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Turning Ligands on Their Side: Computational Investigation into the Binding of N2O and N2 in Transition Metal Complexes

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By

COLE B. DONALD, B.S. Chemistry

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TURNING LIGANDS ON THEIR SIDE: COMPUTATIONAL INVESTIGATION INTO THE BINDING OF N_2O AND N_2 IN TRANSITION METAL COMPLEXES

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Abstract

Common greenhouse gas nitrous oxide (N_2O) is a thermodynamically potent and environmentally benign oxidant, making it a desirable target for metal center activation. Unfortunately, N_2O is a poor ligand for transition metals due to its weak σ-donating and π-accepting properties; as a result, few transition metal complexes capable of interacting with N_2O have been found. As the primary source of all nitrogen in organisms, abundant gas dinitrogen (N_2) is a crucially important tiny molecule and an essential part of daily existence. However, due to its inertness, it has limited practical uses in this form. Through biological and commercial nitrogen fixation processes, one of the most inert substances, N_2, is transformed into an accessible nitrogen supply, such as NH_3, that may be incorporated into all nitrogen-containing biomolecules. Using computational chemistry, this work will highlight the energy differences between new potential N_2O binding modes. Insights into the comparison between the κ-N and κ-O versus the newly reported η^2-NN and η^2-NO binding modes will be discussed. Through the utilization of density functional theory, a low valent cobalt complex possessing N_2O in a η^2-NO coordination is reported. These binding mode comparisons can be employed to develop N_2O as a "green" oxidant given the limited understanding of the coordination of N_2O to metal centers. This study will emphasize the energy disparities between putative N_2 binding mechanisms using computational chemistry. It will also be explored how the κ-N binding mode compares to

the infrequently reported η^2-NN binding mode. Given the partial knowledge of N_2's coordination to metal centers, these binding mode comparisons can be used to improve understanding of N_2's activation.

Dedication

This thesis work is completely dedicated too and would not have been feasible without the unwavering support of my dear parents, Nancy S. Walker-Copland and Therion C. Donald. They have consistently offered their moral, spiritual, and emotional support; and have been a great source of inspiration.

To Dad

Therion C. Donald

6/14/1975 – 7/4/2022

Though you never got to see this

you’re in every page

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Abbreviations

N_2 dinitrogen

CH_4 Methane

CO_2 Carbon dioxide

EPA Environmental Protection Agency

N_2O Nitrous oxide

GWP Global warming potential

CFCs Chlorofluorocarbons

NH_3 Ammonia

FeMo-co FeMo-cofactor

CP^{iPr}_3 Tris(phosphino)alkyl

DFT Density functional theory

MO Molecular orbital

DSC Differential Scanning Calorimetry

ECP Effective core potential

Cp Cyclopentadienyl

Cp* Pentamethylcyclopentadienyl

L Ligands

M Metal

Chapter 1

Small Molecule Activation Through Metal Binding

Since small molecule activation has a significant impact on environmental protection, industrial catalysis, medicine, and biology, chemistry research has long concentrated on the sustainable conversion of molecules like dinitrogen (N_2), methane (CH_4), and carbon dioxide (CO_2) into other compounds. The catalytic activation of generally inert small molecules has maintained a constant presence in the research community from the standpoint of inorganic chemistry.[1]

Although molecules like N_2, and CO_2 are plentiful and easily available, the majority of them are inert, and their chemical transformations are difficult from a thermodynamic and mechanistic standpoint. Such changes frequently occur along difficult-to-control reaction pathways that combine multielectron redox reactions with proton transfers. For the design and development of effective catalysts, it is imperative to understand how these small molecules bind to metals to determine their modes of activation and solve the mechanistic foundation, which provides a significant task for the chemistry community.[1]

Bioinorganic chemistry has been a major source of inspiration for the subject since nature mostly employs metal ions to activate these relatively inert compounds and control their reactivity. But now that industrial processes of small-molecule transformations that encompass enzymatic processes, homogeneous organometallic chemistry, and

heterogeneous catalysis have been developed, attempts to further the catalysis efficiency, utilization, and waste elimination of these processes are currently under investigation.[2]

1.1 Green Oxidation

The current most crucial chemical process for giving a molecule functionality is oxidation. Almost every area of the chemical and related industries will continue to depend on oxidation, particularly selective oxidation, even if hydrocarbons remain our main feedstock. The US Environmental Protection Agency (EPA) launched the Green Chemistry Movement in the early 1990s to persuade businesses and academics to utilize chemistry to stop pollution. The objective of "green chemistry" was to "advance novel chemical technologies that decrease or eliminate the use or creation of hazardous compounds in the design, manufacture, and usage of chemical goods," to be more precise.[5] The employment of metallic oxidants, such as permanganate, is one particularly dangerous and harmful way of oxidation that has a long history in the chemistry of oxidation. The design of cleaner oxidation processes depends critically on the supply of oxygen. The most appealing option is frequently air or oxygen, and hydrogen peroxide, which produces just water as a byproduct, is a good second choice.[4]

Current oxidation chemistry is at a turning point, particularly as it relates to industrial operations. Commodity oxidations generate many megatons of products with a market value of tens of billions of dollars. Due to their high prices and environmental implications, reagents like permanganate and chromate have lost their appeal. The creation of greener

and more effective oxidative processes depends on an understanding of the interactions between metal ions and oxidants.[6]

1.2 Why is N_2O an Attractive Oxidant?

The greatest stratospheric ozone-depleting gas and the third most important anthropogenic greenhouse gas is nitrous oxide (N_2O).[7] Due to its long atmospheric lifespan of approximately 114 years, N_2O, in particular, has a global warming potential (GWP) that is almost 300 times greater than that of CO_2 and depletes the ozone layer at the same time, much like chlorofluorocarbons (CFCs). Therefore, knowledge of its causes and management could significantly aid in the stability of the planet's climate.[8] A third of N_2O production is emitted by industrial sources, including the manufacturing of nitric acid and nylon, as well as from soils, particularly those that have had fertilizer treatment.[5] Agricultural operations account for 4.1 Mt N_2O/yr, or 66 percent of all gross anthropogenic emissions, making them by far the greatest source of N_2O emissions. Agricultural N_2O emissions are mostly caused by manure, synthetic fertilizers, and crop leftovers.[9] Forest fires, burning of crop residues, and burning of biomass for cooking and heating are the main sources of N_2O emissions from biomass. As of 2015, biomass-derived N_2O emissions amount to 0.7 Mt N_2ON/yr, or 11% of all gross anthropogenic emissions (Figure 1.1).[8]

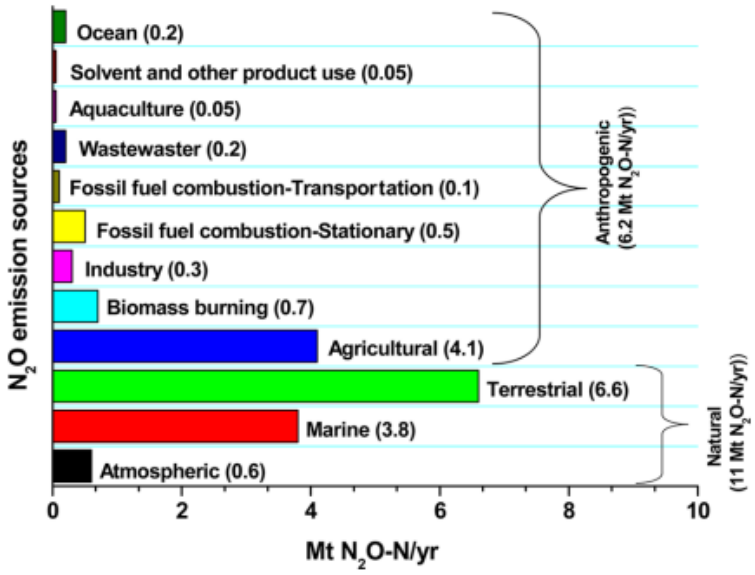

Figure 1.1 N_2O emissions, both natural and man-made, in Mt N_2O/yr (megatons of N_2O in equivalent nitrogen units per year)[8]

Understanding the reactivity of N_2O with metal centers in several contexts, such as the gas phase, solid substrates, enzymes, and soluble complexes in solution has been one key research goal motivated by these metal-promoted reactions. Few transition metal complexes are reported that are capable of interacting with N_2O.[10–16] Given the potential applications of N_2O as an oxidant for O-atom transfer reactions, broadening the scope of this class of compounds would allow for the development of a variety of useful processes.[17] Complexes that can activate nitrous oxide for useful processes are extremely rare. Since N_2O is a potent thermodynamic oxidant and can act as an oxygen-atom transfer reagent giving the ideal chemical byproduct of N_2, it is a preferred oxidant for chemical synthesis. Since N_2O has a strong oxidizing potential and doesn't present the same explosive risks as O_2, it is also considered to be an effective substitute for O_2. Future discoveries could

advance our knowledge of N_2O's known binding properties and open the door to more research on this peculiar and potentially important oxidant.

1.3 Why is N_2 Reduction Important?

N_2 is the main element that makes up the Earth's atmosphere. Thereby, N_2 is a continually abundant molecule around the globe, yet in this form, it has few practical applications due to its inertness. However, molecular nitrogen is the initial source of all nitrogen in organisms, making it a crucial component of life's chemistry. This rich supply of nitrogen is only useful to a few species. Nitrogen fixation is the method by which N_2 is added to biological systems; it involves the nitrogenase enzyme, which has a metal-sulfido cluster in the active site.[18]

One of the most inert compounds, N_2, is converted into a bioavailable nitrogen source, such as NH_3, that may be integrated into all nitrogen-containing biomolecules through biological and industrial nitrogen fixation processes. As a result, nitrogen fixation has drawn close attention from the chemical community for decades since it is crucial to maintaining life on this planet. Currently, it is still not understood mechanistically how the nitrogenase enzymes encourage the biological reduction of nitrogen in the presence of ambient conditions.[6]

The energy-intensive Haber-Bosch process, which produces millions of tons of ammonia each year straight from three equivalents of dinitrogen and dihydrogen molecules with the help of a metal catalyst, is perhaps the most well-known and oldest of these processes.[19] (Equation 1.1). This reaction is exothermic and thermodynamically favorable at ambient

conditions although the process is not kinetically favorable since the feedstock gases must be compressed to several hundred atmospheres to promote ammonia synthesis at the high temperatures currently required.[18] By raising the temperature at which the reaction is conducted, the kinetics can be overcome, but the process's thermodynamics becomes less favorable.

Equation 1.1[18]

$$N_2(g) + 3H_2(g) \underset{\sim 200\ atm, 400°C}{\Longleftrightarrow} 2NH_3(g)$$

In 1886, it was first shown that some species could fix atmospheric N_2. The biological fixation of N_2 by nitrogenase-type enzymes is performed at ambient temperature and pressure, although using a reaction that needs an electron supply, in contrast to the high-temperature commercial procedures mentioned above (Equation 1.2).[18] It takes approximately sixteen equivalents of MgATP to complete this reaction, which is energy-intensive. Even while there have been several attempts to identify new processes that are superior to the Haber-Bosch and nitrogenase processes, none of them have been successful, but future discoveries could advance our knowledge of dinitrogen's reduction by nitrogenase and lead to a greener alternative to the century-old Haber-Bosch process.

Equation 1.2[18]

$$N_2 + 8H^+ + 8e^- + 16MgATP \xrightarrow{nitrogenase} 2NH_3 + H_2 + 16MgADP + 16PO_4^{3-}$$

1.4 Coordination Chemistry

Many ligands in coordination and organometallic chemistry act as π-acceptors, π-donors, or both in addition to being σ-donors. The π^*-orbitals of several ligands that are involved in π-bonding with transition metal centers are unoccupied.[20] As demonstrated for a carbonyl ligand in Figure 1.2,[21] these π*-orbitals overlap with filled metal d-orbitals to produce a lower energy-filled bonding orbital and a higher energy empty antibonding orbital. The interaction between the metal and the ligand π*-orbital results in the shift of electron density from the metal onto the carbonyl ligand because the filled bonding molecular orbital has some carbonyl π* character. This results in the reduction of the CO bond order and more than makes up for the lone pair on carbon's contribution of electron density to the metal. Back bonding is the term for this transfer of electron density from the metal to the π*-orbital. In short, the carbonyl group's infrared stretching frequency is lower than that of free CO, while the C-O distance in carbonyl ligands is longer than that of free

CO. These demonstrate how the back bonding interaction reduces the order of the C-O bonds.[20,21]

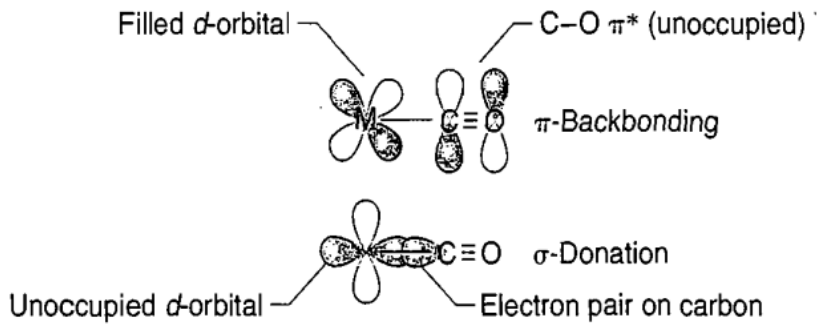

Figure 1.2 Carbonyl ligand orbital interactions involved in binding with a transition metal.[21]

