.382887000	-0.052578000
P	-1.615493000	-1.463203000	-1.742114000
O	-1.175172000	-1.798223000	-3.162870000
O	-2.835758000	-2.449650000	-1.381932000
H	-3.004828000	-2.382500000	-0.376949000
O	-2.435814000	-0.022861000	-1.776582000
P	1.692975000	-1.454619000	1.653387000
P	1.802396000	-1.391513000	-1.640739000
O	2.431797000	0.128947000	-1.799606000
P	-1.667712000	-1.597560000	1.582079000
O	-3.016173000	-2.155788000	1.139383000
O	-1.205630000	-2.462523000	2.859944000
H	-0.220184000	-2.266914000	3.038141000
O	1.352331000	-1.747207000	-3.138950000
H	0.332305000	-1.755724000	-3.222869000
O	3.011628000	-2.263927000	-1.304201000
O	2.969471000	-2.349496000	1.248488000
H	3.072925000	-2.351814000	0.232695000
O	1.265245000	-1.891305000	3.049230000