Olefins are a significant type of π-acceptor ligands that attach to the metal via their π-bonds. The orbital interactions in a metal-olefin complex are depicted in Figure 1.3,[21] which was initially created by Chatt, Dewar, and Duncanson.[20,21] The interactions between the olefin ligand and the metal during metal-olefin binding include both σ-donating and π-accepting interactions. One interaction includes the donation of electron density from the olefin's π-bonding orbital to a metal's open orbital. Since there is no nodal plane along this bond axis, coordination to the olefin's face results in the formation of one σ-bonding interaction. In the second interaction, an occupied orbital at the metal and the olefin's π-antibonding orbital overlap. The overlap between the metal's d-orbitals and the p-orbitals of two carbon atoms at the face of the π-system transpires instead of the overlap between the metal and the π-system of CO through the p-orbital of one atom at the end of the ligand. One nodal plane exists on the face of the π*-orbital of an olefin, and one nodal plane exists

along the bond axis in the orbital that results from the interaction of the filled orbital at the metal with the π*-orbital of the olefin. As a result, this interaction is regarded as a π-bond. The interaction of an olefin's π*-orbital with a full metal orbital results in a flow of electron density into the ligand's π*-orbital and lowers the bond order of the π-bond, similar to the interaction of CO's π*-orbital with a filled metal d-orbital. As a result, the coordination of the olefin in such a complex causes the carbon-carbon bond order to drop and the length of the C-C bond to increase relative to the free olefin. In addition, the olefin's substituents are twisted away from the metal, and hybridization at the olefinic carbons moves from sp^2 to sp^3.[20,21]

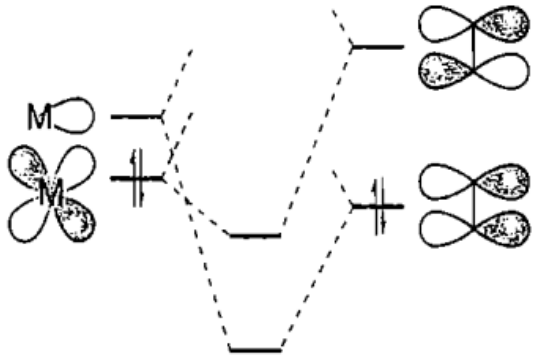

Figure 1.3 Orbital interactions of the olefin binding model by Chatt-Dewar-Duncanson[21]

Alkynes, like olefins, may act as an σ-donor, a π-acceptor, as well as a π-donor. Figure 1.4,[21] illustrates three interactions that can be used to explain the bonding of alkynes: σ-donation by one set of π-bonding orbitals, π-bonding by an orthogonal set of π-bonding orbitals, and π-back bonding into an alkyne's π* orbital.[20,21]

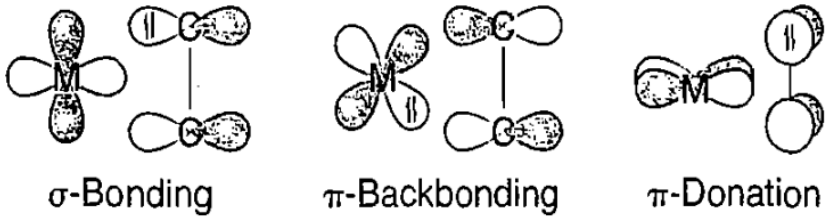

Figure 1.4 Metal-alkyne complexes exhibit σ-donation, π-acceptance, and π-donation[21]

In this research, the electronic and trans-influence characteristics of the metals and ligands are modified. The impact of a ligand on the length of the bond trans to it in the ground state of a complex is known as the *trans*-influence, which is a thermodynamic effect. One ligand, for instance, might have an impact on the length of the metal-ligand bond involving the ligand *trans* to it. Based on the respective σ-donor characteristics of the ligands, the ranking in Figure 1.5 forecasts the order for the trans influence.[20]

$$H^- > PR_3 > SCN^- > I^- \sim CH_3^- \sim CO \sim CN^- > Br^- > Cl^- > NH_3 > OH^-$$

Figure 1.5 Trans influence series[20]

Five isoelectronic hexacarbonyls are shown to have the following CO stretching frequencies in Table 1.1,[20] which illustrate how a complex's electronics affect the CO bond. These numbers can be contrasted with the free CO's 2143 cm^{-1} stretching frequency. From the table, it can be seen that $[Ti(CO)_6]^{2-}$ includes the most highly reduced metal, technically Ti(2-), which indicates that titanium has the greatest potential to back-donate electron density to CO and the least capacity to attract electrons. With $[Fe(CO)_6]^{2+}$, the formal charges on the metals go from -2 for $[Ti(CO)_6]^{2-}$ to +2. With the highest negative formal

charge, the titanium in $[Ti(CO)_6]^{2-}$ has the strongest propensity to donate to CO. The result is a high population of CO's π^* orbitals in $[Ti(CO)_6]^{2-}$ and a weakening of the CO bond. In general, the likelihood of the metal donating electrons to the π^* orbitals of CO increases with the negative charge on the organometallic species, and the energy of the CO stretching vibrations decreases.[20]

Table 1.1 CO stretching frequencies of a variety of hexacarbonyl complexes[20]

Complex	ν(CO), cm^{-1}
$[Ti(CO)_6]^{2-}$	1748
$[V(CO)_6]^{-}$	1859
$Cr(CO)_6$	2000
$[Mn(CO)_6]^{+}$	2100
$[Fe(CO)_6]^{2+}$	2204

1.5 Looking Ahead

The energy differences between putative new N_2O binding modes will be highlighted in Chapter 2 along with comparisons of the previously known κ-N and κ-O binding modes to the recently revealed η^2-NN and η^2-NO binding modes in order to gain a better understanding of how modifying the metal, whether it be through metal identity or ligand changes, relates to small molecule binding preferences. In Chapter 3, N_2 is discussed in relation to how it binds to and is activated by transition metal complexes to reduce the N_2 triple bond.

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Chapter 2

Computational Investigation of the Preferred Binding Modes of N_2O in Group 9 & 10 Metal Complexes

2.1 Introduction

Nitrous oxide (N_2O), a common greenhouse gas, is a thermodynamically powerful and ecologically friendly oxidant that makes it an appealing target for metal center activation.[1] N_2O is a notoriously poor ligand, and its coordination chemistry has been limited to a few terminal, end-on κ-N complexes despite its utility as an oxygen-atom transfer reagent for transition metals.[2] As a result, nitrous oxide is still being studied as a potentially "green" oxidant in inorganic and organometallic systems. Despite its attraction as an oxidant, N_2O's practical utility is limited by its high kinetic stability. Due to a high activation barrier (ca.59 kcal/mol), breaking down N_2O into its constituents, N_2 and O_2, requires considerable temperatures (400 °C) in the absence of catalysts.[3] In the presence of many transition-metal-based systems, however, N_2O has been well-reported as a highly efficient oxygen-atom transfer reagent.[4–6] Tolman's has reported multiple potential binding modes of N_2O to a single metal center (Figure 2.1).[6]

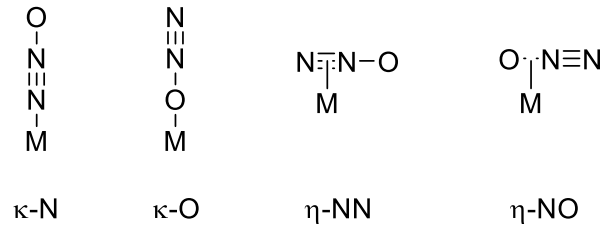


Figure 2.1 Potential monometallic N_2O binding

Characterized complexes of N_2O bond to transition metals are quite rare (Figure 2.2).[1,7–12] The Lehnert lab used vibrational spectroscopy and computational analysis to demonstrate that the first coordination compound with a N_2O unit, $[Ru(NH_3)_5(N_2O)]^{2+}$, reported by Taube [7], is a κ-N isomer.[9] James has also reported a more recent case of a ruthenium octahedral nitrogen-bound N_2O complex found by NMR at low temperatures.[10] X-ray crystallography, NMR spectroscopy, and computational chemistry have been used to describe two nitrogen-bound rhodium(I) pincer complexes.[11] X-ray crystallography and vibrational spectroscopy have also been used to characterize a nitrogen-bound copper (I) complex.[12] Another κ-N isomer of N_2O with a vanadium tris-pyrrolide system, which has been confirmed by X-ray crystallography, vibrational spectroscopy, and computational chemistry, has been reported by the Chang lab.[1] The N_2O binds to the metal through the

nitrogen atom in all of these characterized examples of transition metal complexes with N_2O attached to a terminal atom.

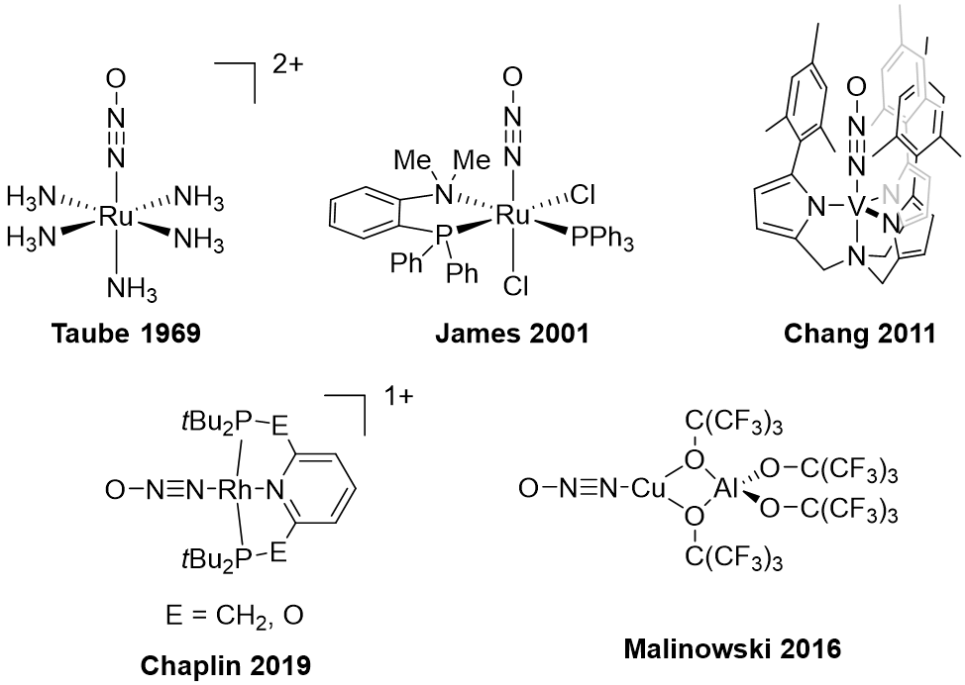


Figure 2.2 Characterized structures with an N_2O unit

The Long lab has reported an iron-based metal-organic framework that can bind N_2O. The N_2O unit has been discovered to bind in both the κ-N and κ-O isomers in this system, and the isomer distribution has been modeled at a 40 percent to 60 percent ratio using powder neutron diffraction.[13] Recent computational studies of this iron-based metal-organic framework have also suggested that organic molecules settling in the pores of the structure may modify the binding preference.[14]

In a previous study, the potential binding effects in a variety of group 8 metal complexes were investigated using density functional theory. Since the N_2O unit is a poor π-acceptor,

it was observed that it preferred to bind in a linear configuration through the terminal nitrogen atom. By changing the nature of the metal center as a π-donor, calculations revealed that the N_2O unit can prefer to bind through the oxygen atom, in which case this binding mode is a σ-donor ligand (Figure 2.3).[15]

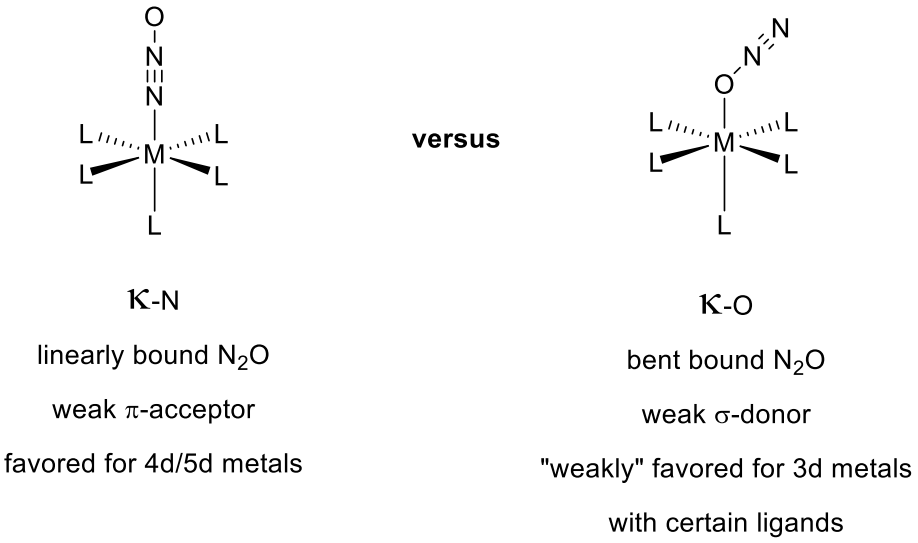


Figure 2.3 N_2O binding modes observed in previous work

In a recent and interesting study by the Roesler lab, a nickel complex possessing a η^2-NN bound N_2O unit was characterized by X-ray crystallography, IR, and solid-state NMR spectroscopy.[16] Also, the Figueroa lab has reported another η^2-NN coordination complex of N_2O with a mononuclear cobalt system that has been characterized by IR spectroscopy and computational chemistry (Figure 2.4).[2] The possible binding effects of a range of group 9 and 10 metal complexes are investigated using density functional theory in this study.

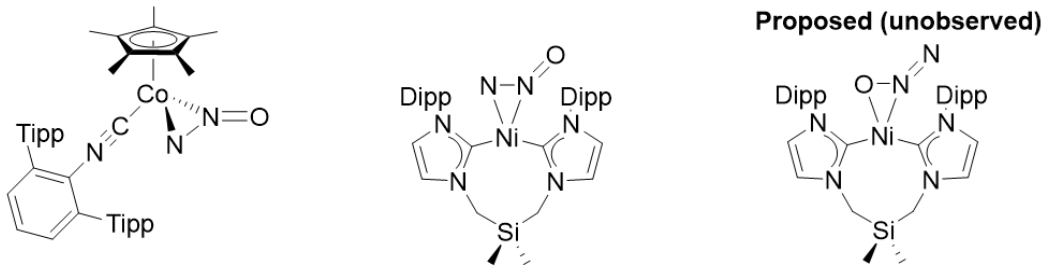


Figure 2.4 Characterized structures with π-bound N_2O unit

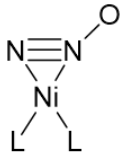
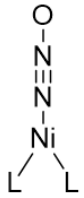
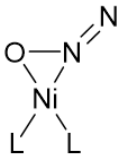
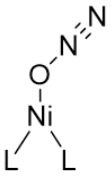
2.2 Computation Details

For all the calculations presented here, the Gaussian16 code was utilized.[17] The level of theory used was B3LYP/6-31G(d). Heavy metals used an effective core potential (ECP) basis set, specifically LANL2DZ. In the gas phase, all singlet spin states were assessed using restricted Kohn-Sham procedures, whereas triplets and quintets were assessed using unrestricted Kohn-Sham techniques. The electronic energy is corrected for enthalpy and entropy using unscaled vibrational frequencies at 1 atm and 298.15 K. By calculating structures with no imaginary frequencies, all stationary points are classified as minima.[15]

2.3 Results and Discussion

The possible binding of N_2O to the previously investigated pseudo-square planar Ni system by the Roselar lab was the first comparison made to better understand the binding of N_2O.[2] Since this approach has been used in the iron, osmium, and ruthenium systems previously studied,[15] the B3LYP/6-31G(d,p) was chosen as the suitable level of theory. With this system, the impact of altering ligands *cis* to the N_2O unit was investigated to determine the influence on binding preference. Interestingly, despite the Roselar lab's

proposal of η^2-NO as an intermediate, the η^2-NO binding mode could not be optimized without geometric restrictions of the N_2O unit in four of the five systems. The κ-O binding mode could not be successfully optimized as the structure favored the formation of a metal oxo. In the system with the CO-supporting ligand, all proposed N_2O binding mechanisms were optimized.[6] The η^2-NN bound N_2O unit is the energetically favored binding mode with the majority of the ligands, according to the data in Figure 2.5.

				
L=NHC	0.0 kcal/mol	+ 15.6 kcal/mol	IS	oxo
L=PMe_3	0.0 kcal/mol	+ 14.8 kcal/mol	IS	+ 38.1 kcal/mol
L=PH_3	0.0 kcal/mol	+ 8.9 kcal/mol	IS	+ 30.2 kcal/mol
L=CNMe	0.0 kcal/mol	+ 5.7 kcal/mol	IS	+ 22.3 kcal/mol
L=CO	+ 5.4 kcal/mol	0.0 kcal/mol	+ 18.4 kcal/mol	+ 12.5 kcal/mol

"oxo" represents the formation of a metal oxo due to NO bond breaking and "IS" represents an incorrect structure.

Figure 2.5 Ligand modification effect on binding energy in $[Ni(L)_2(N_2O)]$

As one progresses from an electron-rich to an electron-deficient metal system through donating supporting ligands, the relative energy difference between η^2-NN and κ-N decreases. This observation is supported by the vibrational frequencies of the κ-CO and η^2-C_2H_2 complexes of $[Ni(L)_2]$ as seen in Table 2.1. When the ligand *cis* to the N_2O unit

is substituted with CO, the binding preference favors the κ-N bound N_2O unit by 5.4 kcal/mol.

Table 2.1 C-O and C-C stretch vibrational frequencies (in cm^{-1}) for $[Ni(L)_2(CO)]$ and $[Ni(L)_2(CH)_2]$ complexes

Complex	**ν_{CO} (cm^{-1})**	**ν_{CC} (cm^{-1})**
$[NiC_{10}N_4H_{16}]$	2009.4	1652.2
$[Ni(PMe_3)_2]$	2036.0	1672.0
$[Ni(PH_3)_2]$	2071.0	1696.4
$[Ni(CNMe)_2]$[a]	2061.8	1709.4
$[Ni(CO)_2]$[b]	2100.0, 2102.1, 2189.0	1749.9

[a]The C-O stretch vibrational frequency for $[Ni(CNMe)_2(CO)]$ does not follow the trend as the structure breaks planarity. [b]The $[Ni(CO)_2(CO)]$ complex has three C-O stretch vibrational frequencies due to symmetry coupling.

In an attempt to get a better understanding of the preference between the η^2-NN and η^2-NO binding modes, the next system investigated was one similar to the Figueroa lab.[2] Of the proposed binding modes of N_2O by Tolman, all binding modes were optimized.[6] The η^2-NN isomer was calculated to be the most stable in the [CoCp*CNMe] system by 6.2 kcal/mol (Figure 2.6), which is consistent with the Figueroa lab observations in which the η^2-NN isomer was experimentally characterized and computationally shown to be the most stable isomer.[2]

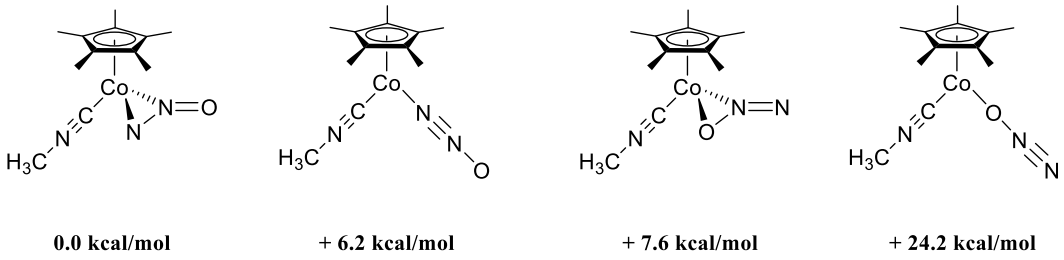
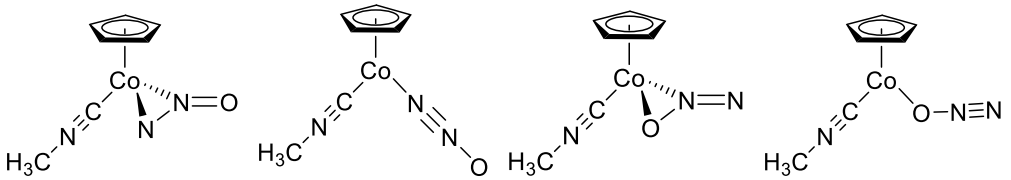


Figure 2.6 Ligand modification effect on binding in [Co(η^5-Cp*)(N_2O)]

The pentamethylcyclopentadienyl (Cp*) ligand was replaced with a cyclopentadienyl (Cp) ligand to see if the electronics of the system altered the η^2-NN or κ-N binding preference. The η^2-NN isomer was determined to be the most stable by 2.9 kcal/mol in the [CoCpCNMe] system, as shown in Figure 2.7, which is consistent with the previously examined system. The relative energy difference between the preferred binding mode and the subsequent mode diminishes when a supportive ligand is switched from an electron-rich Cp* to a more electron-deficient Cp. This is comparable to what was observed with the initial Ni system. To evaluate the ligand's influence on the preferred binding mode, the effects of altering the ligand *cis* to the N_2O unit were investigated. The η^2-NN bound N_2O unit is the energetically favored binding mode with the majority of the ligands, as shown by the data in Figure 2.7.



L=PMe_3	0.0 kcal/mol	+ 6.6 kcal/mol	+ 7.5 kcal/mol	+ 31.2 kcal/mol
L=PH_3	0.0 kcal/mol	+ 6.0 kcal/mol	+ 9.2 kcal/mol	+ 26.4 kcal/mol
L=CNMe	0.0 kcal/mol	+ 2.9 kcal/mol	+ 11.2 kcal/mol	+ 21.0 kcal/mol
L=CO	+ 3.3 kcal/mol	0.0 kcal/mol	+ 12.5 kcal/mol	+ 17.1 kcal/mol

Figure 2.7 Ligand modification effect on binding energy in [Co(η^5-Cp)(L)(N_2O)]

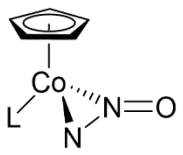
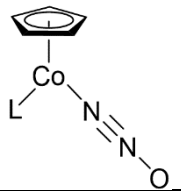
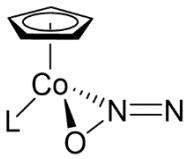
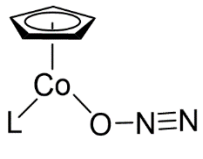
When the ligand *cis* to the N_2O unit is substituted with CO, however, the binding preference favors the κ-N bound N_2O unit by 3.3 kcal/mol. This is not unexpected considering CO is a strong π-acceptor that efficiently lowers the electron richness of the low valent Co metal center, giving favorability to the κ-N bound binding state. This observation is supported by the vibrational frequencies of the κ-CO and η^2-C_2H_2 complexes of [Co(η^5-Cp)(L)] as seen in Table 2.2, which follows a similar trend seen with the previously investigated Ni systems.

Table 2.2 C-O and C-C stretch vibrational frequencies (in cm^{-1}) for [Co(η^5-Cp)(L)(CO)] and [Co(η^5-Cp)(L)$(CH)_2$] complexes

Complex	ν_{CO} (cm^{-1})	ν_{CC} (cm^{-1})
[Co(η^5-Cp)(PMe_3)]	2032.4	1739.5
[Co(η^5-Cp)(PH_3)]	2049.2	1749.1
[Co(η^5-Cp)(CNMe)]	2062.5	1765.2
[Co(η^5-Cp)(CO)][a]	2071.2, 2117.6	1780.7

[a]The [Co(η^5-Cp)$(CO)_2$] complex has two C-O stretch vibrational frequencies due to symmetry coupling.

Several para-substituted pyridine ligands *cis* to the N_2O unit in the [CoCp] system were studied to determine the influence of preference for η^2-NN or κ-N binding with minimal impact from sterics. According to the results in Figure 2.8, the η^2-NN bound isomer is energetically preferred over the κ-N isomer, independent of the ligand identity. Because the structures formed a metal oxo complex, energy estimates for the O-bound isomers of the [Co(Cp)$(NMe)_2(N_2O)$] and [Co(Cp)$(NO)_2(N_2O)$] systems could not be determined without constraining the N_2O unit.

				
L= py(p-NMe)$_2$	0.0 kcal/mol	+ 9.7 kcal/mol	oxo	oxo
L=py	0.0 kcal/mol	+ 9.0 kcal/mol	oxo	+ 30.3 kcal/mol
L= py(p-NO)$_2$	0.0 kcal/mol	+ 5.3 kcal/mol	+ 6.6 kcal/mol	+ 21.6 kcal/mol

"oxo" represents the formation of a metal oxo due to NO bond breaking.

Figure 2.8 Para-substituted pyridine ligand modification effect on binding energy in [Co(η^5-Cp)(L)(N_2O)]

The metal center was then exchanged with other metals in the [[M]Cp(CNMe)(N_2O)] complexes to understand how it affected the binding preference (Figure 2.9). Interestingly with Ir and Rh, the preferred binding mode was calculated to be the κ-N isomer with a linear orientation.

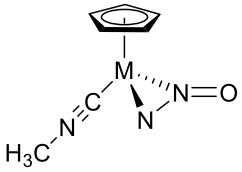
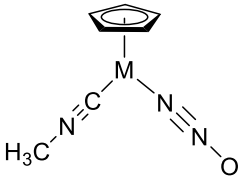
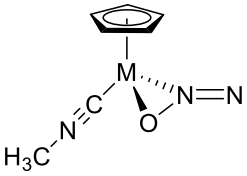
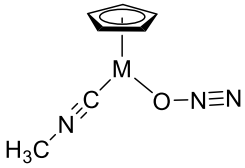
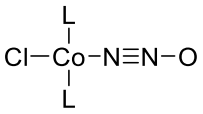
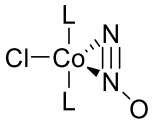
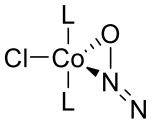
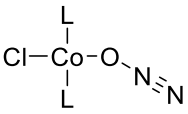
				
M=Co	0.0 kcal/mol	+ 2.9 kcal/mol	+ 11.2 kcal/mol	+ 21.0 kcal/mol
M-Rh	+ 6.0 kcal/mol	0.0 kcal/mol	+ 14.2 kcal/mol	+ 11.4 kcal/mol
M=Ir	+ 3.5 kcal/mol	0.0 kcal/mol	+ 14.9 kcal/mol	+ 16.2 kcal/mol

Figure 2.9 Metal identity modification effect on η-NN binding in [[M]CNMe(η^5-Cp)(N_2O)]

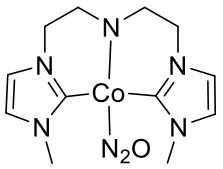
A series of square planar $[Co(L)_2Cl(N_2O)]$ complexes were investigated using a variety of ligands (L) in an effort to reduce the relative energy gap between the η^2-NN and η^2-NO binding modes using the observations made (Figure 2.10). Similar to the observations in the $[CoCp(L)_2(N_2O)]$ and $[Ni(L)_2(N_2O)$ systems, it is evident that the relative energy difference between η^2-NN and η^2-NO reduces as one moves from an electron-rich to an electron-deficient system. The κ-O binding modes for 4 out of the 5 systems investigated could not be obtained without geometric restrictions of the N_2O unit, as they originally optimized to the η^2-NO binding mode. These complexes are indicated by the symbol "IS". By continuing with a pseudo-square planar geometry, similar to the Figueroa lab system, and making the metal center more electron-rich, the relative energy difference between η^2-NN and η^2-NO binding modes was decreased. It should also be noted that the second most favored binding mode of N_2O is η^2-NO in both the $[Co(PH_3)_2(N_2O)Cl]$ and $[Co(PMe_3)_2(N_2O)Cl]$ systems, which has not been seen before. Previously, κ-N and η^2-NN have been the two most favored binding modes.

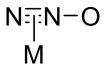
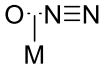
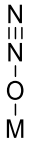
				
L=PMe_3	+ 7.8 kcal/mol	0.0 kcal/mol	+ 2.5 kcal/mol	IS
L=PH_3	+ 3.4 kcal/mol	0.0 kcal/mol	+ 3.1 kcal/mol	IS
L=CNMe	0.0 kcal/mol	+ 1.0 kcal/mol	+ 5.6 kcal/mol	IS
L=CO	0.0 kcal/mol	+ 9.1 kcal/mol	+ 13.5 kcal/mol	+ 12.7 kcal/mol

"IS" represents an incorrect structure.

Figure 2.10 Ligand identity modification effect on binding energy in [[Co](L)$_2$Cl(N_2O)]

In view of the decrease in the relative energy difference between not only η^2-NN and κ-N but also η^2-NN and η^2-NO by changing the geometry and electronics of the metal system, more attempts were made to locate a system in which η^2-NO was the favored binding mode. To perhaps shift the electronics in favor of the η^2-NO binding mode while maintaining the pseudo square planar geometry, the PMe_3 supporting ligands were substituted for an N-heterocyclic carbene (NHC). Figure 2.11's results over [Co($C_4N_2H_5$)$_2$(NC_4H_8)(N_2O)] show that the η^2-NN binding mode is still the energetically preferred one by 0.9 kcal/mol. The κ-O binding mode could not be successfully optimized as the structure favored the formation of a metal oxo.



				
	κ-N	η-NN	η-NO	κ-O
	+ 8.3 kcal/mol	0.0 kcal/mol	+ 0.9 kcal/mol	oxo

"oxo" represents the formation of a metal oxo due to NO bond breaking.

Figure 2.11 Ligand modification effect on binding in $[Co(C_4N_2H_5)_2(NC_4H_8)(N_2O)]$

The twisting of the pincer ligand in the $[Co(C_4N_2H_5)_2(NC_4H_8)(N_2O)]$ system is shown in Figure 2.12a. This resulted in the N_2O unit being driven up out of plane by the steric bulk of the methyl groups, which significantly reduced the relative energy disparity between the η^2-NN and η^2-NO binding modes. In correspondence to this observation, the methyl groups on the NHCs were altered to t-butyl in a last attempt to pinpoint a system in which η^2-NO is the favored binding mode. As seen in Figure 2.12b, the substitution of methyl groups for t-butyl groups caused the pincer ligand to twist further, and in turn, caused the N_2O unit to rise higher out of plane.

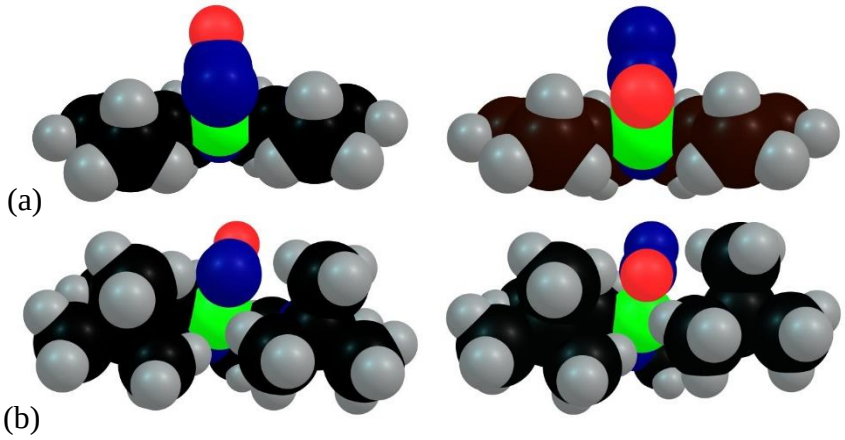
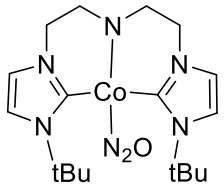
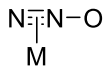
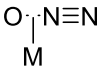
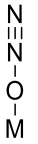


Figure 2.12 (**a**) Space-filling model of $[Co(C_4N_2H_5)_2(NC_4H_8)]$ in both the η^2-NN and η^2-NO configuration, (**b**) Space-filling model of $[Co(C_6N_2H_{11})_2(NC_4H_8)]$ in both the η^2-NN and η^2-NO configuration

Color Scheme: green = cobalt, blue = nitrogen, red = oxygen, black = carbon, grey = hydrogen

Figure 2.13's results over $[Co(C_6N_2H_{11})_2(NC_4H_8)(N_2O)]$ show that the η^2-NO is in energetic equilibrium with the η^2-NN binding mode. It should be noted that for "consistency", the values are reported to one decimal place, making the η^2-NN and η^2-NO appear in energetic equilibrium. However, these two binding modes vary by 0.04 kcal/mol, giving preference to the η^2-NO binding mode, which has not previously been seen. This being said, the 0.04 kcal/mol difference between the η^2-NN and η^2-NO binding modes falls into the margin of error for density functional theory (DFT) calculations.



				
	κ-N	η-NN	η-NO	κ-O
	+ 5.4 kcal/mol	0.0 kcal/mol	0.0 kcal/mol	oxo

"oxo" represents the formation of a metal oxo due to NO bond breaking.

Figure 2.13 Ligand modification effect on binding in $[Co(C_6N_2H_{11})_2(NC_4H_8)(N_2O)]$

2.4 Conclusion

The N_2O unit often prefers to be bonded through both nitrogens in a bent configuration to low valent metal centers, according to this study's use of computational chemistry. This favored binding mode is associated with a low valent metal's strong π-donor characteristics. Alternately, by increasing the electron deficiency of the metal complexes, this binding preference can be switched to the κ-N binding mode. It was interestingly observed that the geometry and electronics of the structure also had an impact on the preference between the η^2-NN and η^2-NO binding modes. Binding between the nitrogen and oxygen atoms of the N_2O can be favored by utilizing a pseudo-square planar geometry, similar to the Figueroa lab system, and making the metal center more electron-rich. These insights aid in understanding the known binding properties of N_2O, opening the door for further research into the chemistry of this peculiar and potentially major oxidant.

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Chapter 3

Computational Investigation into the Activation of N_2 Through Binding in Transition Metal Complexes

3.1 Introduction

One of the essential elements for the existence of all living things is nitrogen. It is a need for the formation of several classes of biomolecules, such as proteins, DNA, and chlorophyll. Although nitrogen is present in the atmosphere in huge quantities as dinitrogen gas (N_2), most organisms cannot access it in this form, making it a limited resource and frequently restricting primary production in many ecosystems. Nitrogen is not readily accessible to primary producers like plants until it is changed from dinitrogen gas into ammonia (NH_3).[1]

Along with N_2 and NH_3, nitrogen may also take on inorganic (such as nitrate) and organic (such as amino and nucleic acids) forms. Thus, when organisms use nitrogen for development and, in certain circumstances, energy, it passes through a variety of distinct changes throughout the environment. Nitrogen is transformed primarily by nitrogen fixation, nitrification, denitrification, ammonification, and anammox (Figure 3.1). The productivity of the biosphere depends heavily on the oxidation of nitrogen into its many oxidation states, which is carried out by a wide variety of microorganisms including bacteria, archaea, and fungi. [1]

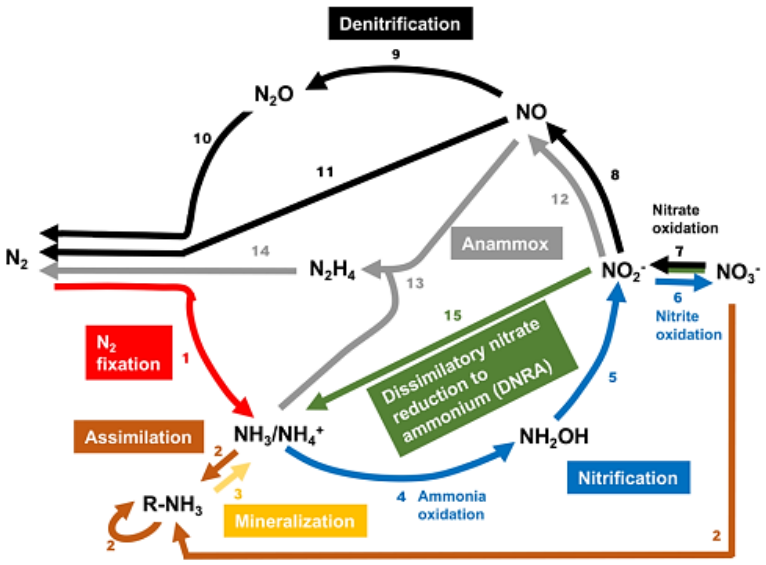


Figure 3.1 Major transformations in the nitrogen cycle

Diazotrophic bacteria carry out biological nitrogen fixation, which is the conversion of N_2 into two NH_3 molecules, an accessible source of nitrogen. These specialized microbes can exist independently or in symbiotic partnerships with specific animals and plants, such as legumes (e.g., termites).[1] Before the development of the Haber-Bosch process for the synthesis of commercial ammonia, these microorganisms were the primary source of the majority of nitrogen atoms in living things. They possess nitrogenase enzymes, which are the only kind of enzymes capable of carrying out the crucial N_2-reducing process.[2–12] Despite being an exergonic process under ambient conditions, the full reduction of atmospheric N_2 gas to two molecules of NH_3 is kinetically unfavorable due to the high energy barrier for activating the inert N_2 triple bond.[13–17]

The well-known Haber-Bosch process, which sustains the reaction of N_2 and H_2 on an iron catalyst at high temperature and pressure, is the technical answer to dinitrogen

fixation.[18] Due to the process, ammonia fertilizer became widely available, which contributed to a rise in the global population by hastening the rate at which agricultural yields rose. Unfortunately, although being a significant technological development, the Haber-Bosch process has always been energy-intensive, leaving a significant carbon footprint. The reaction consumes around 1% of the world's total energy production while operating at temperatures of around 500 °C and pressures of up to 20 MPa.[19,20] According to the Institute for Industrial Productivity, it released up to 451 million tons of CO_2 in 2010. More than any other industrial chemical-making process, this sum is responsible for around 1.4% of the world's yearly CO_2 emissions.[19,20] On the other hand, biological nitrogen fixation is limited to ambient circumstances and the usage of ATP, a biological energy source. At the active site of the proteins, metal ions like molybdenum and iron are often present, which are essential for activating N_2.[21–28] Metalloenzyme nitrogenase, which is made up of the electron-donating Fe cluster and the catalytic MoFe active site, serves as a catalyst for biological N_2 fixation. N_2 is reduced at the FeMo-cofactor (FeMo-co) active

site of the MoFe protein, [7Fe-9S-Mo-C-homocitrate], on the particular 4Fe-face picture in Figure 3.2.[2]

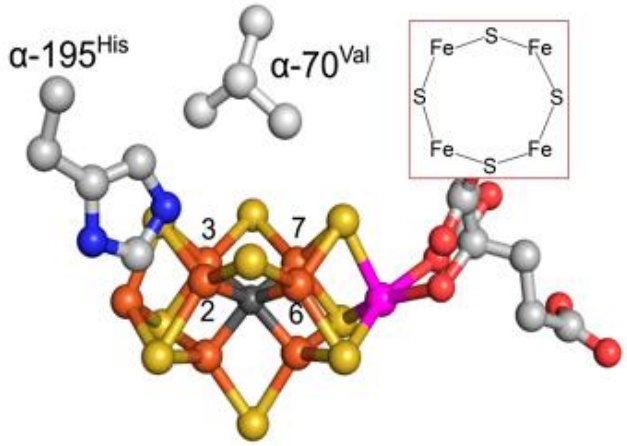


Figure 3.2 FeMo-co, [7Fe-9S-Mo-C-homocitrate], with a cartoon of active Fe 2,3,6,7 FeMo-co face. PDB: 2AFI

Exploring the most efficient catalysts for use in industry while drawing lessons from nature has proven to be one of the biggest obstacles. Numerous investigations have been done on metal-containing catalysts for nitrogen fixation at mild temperatures and pressures (298 K and 1 atm), where the metallic elements play important roles.[22,29–41]

The reduction of N_2 to ammonia using molybdenum catalysts that include tetradentate $[HIPTN_3N]^{3-}$ triamidoamine ligands discovered by X-ray crystallography was reported by the Schrock lab at room temperature and 1 atmosphere.[37] The Peters team also reported the structurally and computationally supported reduction of N_2 to ammonia through the Fe complex with tris(phosphino)alkyl (CP^{iPr}_3) ligand containing an axial carbon donor.[42] A report on terminal vs bridging end-on N_2 coordination in transition metal complexes was published by the Goldman, Miller, and Holland laboratories. They use both quantitative

DFT and qualitative molecular orbital (MO) analyses to elucidate the fundamental factors governing the two binding modes and determine which is preferred for a given metal-ligand system. They concluded that an electronic factor, such as the number of π-bonds in the triatomic MNN moiety of an MNN complex, plays a critical role in determining these trends.[40]

In a prior, yet intriguing, investigation, the Lappert group used IR and ESR spectroscopy to analyze a zirconium complex that contained a η^2-NN bound N_2 unit.[43] The Sutton group has reported side-bound coordination of N_2 with a mononuclear rhenium system that has been characterized by NMR spectroscopy.[44] A η^2-NN coordination complex of N_2 has been reported by the Coppens lab using the photocrystallographic method, which enables the study of metastable or transient species formed by in situ laser irradiation of diffractometer-mounted samples at low temperatures. These findings have been supported by low-temperature IR and Differential Scanning Calorimetry (DSC) measurements as well as by quantum mechanical calculations.[45] The Bercaw lab has reported the discovery of yet another η^2-NN bound N_2 unit with a mononuclear titanium system that has been characterized by IR and NMR spectroscopy.[46] We hope to shed some insight on yet another significant small molecule and its binding and activation towards bond reduction with transition metal complexes based on our earlier research on terminal vs side-on N_2O coordination in transition metal complexes.

3.2 Computation Details

For all the calculations presented here, the Gaussian16 code was utilized.[47] The level of theory used was B3LYP/6-31G(d). Heavy metals used an effective core potential (ECP) basis set, specifically LANL2DZ. In the gas phase, all singlet spin states were assessed using restricted Kohn-Sham procedures, whereas triplets and quintets were assessed using unrestricted Kohn-Sham techniques. The electronic energy is corrected for enthalpy and entropy using unscaled vibrational frequencies at 1 atm and 298.15 K. By calculating structures with no imaginary frequencies, all stationary points are classified as minima.[48]

3.3 Results and Discussion

The initial systems investigated involved the potential binding of N_2 to the previously studied [Ni(L)$_2$)] in our lab. These systems were chosen as they are known to bind small molecules in both the terminal and side-bound coordination, as seen with the Roselar lab's work with N_2O.[49] This initial comparison, which was done to better understand the binding and activation of N_2, included a pseudo-trigonal planar Ni system. The B3LYP/6-31G(d,p) level of theory was selected as it has been employed in the iron, osmium, and ruthenium systems previously studied.[48] With this system, the effect of changing the ligands' *cis* to the N_2 unit was examined to assess its impact on bond activation and binding. The findings in Figure 3.3 show that the energetically preferred binding mode for all of the ligands is the κ-N bound N_2 unit.

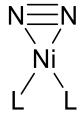
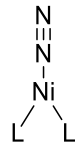
		
L=NHC	0.0 kcal/mol	+3.3 kcal/mol
L=PMe3	0.0 kcal/mol	+1.7 kcal/mol
L=PH3	0.0 kcal/mol	+3.8 kcal/mol
L=CNMe	0.0 kcal/mol	+4.7 kcal/mol
L=CO	0.0 kcal/mol	+6.8 kcal/mol

Figure 3.3 Ligand modification effect on binding energy in $[Ni(L)_2(N_2)]$

The relative energy difference between η^2-NN and κ-N increases as one moves from an electron-rich to an electron-deficient metal system through donating supporting ligands. The NHC ligand deviates from the trend because of the steric encumbrance in the complex. This observation is supported by the vibrational frequencies of the κ-CO and η^2-C_2H_2 complexes of $[Ni(L)_2]$ as seen in Table 3.1. It can be seen from the data that with this Ni^0 system, the relative energy between the η^2-NN and κ-N binding modes is fairly small, indicating that the η^2-NN binding mode on N_2 is achievable, as seen with the Figueroa and Roselar labs.

Table 3.1 C-O and C-C stretch vibrational frequencies (in cm^{-1}) for $[Ni(L)_2(CO)]$ and $[Ni(L)_2(CH)_2]$ complexes

Complex	ν_{CO} (cm^{-1})	ν_{CC} (cm^{-1})
$[NiC_{10}N_4H_{16}]$	2009.4	1652.2
$[Ni(PMe_3)_2]$	2036.0	1672.0
$[Ni(PH_3)_2]$	2071.0	1696.4
$[Ni(CNMe)_2]$[a]	2061.8	1709.4
$[Ni(CO)_2]$[b]	2100.0, 2102.1, 2189.0	1749.9

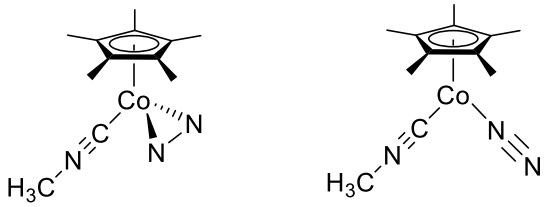
[a]The C-O stretch vibrational frequency for $[Ni(CNMe)_2(CO)]$ does not follow the trend as the structure breaks planarity. [b]The $[Ni(CO)_2(CO)]$ complex has three C-O stretch vibrational frequencies due to symmetry coupling.

In this $[Ni(L)_2(N_2)]$ series, the N-N bond distance decreases from 1.13 Å in the terminal bound $[Ni(NHC)_2(N_2)]$ complex to 1.12 Å in the terminal bound $[Ni(CO)_2(N_2)]$ complex while the N-N stretching frequency in the terminal bound $[Ni(NHC)_2(N_2)]$ complex increases from 2194.0 cm^{-1} to 2331.4 cm^{-1} in the terminal bound $[Ni(CO)_2(N_2)]$ complex. Similar observations can be seen with the side-bound N_2 unit (Table 3.2), in which the N-N bond distance decreases from 1.18 Å in the side-bound $[Ni(NHC)_2(N_2)]$ complex to 1.15 Å in the side-bound $[Ni(CO)_2(N_2)]$ complex while the N-N stretching frequency in the side-bound $[Ni(NHC)_2(N_2)]$ complex increases from 1882.9 cm^{-1} to 2068.3 cm^{-1} in the side-bound $[Ni(CO)_2(N_2)]$ complex. This demonstrates that the N-N bond distance decreases as the N-N stretching frequency increases when a supporting ligand is switched from an electron-rich to an electron-deficient alternative.

Table 3.2 N-N bond distances (in Å) and N-N stretch vibrational frequencies (in cm^{-1}) for $[Ni(L)_2(N_2)]$ complexes

	κ-N		**η^2-NN**	
$[Ni(L)_2(N_2)]$	**N-N (Å)**	**ν_{NN} (cm^{-1})**	**N-N (Å)**	**ν_{NN} (cm^{-1})**
L=NHC	1.13	2194.0	1.18	1882.9
$L=PMe_3$	1.13	2217.7	1.17	1917.5
$L=PH_3$	1.13	2249.1	1.17	1955.3
L=CNMe	1.12	2217.9	1.16	1988.6
L=CO	1.12	2331.4	1.15	2068.3

The next system examined, which was another that has been shown to bind small molecules in both the terminal and side-bound coordination, was comparable to the Figueroa lab to gain a better grasp of the η^2-NN and κ–N binding modes.[50] According to calculations, the κ–N isomer is 8.6 kcal/mol more stable in the $[Co(\eta^5\text{-Cp*})(CNMe)]$ system (Figure 3.4).



0.0 kcal/mol **+ 8.6 kcal/mol**

Figure 3.4 Ligand modification effect on binding in $[Co(\eta^5\text{-Cp*})(CNMe)(N_2)]$

In this [Co(η^5-Cp*)(CNMe)(N_2)] series, the N-N bond distance increases from 1.13 Å in the terminal N_2 bound complex to 1.16 Å in the side-bound N_2 complex (Table 3.3). From this, it can be seen that the N-N stretching frequency in the terminal N_2 bound complex decreases from 2257.7 cm^{-1} to 2003.7 cm^{-1} in the side-bound N_2 complex. The relative energy difference and N-N stretching frequency in the preceding Ni system are less than those in the [Co(η^5-Cp*)(CNMe)(N_2)] system, indicating that this system does not activate the N_2 bond as much as the previous systems.

Table 3.3 N-N bond distances (in Å) and N-N stretch vibrational frequencies (in cm^{-1}) for [Co(η^5-Cp*)(CNMe)(N_2)]

	κ-N		**η^2-NN**	
[Co(Cp*)(CNMe)(N_2)]	**N-N (Å)**	**ν_{NN} (cm^{-1})**	**N-N (Å)**	**ν_{NN} (cm^{-1})**
CNMe	1.13	2257.7	1.16	2003.7

To determine if the electronics of the system changed the binding of η^2-NN or κ–N as well as N_2 activation, the cyclopentadienyl (Cp) ligand was substituted with the pentamethylcyclopentadienyl (Cp*) ligand. In the [CoCpCNMe] system, as seen in Figure 3.5, the κ–N isomer was shown to be the most stable by 12.5 kcal/mol. When a supporting ligand is changed from an electron-rich to a more electron-deficient alternative, the relative energy gap between the favored binding mode and the succeeding mode increases. Similar results were seen with the original Ni system. The impacts of changing the ligand's *cis* to the N_2 unit were examined to assess the ligand's impact on the binding mode and N_2

activation. According to the results in Figure 3.5, the κ–N bound N_2 unit is the energetically preferred binding form with all of the ligands. Due to the ligand's broken linearity, which caused some distortion in the relative energy, the CNMe supporting ligand did not follow the trend.

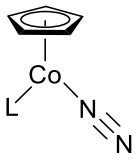
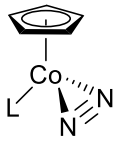
		
L=PMe_3	0.0 kcal/mol	+ 9.7 kcal/mol
L=PH_3	0.0 kcal/mol	+ 9.9 kcal/mol
L=CNMe	0.0 kcal/mol	+ 12.5 kcal/mol
L=CO	0.0 kcal/mol	+ 10.7 kcal/mol

Figure 3.5 Ligand modification effect on binding energy in [Co(η^5-Cp)(L)(N_2)]

The binding preference varies by 10.7 kcal/mol when CO is replaced for the ligand *cis* to the N_2 unit. This is not unexpected considering CO is a strong π-acceptor that efficiently lowers the electron richness of the low valent Co metal center, giving favorability to the κ-N bound binding mode. The vibrational frequencies of the κ-CO and η^2-C_2H_2 complexes of [Co((η^5-Cp)(L)] shown in Table 3.4 complement this observation and show a similar pattern to the Ni systems that were previously studied.

Table 3.4 C-O and C-C stretch vibrational frequencies (in cm^{-1}) for [Co(η^5-Cp)(L)(CO)] and [Co(η^5-Cp)(L)$(CH)_2$] complexes

Complex	ν_{CO} (cm^{-1})	ν_{CC} (cm^{-1})
[Co(η^5-Cp)(PMe_3)]	2032.4	1739.5
[Co(η^5-Cp)(PH_3)]	2049.2	1749.1
[Co(η^5-Cp)(CNMe)]	2062.5	1765.2
[Co(η^5-Cp)(CO)][a]	2071.2, 2117.6	1780.7

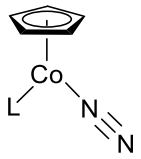
[a]The [Co(η^5-Cp)$(CO)_2$] complex has two C-O stretch vibration frequencies due to symmetry coupling.

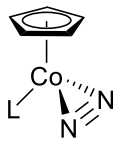
In this [Co(η^5-Cp)(L)(N_2)] series, the N-N bond distance decreases from 1.13 Å in the terminal bound [Co(η^5-Cp)(PMe_3)(N_2)] complex to 1.12 Å in the terminal bound [Co(η^5-Cp)(CO)(N_2)] complex, similar observations can be seen with the side-bound N_2 unit (Table 3.5). From this, it can be seen that the N-N stretching frequency in the terminal bound [Co(η^5-Cp)(PMe_3)(N_2)] complex increases from 2226.8 cm^{-1} to 2294.9 cm^{-1} in the terminal bound [Co(η^5-Cp)(CO)(N_2)] complex, similar observations can be seen with the side-bound N_2 coordination. It can be seen that changing the electronics of the metal system had quite an effect on N_2 activation, however, this observation is complicated by the bending of the CNMe.

Table 3.5 N-N bond distances (in Å) and N-N stretch vibrational frequencies (in cm^{-1}) for $[Co(\eta^5\text{-}Cp)(L)(N_2)]$

	κ-N		**η^2-NN**	
$[Co(Cp)(L)(N_2)]$	**N-N (Å)**	**ν_{NN} (cm^{-1})**	**N-N (Å)**	**ν_{NN} (cm^{-1})**
L=PMe_3	1.13	2226.8	1.16	1975.7
L=PH_3	1.13	2244.4	1.16	1992.8
L=CNMe	1.12	2274.7	1.15	2022.3
L=CO	1.12	2294.9	1.15	2048.9

In order to ascertain the influence that the electronics have on η^2-NN or κ-N binding as well as N_2 activation with consistent steric influence, a number of para-substituted pyridine ligands *cis* to the N_2 unit in the $[Co(\eta^5\text{-}Cp)(L)(N_2)]$ system were examined. According to the findings in Figure 3.6, regardless of the kind of ligand, the κ-N bound isomer is energetically favored over the η^2-NN isomer.





L= py-$(p\text{-}NMe)_2$	0.0 kcal/mol	+6.2 kcal/mol
L=py	0.0 kcal/mol	+6.7 kcal/mol
L= py-$(p\text{-}NO)_2$	0.0 kcal/mol	+8.4 kcal/mol

Figure 3.6 Ligand modification effect on binding energy in $[Co(\eta^5\text{-}Cp)(L)(N_2)]$

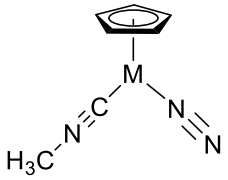
The N-N bond distance reduces in this [Co(η^5-Cp)(L)(N_2)] series from 1.13 Å in the terminal bound [Co(η^5-Cp)py-(p-NMe)$_2$(N_2)] complex to 1.13 Å in the terminal bound [Co(η^5-Cp)py-(p-NO)$_2$(N_2)] complex. Similar findings may be made with the side-bound N_2 unit (Table 3.6). In contrast, the terminal bound [Co(η^5-Cp)py-(p-NO)$_2$(N_2)] complex has a higher N-N stretching frequency than the terminal bound [Co(η^5-Cp)py-(p-NMe)$_2$(N_2)] complex, increasing from 2216.3 cm^{-1} to 2248.4 cm^{-1}. Similar findings may be made for the side-bound N_2 coordination. It is clear from the minimal steric interference that the earlier observation—that the N_2 bond length and activation were mostly unaffected by electronic factors—was correct.

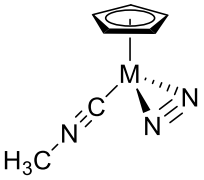
Table 3.6 N-N bond distances (in Å) and N-N stretch vibrational frequencies (in cm^{-1}) for para-substituted pyridine series [Co(η^5-Cp)(L)(N_2)]

	κ-N		**η^2-NN**	
[Co(η^5-Cp)(L)(N_2)]	**N-N (Å)**	**ν_{NN} (cm^{-1})**	**N-N (Å)**	**ν_{NN} (cm^{-1})**
L= py-(p-NMe_2)	1.13	2216.3	1.16	1963.7
L=py	1.13	2225.3	1.16	1972.7
L= py-(p-NO_2)	1.13	2248.4	1.16	2003.0

To examine the periodic trend in previously investigated systems, the metal center was then replaced with other metals in the [[M](η^5-Cp)(CNMe)(N_2)] complexes (Figure 3.7). Interestingly, it was observed that the preferred binding mode for all three metal centers was the κ-N isomer with a linear orientation. With respect to Co and Ir, the data in the table

shows a periodic trend where the relative energy between the η^2-NN or κ-N binding mode increases as one descends the group. It should also be noted that Rh does not follow any sort of trend, which is similar to observations in chapter 2 as well as in previous work.[48]





M=Co	0.0 kcal/mol	+12.5 kcal/mol
M=Rh	0.0 kcal/mol	+9.4 kcal/mol
M=Ir	0.0 kcal/mol	+15.6 kcal/mol

Figure 3.7 Metal identity modification effect on binding energy in [[M]CNMe(η^5-Cp)(N_2)]

In this [[M](η^5-Cp)(CNMe)(N_2)] series, the N-N bond distance in all the terminal bound complexes is 1.12 Å, similar observations can be seen with the side-bound N_2 unit (Table 3.7). From this, it can be seen that the N-N stretching frequency in the terminal [Co(η^5-Cp)(CNMe)(N_2)] complex decreases from 2274.7 cm^{-1} to 2264.0 cm^{-1} in the terminal bound [Ir(η^5-Cp)(CNMe)(N_2)] complex, opposite observations can be seen with the side-bound N_2 coordination.

Table 3.7 N-N bond distances (in Å) and N-N stretch vibrational frequencies (in cm^{-1}) for [[M](η^5-Cp)(CNMe)(N_2)]

	κ-N		**η^2-NN**	
[[M](η^5-Cp)(CNMe)(N_2)]	**N-N (Å)**	**ν_{NN} (cm^{-1})**	**N-N (Å)**	**ν_{NN} (cm^{-1})**
M=Co	1.12	2274.7	1.15	2022.3
M=Rh	1.12	2300.1	1.14	2134.7
M=Ir	1.12	2264.0	1.15	2040.6

Sticking with a d^8 system that has a similar geometry as the previously studied system, a number of square planar [$Co(L)_2Cl(N_2)$] complexes were studied employing a range of ligands (L) (Figure 3.8). It is clear that the relative energy difference between η^2-NN and κ-N grows as one advances from an electron-rich to an electron-deficient system, which is in line with the observations in the [$CoCp(L)_2(N_2)$] and [$Ni(L)_2(N_2)$] systems.

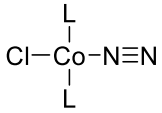
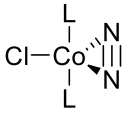
		
L=PMe_3	0.0 kcal/mol	+10.3 kcal/mol
L=PH_3	0.0 kcal/mol	+10.9 kcal/mol
L=CNMe	0.0 kcal/mol	+11.8 kcal/mol
L=CO	0.0 kcal/mol	+12.9 kcal/mol

Figure 3.8 Ligand identity modification effect on binding energy in [$Co(L)_2Cl(N_2)$]

In this $[Co(L)_2Cl(N_2)]$ series, the N-N bond distance decreases from 1.13 Å in the terminal bound $[Co(PMe_3)_2Cl(N_2)]$ complex to 1.12 Å in the terminal bound $[Co(CO)_2Cl(N_2)]$ complex, similar observations can be seen with the side-bound N_2 unit (Table 3.8). From this, it can be seen that the N-N stretching frequency in the terminal $[Co(PMe_3)_2Cl(N_2)]$ complex increases from 2209.1 cm^{-1} to 2335.8 cm^{-1} in the terminal bound $[Co(CO)_2Cl(N_2)]$ complex, similar observations can be seen with the side-bound N_2 coordination.

Table 3.8 N-N bond distances (in Å) and N-N stretch vibrational frequencies (in cm^{-1}) for $[Co(L)_2Cl(N_2)]$

	κ-N		**η^2-NN**	
$[Co(L)_2Cl(N_2)]$	**N-N (Å)**	**ν_{NN} (cm^{-1})**	**N-N (Å)**	**ν_{NN} (cm^{-1})**
L=PMe_3	1.13	2209.1	1.16	1965.5
L=PH_3	1.13	2241.9	1.16	1991.8
L=CNMe	1.12	2264.3	1.15	2050.0
L=CO	1.12	2335.8	1.14	2095.8

In an effort to further comprehend the reduction in energy differences between the η^2-NN and κ-N binding modes utilizing the findings made, a number of pseudo-trigonal planar $[[M]((\eta^5\text{-}Cp^*)_2(N_2)]$ complexes were studied (Figures 3.9). These systems were picked since it has been shown experimentally that the respective binding energies of N_2's η^2-NN and κ-N binding modes are generally close to one another and occasionally even in

equilibrium as well as that the relative energy for the η^2-NN and κ-N binding modes and N_2 activation depended on the structure's shape, electronics, the metals oxidation state, and the number of electrons. As demonstrated by the work of the Chirik and Bercaw laboratories, these structures are also known to favor the binding of N_2 in a side-bound coordination.[46,51] These systems were chosen when it was discovered that the relative energy for the η^2-NN and κ-N binding modes and N_2 activation depended on the structure's shape, electronics, the metals oxidation state, and the number of electrons. According to the results, the κ-N binding mode is the energetically favored binding mode for the triplet and singlet forms of $[Ti(\eta^5\text{-}Cp^*)_2(N_2)]$ as well as for $[Zr(\eta^5\text{-}Cp^*)_2(N_2)]$ as a triplet. It's interesting to note that the η^2-NN binding mode was discovered to be N_2's preferred energetic binding mode for $[Zr(\eta^5\text{-}Cp^*)_2(N_2)]$ as a singlet. It should be noticed that when one moves from Ti to Zr, the relative energy between the η^2-NN and κ-N binding modes diminishes.

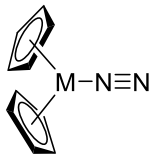
	Multiplicity		
M=Ti	1	0.0 kcal/mol	+0.9 kcal/mol
M=Ti	3	0.0 kcal/mol	+8.7 kcal/mol
M=Zr	1	+2.6 kcal/mol	0.0 kcal/mol
M=Zr	3	0.0 kcal/mol	+4.0 kcal/mol

Figure 3.9 Metal identity modification effect on binding energy in $[[M](\eta^5\text{-}Cp^*)_2(N_2)]$

In this [[M](η^5-Cp^*)$_2$(N_2)] series, the N-N bond distance is 1.14 Å in the terminal bound [Ti(η^5-Cp^*)$_2$(N_2)] singlet complex and the terminal bound [Zr(η^5-Cp^*)$_2$(N_2)] singlet complex but increases from 1.13 Å in the terminal bound [Ti(η^5-Cp^*)$_2$(N_2)] triplet complex to 1.14 Å in the [Zr(η^5-Cp^*)$_2$(N_2)] triplet complex, similar observations can be seen with the side-bound N_2 unit (Table 3.9). In direct contrast, the N-N stretching frequency in the terminal [Ti(η^5-Cp^*)$_2$(N_2)] singlet decreases from 2117.0 cm^{-1} to 2101.9 cm^{-1} in the terminal bound [Zr(η^5-Cp^*)$_2$(N_2)] singlet complex and from 2101.9 cm^{-1} in the terminal bound [Ti(η^5-Cp^*)$_2$(N_2)] triplet complex to 2076.5 cm^{-1} in the [Zr(η^5-Cp^*)$_2$(N_2)] triplet complex, similar observations can be seen with the side-bound N_2 coordination.

Table 3.9 N-N bond distances (in Å) and N-N stretch vibrational frequencies (in cm^{-1}) for [[M](η^5-Cp^*)$_2$(N_2)]

		κ-N		**η^2-NN**	
[[M](η^5-Cp^*)$_2$(N_2)]	**Multiplicity**	**N-N (Å)**	**ν_{NN} (cm^{-1})**	**N-N (Å)**	**ν_{NN} (cm^{-1})**
M=Ti	1	1.14	2117.0	1.18	1877.2
M=Ti	3	1.13	2101.9	1.15	2030.4
M=Zr	1	1.14	2101.9	1.18	1815.7
M=Zr	3	1.14	2076.5	1.15	1999.2

As these complexes are known to favor the side-bound N_2 unit or for the η^2-NN and κ-N binding modes of N_2 to be in equilibrium, the next two systems to be examined were ones similar to the Sutton lab.[44] The κ-N isomer is 19.4 kcal/mol more stable in the [Re(η^5-

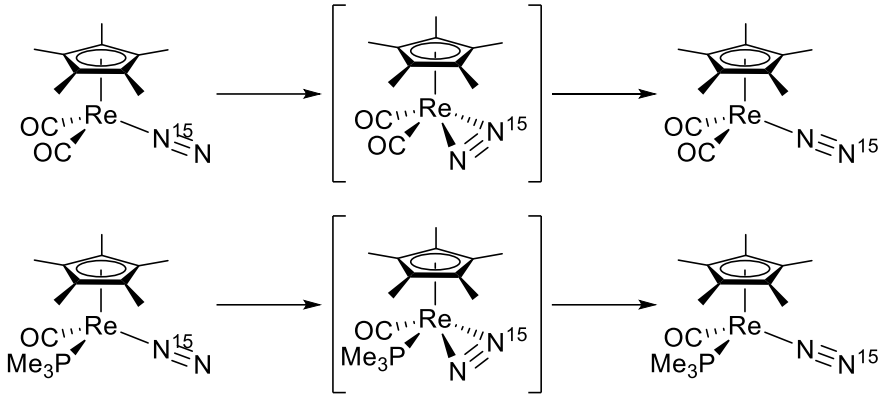
Cp*)$(CO)_2$] system, according to calculations (Figure 3.10). It can also be seen that the κ–N isomer is 20.3 kcal/mol more stable in the [Re(η^5-Cp*)(CO)(PMe_3)] system.

κ-N	**η^2-NN**	**κ-N**	**η^2-NN**
0.0 kcal/mol	+19.4 kcal/mol	0.0 kcal/mol	+20.3 kcal/mol

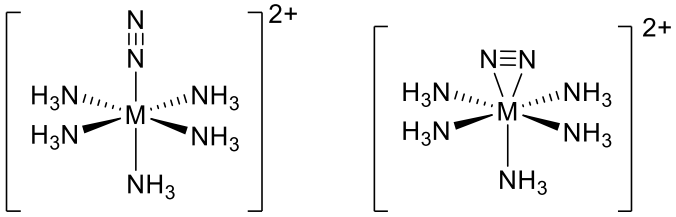
Figure 3.10 Ligand modification effect on binding in [Re(η^5-Cp*)$(CO)_2$] and [Re(η^5-Cp*)(CO)(PMe_3)]

Through a time-dependent study by the Sutton lab, using ^{15}N spectroscopy, the formation of [Re(η^5-Cp*)$(CO)_2$] occurred after 7 hours at room temperature, while the formation of [Re(η^5-Cp*)(CO)(PMe_3)] was not observed at room temperature, formation did occurred after 3 hours at 330 K (Scheme 3.1).[44] It can be understood that the faster formation corresponds to the molecule that is lower in energy and thereby, more accessible. This rhenium data agrees with the finding of the Sutton lab in which [Re(η^5-Cp*)$(CO)_2$] was observed to be lower in energy than [Re(η^5-Cp*)(CO)(PMe_3)].

Scheme 3.1 Isomerization of [Re(η^5-Cp*)$(CO)_2$] and [Re(η^5-Cp*)(CO)(PMe_3)] by the Sutton lab[44]



In an effort to comprehend how the geometry of the structure, the d electron count, and the metal center's oxidation state impact the relative binding of the two binding modes and N_2 activation, a number of octahedral [[M]$(NH_3)_5(N_2)]^{2+}$ complexes were studied (Figure 3.11). As one goes down the group, as was the case in the prior systems, it can be seen that the relative energy between the η^2-NN and κ–N binding modes rises.



M=Fe	0.0 kcal/mol	+17.2 kcal/mol
M=Ru	0.0 kcal/mol	+15.9 kcal/mol
M=Os	0.0 kcal/mol	+23.7 kcal/mol

Figure 3.11 Metal identity modification effect on binding energy in [[M]$(NH_3)_5(N_2)$]

In this $[[M](NH_3)_5(N_2)]^{2+}$ series, the N-N bond distance increases from 1.11 Å in the terminal bound $[Fe(NH_3)_5(N_2)]^{2+}$ complex to 1.12 Å in the terminal bound $[Os(NH_3)_5(N_2)]^{2+}$ complex, similar observations can be seen with the side-bound N_2 unit (Table 3.10). From this, it can be seen that the N-N stretching frequency in the terminal $[Fe(NH_3)_5(N_2)]^{2+}$ complex decreased from 2347.0 cm^{-1} to 2268.5 cm^{-1} in the terminal-bound $[Os(NH_3)_5(N_2)]^{2+}$ complex, similar observations can be seen with the side-bound N_2 coordination.

Table 3.10 N-N bond distances (in Å) and N-N stretch vibrational frequencies (in cm^{-1}) for $[[M](NH_3)_5(N_2)]$

	κ-N		**η^2-NN**	
$[[M](NH_3)_5(N_2)]^{2+}$	**N-N (Å)**	**ν_{NN} (cm^{-1})**	**N-N (Å)**	**ν_{NN} (cm^{-1})**
M=Fe	1.11	2347.0	1.12	2309.9
M=Ru	1.11	2339.8	1.12	2311.6
M=Os	1.12	2268.5	1.14	2139.4

From the data in chapter 2 over N_2O, and previous work,[48] it can be seen that η^2-NN is a better π-acceptor than κ-N. The favorability of η^2-NN was observed in low oxidation states systems with a good electron-rich π-donor metal. Lastly, in view of the decrease in the relative energy between the η^2-NN and κ–N binding modes and N_2 activation by changing the electronics, and oxidation state of the metal system, more attempts were made to locate a system in which the η^2-NN mode of N_2 was not plausible. To do this, a series

of $[[M](\eta^5\text{-Cp})(N_2)Cl_2]^{3+}$ complexes similar to the previous system were investigated however, an additional supporting ligand was added to increase the oxidation state of the metal center. It should be noted that the η^2-NN binding mode could not be successfully optimized as the N_2 unit broke off of the metal center in all three systems, which is a similar observation from previous work.[48] It can be seen in Table 3.11 that the N_2 bond distance and stretching frequency of the κ-N binding mode do not follow any periodic trend.

Table 3.11 N-N bond distances (in Å) and N-N stretch vibrational frequencies (in cm^{-1}) for $[[M](\eta^5\text{-Cp})(N_2)Cl_2]$

		κ-N
$[[M](\eta^5\text{-Cp})(N_2)Cl_2]^{3+}$	**N-N (Å)**	**ν_{NN} (cm^{-1})**
M=Co	1.11	2416.2
M=Rh	1.11	2427.7
M=Ir	1.11	2378.1

3.4 Conclusion

According to this study's use of computational chemistry, the linear configuration of the N_2 unit bonding through the terminal nitrogen is preferred. However, it was shown that the strong π-donor properties of a low valent metal might alter the preference in favor of η^2-NN. It was interestingly shown that the geometry and electronics of the structure also affected the favorability between the η^2-NN and κ-N binding modes. It may be said that η^2-NN is a superior π-acceptor than κ-N and requires a suitable electron-rich low valent π-

donor metal in order to be possibly favorable. These observations help to explain the N_2's known binding characteristics and pave the way for more investigation into the chemistry of this remarkable small molecule.

3.5 References

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Chapter 4

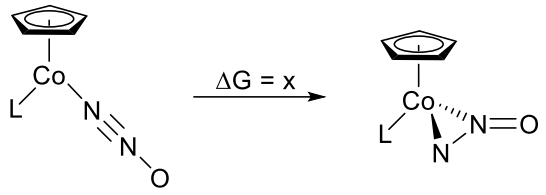
Conclusions and Future Prospects

4.1 Conclusions

The activation of N_2O and N_2 has long caught the considerable interest of inorganic chemists.[1,2] Despite being a potentially effective oxygen-atom transfer agent for transition metals, N_2O is a notably poor ligand, and the coordination chemistry of just a few terminal, end-on κ-N, and side-bound η^2-NN complexes has been characterized.[1] Despite the fact that molecular nitrogen is abundant in the atmosphere as N_2, many organisms cannot access it, making it a limited resource that frequently restricts primary production in many ecosystems.[2] This work used computational chemistry to examine the binding of these two small molecules to various transition metal complexes in an effort to understand the binding properties of N_2O and N_2.

This study demonstrates that the N_2O unit prefers to connect across both nitrogens in a bent configuration to low valent metal centers. The strong π-donor properties of a metal with a low valent electron configuration can alter the preference for η^2-NN over κ-N as seen in Table 4.1.

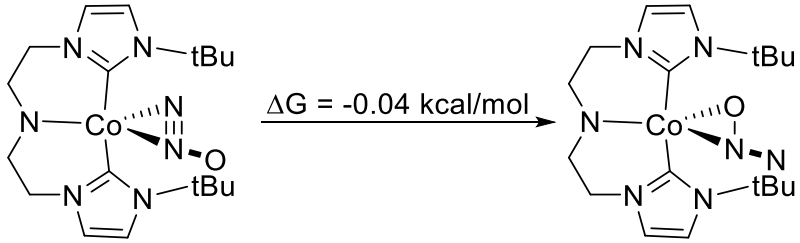
Table 4.1 Trans ligand modification effect on terminal nitrogen vs oxygen binding



Ligand (L)	Energy (ΔG in kcal/mol)
PMe_3	-6.6
PH_3	-6.0
CMNe	-2.9
CO	+3.3

The binding between the nitrogen and oxygen atoms of the N_2O can be enhanced by using a pseudo-square planar geometry, similar to the Figueroa lab system, and making the metal center more electron-rich as seen in Scheme 4.1.

Scheme 4.1 Binding between the nitrogen and oxygen atoms of the N_2O

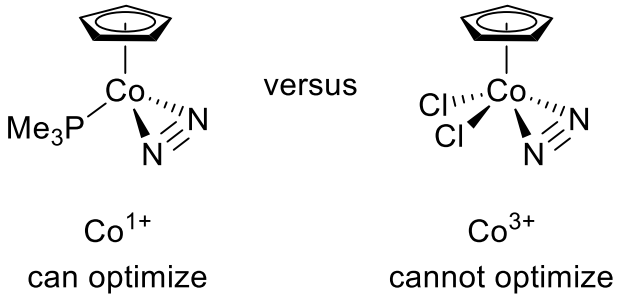


One may conclude that η^2-NN is a better π-acceptor than κ-N and requires a suitable low valent π-donor metal that is electron-rich in order to be the favored isomer. These

discoveries help to explain the well-known binding characteristics of N_2O and N_2, and they pave the way for more investigation into the chemistry of these incredible small molecules.

This study showed that the N_2 unit prefers to bind via the terminal nitrogen in a linear arrangement. It was demonstrated, nonetheless, that the strong π-donor characteristics of a low valent metal might change the choice for η^2-NN. It should also be noted that the weak π-donor characteristics of a high valent metal will not bind N_2 in side-bound coordination as seen in Scheme 4.2.

Scheme 4.2 Electronic effect on N_2 binding



4.2 Future Prospects

While this work offers significant insight into the potential binding of N_2O and N_2, many questions and research directions remain to be studied. The use of N_2O is desirable as it is a relatively "green oxidant".[1] However, understanding of its binding, specifically in a side-bound configuration is fairly limited as few complexes have been characterized. As such, future work could continue to investigate the η^2-NO binding mode of N_2O in order to find a system in which it is favored far more than the terminal-bound isomers. Likely metals to

investigate could be low oxidation state early metals because the metal needs to be a good electron rich π-donor.

Terminal and side-on coordination of N_2 to transition metal complexes offer possibilities for distinct pathways in ammonia synthesis and N_2 functionalization. Additionally, further investigation into the activation of N_2 through transition metal binding would be worthwhile. One could start, similar to N_2O, with low oxidation state early metals because the metal needs to be a good electron rich π-donor.

Furthermore, future work could consist of a computational examination of the transfer of an oxygen atom from N_2O to a metal core, with the systems from chapter 2. This study on how the preferred binding mechanism relates to the kinetics of O-atom transfer could be an important step toward making this potentially green oxidant more widely used.

4.3 References

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Appendix

XYZ Coordinates – Calculated Structures

$[Ni(C_{10}N_4H_{16})_2(N_2O)]$

κ-N

6	-2.140938000	-2.045558000	-0.818745000
6	-0.597413000	-0.516911000	-0.111296000
1	-2.535948000	-2.838825000	-1.434993000
6	4.604443000	-0.996899000	-0.199216000
6	4.104148000	-1.802056000	0.771188000
6	2.457791000	-0.338163000	0.175108000
7	3.593986000	-0.118061000	-0.554914000
1	5.576652000	-0.976256000	-0.666783000
1	4.554884000	-2.613072000	1.322204000
7	2.792707000	-1.397442000	0.979695000
6	1.918110000	-1.959256000	1.994820000
6	3.757699000	0.987737000	-1.497664000
1	3.007927000	0.919337000	-2.290250000
1	3.647545000	1.949267000	-0.974583000
1	4.752983000	0.914638000	-1.943306000
7	-1.746334000	-0.445961000	0.636716000

7	-0.866605000	-1.525188000	-0.999916000
6	-2.693897000	-1.366921000	0.218205000
1	-3.660759000	-1.461646000	0.688586000
6	-1.933207000	0.519467000	1.710771000
1	-2.891546000	1.033998000	1.592680000
1	-1.902470000	0.030792000	2.690830000
1	-1.119745000	1.244542000	1.635992000
6	0.045119000	-1.942241000	-2.053796000
28	0.884452000	0.645459000	0.081653000
1	1.065266000	-1.730712000	-1.731456000
1	-0.067393000	-3.015627000	-2.232546000
1	-0.155249000	-1.400475000	-2.984684000
1	1.981725000	-1.389901000	2.928697000
1	0.889733000	-1.929645000	1.631805000
1	2.207423000	-2.996140000	2.187892000
7	1.225795000	2.311947000	0.185097000
7	1.725627000	3.408243000	0.033361000
8	2.950878000	3.725566000	-0.058440000

κ-O

NA

η-NN

6	-2.418633000	-0.761678000	-1.190271000
6	-0.889392000	0.776777000	-0.472671000
1	-2.796740000	-1.570501000	-1.796635000
6	4.293745000	0.153009000	-0.255833000
6	3.695678000	-0.565299000	0.727348000
6	2.135567000	0.876090000	-0.114636000
7	3.336986000	1.021400000	-0.754774000
1	5.301618000	0.122105000	-0.640068000
1	4.080073000	-1.336999000	1.376372000
7	2.382707000	-0.120347000	0.794704000
6	1.421289000	-0.587084000	1.781128000
6	3.587023000	2.006968000	-1.806951000
1	3.052716000	1.731913000	-2.721737000
1	3.260872000	2.995979000	-1.469296000
1	4.659495000	2.022536000	-2.015643000
7	-2.063647000	0.886143000	0.222717000
7	-1.131618000	-0.260197000	-1.334544000
6	-3.004052000	-0.040734000	-0.202022000
1	-3.990066000	-0.106270000	0.232031000
6	-2.300729000	1.875213000	1.266600000
1	-3.253564000	2.381838000	1.088247000

1	-2.323182000	1.400162000	2.254055000
1	-1.494633000	2.606869000	1.217404000
6	-0.186008000	-0.717168000	-2.341531000
28	0.603344000	1.941251000	-0.377514000
1	0.825826000	-0.589575000	-1.955318000
1	-0.366071000	-1.774609000	-2.555168000
1	-0.289117000	-0.140873000	-3.267271000
1	1.447622000	0.037737000	2.680557000
1	0.421371000	-0.544142000	1.349309000
1	1.657261000	-1.619090000	2.055635000
7	-0.133317000	3.670750000	-0.568086000
7	1.099538000	3.663962000	-0.507858000
8	2.024420000	4.513930000	-0.538336000

η-NO (constrained)

6	-2.966131000	0.017230000	0.575884000
6	-1.334130000	1.342441000	-0.319307000
1	-3.414151000	-0.646660000	1.299542000
6	3.826180000	0.836456000	0.282525000
6	3.379119000	-0.062461000	-0.629785000
6	1.733705000	1.495415000	-0.337207000
7	2.819685000	1.773954000	0.447310000

1	4.759612000	0.892044000	0.821096000
1	3.847338000	-0.938360000	-1.051620000
7	2.102395000	0.346306000	-0.990424000
6	1.294833000	-0.309151000	-2.006113000
6	2.920281000	2.954548000	1.306090000
1	2.674626000	3.846349000	0.719066000
1	2.242783000	2.864291000	2.161164000
1	3.946435000	3.025833000	1.674654000
7	-2.458577000	1.346406000	-1.100070000
7	-1.672568000	0.503398000	0.708457000
6	-3.460261000	0.547132000	-0.571231000
1	-4.419782000	0.425121000	-1.050481000
6	-2.582665000	2.107236000	-2.338445000
1	-2.535960000	1.442083000	-3.208083000
1	-3.535189000	2.644796000	-2.348102000
1	-1.766598000	2.829231000	-2.372348000
6	-0.809634000	0.215033000	1.844344000
28	0.187915000	2.513680000	-0.535026000
1	0.226693000	0.348768000	1.534182000
1	-1.022757000	0.889947000	2.680480000
1	-0.964772000	-0.817989000	2.169635000

1	1.579499000	-1.363137000	-2.069158000
1	0.243136000	-0.230272000	-1.727201000
1	1.438687000	0.160003000	-2.985458000
7	0.726715000	4.249617000	-0.783700000
7	1.585728000	5.075605000	-0.797114000
8	-0.512094000	4.204249000	-0.944310000

$[Ni(PMe_3)_2(N_2O)]$

κ-N

28	2.497864000	0.050376000	-0.276226000
15	1.354148000	1.854317000	-0.123853000
15	1.313071000	-1.712046000	0.043613000
6	0.869197000	2.371838000	1.588249000
1	0.276560000	3.294620000	1.585627000
1	0.288280000	1.577009000	2.066829000
1	1.772944000	2.534854000	2.184251000
6	2.125038000	3.416198000	-0.759297000
1	2.361619000	3.294133000	-1.821227000
1	1.468501000	4.287495000	-0.638736000
1	3.064337000	3.600065000	-0.228471000
6	-0.268593000	1.913855000	-1.021024000
1	-0.930717000	1.123023000	-0.653185000

1	-0.772607000	2.880755000	-0.902210000
1	-0.094850000	1.738170000	-2.088021000
6	-0.025119000	-1.676899000	1.328255000
1	-0.758014000	-0.899931000	1.086373000
1	-0.546088000	-2.638350000	1.414984000
1	0.418245000	-1.430077000	2.299004000
6	2.230498000	-3.227417000	0.588837000
1	1.571455000	-4.097160000	0.703727000
1	3.011164000	-3.465855000	-0.140504000
1	2.720057000	-3.026272000	1.547442000
6	0.400866000	-2.352074000	-1.436993000
1	1.118818000	-2.587348000	-2.229270000
1	-0.178308000	-3.254044000	-1.204915000
1	-0.277490000	-1.581117000	-1.816223000
7	4.186574000	0.007649000	-0.632770000
7	5.321333000	-0.217653000	-0.842475000
8	6.447484000	0.213447000	-1.088758000

κ-O

28	2.450765000	0.133874000	-0.089502000
15	1.380653000	1.927466000	-0.148844000
15	1.461742000	-1.698798000	0.066043000

6	0.803635000	2.570258000	1.497671000
1	0.139366000	3.437240000	1.390937000
1	0.272143000	1.780529000	2.038399000
1	1.670848000	2.863289000	2.098741000
6	2.062802000	3.497258000	-0.888849000
1	2.323618000	3.313791000	-1.936990000
1	1.354920000	4.335914000	-0.845879000
1	2.978876000	3.783154000	-0.360617000
6	-0.234004000	1.873102000	-1.073324000
1	-0.877958000	1.094850000	-0.650569000
1	-0.767374000	2.831972000	-1.038442000
1	-0.042305000	1.616402000	-2.120891000
6	0.240289000	-1.801482000	1.465921000
1	-0.485217000	-0.985391000	1.386992000
1	-0.298701000	-2.757471000	1.474225000
1	0.768875000	-1.688837000	2.418607000
6	2.331057000	-3.330601000	0.327937000
1	1.638053000	-4.178993000	0.408627000
1	3.014099000	-3.517181000	-0.508338000
1	2.929100000	-3.280944000	1.244736000
6	0.390924000	-2.173009000	-1.378227000

1	1.024703000	-2.345206000	-2.254698000
1	-0.190309000	-3.082754000	-1.180488000
1	-0.296359000	-1.355757000	-1.617627000
8	4.395950000	0.199487000	0.091521000
7	5.360573000	-0.295806000	-0.438946000
7	6.274457000	-0.756218000	-0.943251000

η-NN

28	5.394728000	0.209776000	-0.375478000
15	4.240093000	2.034484000	-0.065491000
15	4.219556000	-1.550714000	0.074841000
6	3.843270000	2.497586000	1.680972000
1	3.304283000	3.450332000	1.741259000
1	3.237024000	1.716562000	2.150725000
1	4.778128000	2.584723000	2.244214000
6	5.110556000	3.543598000	-0.669476000
1	5.293889000	3.446873000	-1.743842000
1	4.534412000	4.456929000	-0.480756000
1	6.085060000	3.617654000	-0.178344000
6	2.605713000	2.190129000	-0.919792000
1	1.925322000	1.398883000	-0.588279000
1	2.133822000	3.162050000	-0.733669000

1	2.758298000	2.073912000	-1.997920000
6	2.801707000	-1.483166000	1.261281000
1	2.020243000	-0.814252000	0.885169000
1	2.362400000	-2.473331000	1.430073000
1	3.155358000	-1.089990000	2.220255000
6	5.276667000	-2.864680000	0.820012000
1	4.761288000	-3.830092000	0.882654000
1	6.185833000	-2.957692000	0.216972000
1	5.572633000	-2.553638000	1.827710000
6	3.477839000	-2.391459000	-1.393870000
1	4.272823000	-2.620109000	-2.110538000
1	2.968611000	-3.322148000	-1.117674000
1	2.760968000	-1.723000000	-1.881650000
7	7.077441000	0.813517000	-0.947534000
7	7.001109000	-0.413360000	-0.880566000
8	7.704974000	-1.422198000	-1.079341000

η-NO (constrained)

28	8.371732000	0.255442000	-0.326971000
15	7.162060000	2.102090000	-0.051057000
15	7.188766000	-1.475534000	0.122631000
6	6.734142000	2.614740000	1.674250000

1	6.215353000	3.580188000	1.702695000
1	6.099889000	1.857504000	2.146063000
1	7.657100000	2.693143000	2.258197000
6	8.081448000	3.578870000	-0.667978000
1	8.289764000	3.454176000	-1.735117000
1	7.521932000	4.509069000	-0.515632000
1	9.044555000	3.646296000	-0.152943000
6	5.553613000	2.270700000	-0.950981000
1	4.848237000	1.502993000	-0.616005000
1	5.096875000	3.256618000	-0.804185000
1	5.730800000	2.121107000	-2.021240000
6	5.795260000	-1.363051000	1.332927000
1	5.035706000	-0.658781000	0.976784000
1	5.319169000	-2.336411000	1.498664000
1	6.180813000	-0.995039000	2.289567000
6	8.210721000	-2.832850000	0.830025000
1	7.676724000	-3.789510000	0.851175000
1	9.123936000	-2.920400000	0.228842000
1	8.503371000	-2.564347000	1.850785000
6	6.394324000	-2.265694000	-1.346310000
1	7.170696000	-2.515377000	-2.076343000

1	5.854260000	-3.180118000	-1.074628000
1	5.696829000	-1.564417000	-1.815679000
7	9.978914000	-0.460750000	-0.807618000
7	10.668441000	-1.402402000	-0.983941000
8	10.046196000	0.834403000	-0.897358000

$[Ni(PH_3)_2(N_2O)]$

κ-N

28	-0.643771000	0.126938000	0.071479000
15	-1.739599000	1.923641000	-0.031528000
15	-1.779718000	-1.644962000	0.168721000
1	-1.227232000	-2.959405000	0.213292000
1	-2.672373000	-1.858514000	1.254897000
1	-2.715701000	-1.952463000	-0.856803000
1	-2.669811000	2.135330000	-1.086137000
1	-1.157552000	3.222003000	-0.133806000
1	-2.625742000	2.277639000	1.022827000
7	1.123182000	0.104083000	0.016617000
7	2.217631000	0.072642000	-0.323227000
8	3.385552000	0.042355000	-0.629056000

κ-O

28	-0.667513000	-0.096803000	-0.042343000

15	-1.469449000	1.802129000	-0.043900000
15	-1.897455000	-1.743833000	0.145820000
1	-1.530772000	-3.129046000	0.180832000
1	-2.743189000	-1.844086000	1.287567000
1	-2.927869000	-1.944950000	-0.816759000
1	-2.439005000	2.138202000	-1.032109000
1	-0.788811000	3.060235000	-0.156982000
1	-2.243932000	2.222998000	1.075297000
7	2.189534000	0.360076000	-0.313672000
8	1.239427000	-0.383769000	-0.231058000
7	3.100412000	1.033914000	-0.393178000

η-NN

28	-0.995579000	0.309165000	0.051600000
15	-2.196648000	2.122489000	-0.092930000
15	-2.256365000	-1.432417000	0.134774000
1	-1.590611000	-2.676936000	0.230489000
1	-3.173608000	-1.642769000	1.194785000
1	-3.124785000	-1.780036000	-0.930211000
1	-3.052290000	2.376040000	-1.194720000
1	-1.475394000	3.337284000	-0.152994000
1	-3.104296000	2.511551000	0.924476000

7	0.747456000	0.968827000	0.049463000
7	0.710937000	-0.255961000	0.127889000
8	1.444133000	-1.246405000	0.209164000

η-NO (constrained)

28	-1.062841000	0.250814000	0.053524000
15	-2.344848000	2.059593000	-0.095864000
15	-2.265627000	-1.501736000	0.154835000
1	-1.527741000	-2.707650000	0.253399000
1	-3.164050000	-1.743512000	1.224520000
1	-3.125941000	-1.893948000	-0.901517000
1	-3.214030000	2.291140000	-1.192203000
1	-1.657989000	3.295666000	-0.169791000
1	-3.251906000	2.438853000	0.926126000
7	0.629340000	-0.446430000	0.132094000
7	1.313148000	-1.395442000	0.209151000
8	0.692654000	0.849092000	0.044832000

$[Ni(CNMe)_2(N_2O)]$

κ-N

1	-3.067067000	-2.777803000	2.256621000
1	-1.752096000	-2.439794000	3.408420000
1	-3.252306000	-1.488580000	3.470945000

6	-1.311107000	-0.618611000	-4.280974000
1	-0.341261000	-0.884778000	-4.716541000
1	-1.944727000	-1.513601000	-4.265233000
1	-1.783671000	0.133062000	-4.923712000
7	0.474954000	1.890555000	0.291828000
7	1.494935000	2.336944000	0.555396000
8	2.557917000	2.834834000	0.836288000
28	-0.829782000	0.723694000	-0.159989000
6	-1.584156000	-0.259477000	1.115158000
6	-1.064526000	0.317235000	-1.875041000
7	-1.986149000	-1.046151000	1.901616000
7	-1.137990000	-0.105166000	-2.977381000
6	-2.540999000	-1.983440000	2.799700000

κ-O

28	-1.717791000	4.417905000	0.133446000
6	-1.985515000	2.704503000	0.089629000
6	-0.183359000	5.240067000	0.221466000
7	-2.030050000	1.511989000	0.167337000
7	0.921591000	5.652241000	0.375104000
6	-1.453570000	0.212815000	0.188678000
1	-1.762174000	-0.321559000	1.094210000

1	-1.797744000	-0.365919000	-0.676233000
1	-0.357112000	0.261477000	0.165596000
6	2.327482000	5.773906000	0.467110000
1	2.706599000	6.413626000	-0.338541000
1	2.607613000	6.230594000	1.423359000
1	2.814668000	4.793022000	0.392877000
7	-4.507570000	5.263066000	0.357709000
8	-3.356975000	5.623260000	0.334705000
7	-5.588002000	4.921427000	0.382738000

η-NN

1	-5.321995000	2.211817000	-3.505499000
1	-5.594407000	1.091246000	-2.147499000
1	-5.254447000	2.811821000	-1.827974000
6	0.690674000	-1.941789000	-4.821855000
1	0.188080000	-2.887846000	-4.596306000
1	0.515950000	-1.688523000	-5.872490000
1	1.766217000	-2.060785000	-4.657512000
7	-0.199162000	2.546689000	-0.878365000
7	0.764266000	1.897774000	-1.264627000
8	1.984067000	1.787154000	-1.097441000
28	-0.688618000	1.265391000	-2.169017000

6	-2.484301000	1.486497000	-2.361347000
6	-0.182592000	-0.057499000	-3.277820000
7	-3.637718000	1.682421000	-2.435307000
7	0.186746000	-0.915398000	-3.986995000
6	-5.024899000	1.964373000	-2.481447000

η-NO (constrained)

28	-1.843051000	0.716617000	0.303002000
6	-2.630034000	-0.915539000	0.680651000
6	-0.126677000	0.572949000	0.748644000
7	-3.102591000	-1.988679000	0.637712000
7	1.015479000	0.467413000	1.000688000
6	-3.726738000	-3.260573000	0.620462000
1	-4.607885000	-3.233584000	-0.028075000
1	-3.028672000	-4.014763000	0.243799000
1	-4.037100000	-3.536663000	1.633268000
6	2.398494000	0.414278000	1.295190000
1	2.971871000	0.862046000	0.477034000
1	2.604777000	0.968745000	2.216569000
1	2.717539000	-0.624809000	1.427511000
7	-2.005615000	2.373252000	-0.566134000
7	-1.503401000	3.359274000	-0.948528000

8	-3.155283000	1.768035000	-0.521700000

$[Ni(CO)_2(N_2O)]$

κ-N

28	0.133079000	0.709473000	0.131772000
6	-0.560090000	2.279021000	0.471436000
8	-0.896253000	3.371531000	0.622835000
6	1.868883000	0.583154000	-0.042559000
8	3.008957000	0.644989000	-0.203532000
7	-0.952614000	-0.705349000	-0.330872000
7	-1.593055000	-1.446127000	-0.913304000
8	-2.269338000	-2.237406000	-1.498408000

κ-O

28	-0.002559000	1.019250000	0.032347000
6	-0.394210000	2.634920000	0.482144000
8	-0.407340000	3.742371000	0.816276000
6	1.635729000	0.498375000	0.033698000
8	2.784880000	0.380747000	0.110923000
7	-1.420949000	-1.413637000	-0.832022000
8	-1.507360000	-0.257682000	-0.492309000
7	-1.361636000	-2.495293000	-1.151856000

η-NN

28	-0.384295000	0.050650000	0.295663000
6	-1.003355000	1.733444000	0.415660000
8	-1.397100000	2.803786000	0.492050000
6	1.370090000	0.139711000	0.054996000
8	2.500913000	0.232620000	-0.095083000
7	-1.916687000	-1.043554000	0.494809000
7	-0.931908000	-1.733598000	0.342151000
8	-0.500603000	-2.874548000	0.260638000

η-NO

8	1.896787000	-0.120699000	0.027297000
7	-1.624903000	-1.883798000	0.295462000
7	-1.318630000	-2.989415000	0.434820000
8	-2.594567000	-1.024917000	0.136384000
28	-0.989641000	-0.003871000	0.193691000
6	-1.375962000	1.711310000	0.620752000
8	-1.470399000	2.723934000	1.147964000
6	0.750206000	-0.128250000	0.089923000

[Co(η^5-Cp*)(CNMe)(N_2O)]

κ-N

6	-0.077040000	2.318317000	-0.162358000
6	-1.070686000	3.326605000	-0.111411000

6	-2.357152000	2.658256000	-0.111363000
6	-2.144952000	1.234454000	-0.053381000
6	-0.742059000	1.026126000	-0.145842000
27	-1.376003000	2.131262000	-1.811666000
7	-0.300720000	1.410906000	-3.068295000
7	0.439373000	1.009898000	-3.837446000
8	1.172641000	0.504416000	-4.656614000
6	-2.466275000	2.922183000	-2.941177000
7	-3.147093000	3.574507000	-3.678241000
6	-4.319990000	3.611439000	-4.498058000
1	-4.867971000	2.661040000	-4.463444000
1	-4.982082000	4.415696000	-4.160859000
1	-4.038707000	3.820898000	-5.535281000
6	-3.684991000	3.349454000	0.027008000
1	-4.501227000	2.739671000	-0.372722000
1	-3.909740000	3.551699000	1.083261000
1	-3.699215000	4.306919000	-0.502537000
6	-0.856313000	4.809846000	-0.012292000
1	-1.621226000	5.366308000	-0.562898000
1	-0.894141000	5.147697000	1.033705000
1	0.116301000	5.106139000	-0.417401000

6	1.411994000	2.519432000	-0.157270000
1	1.684981000	3.524321000	-0.493772000
1	1.827039000	2.384870000	0.851638000
1	1.923369000	1.805292000	-0.812100000
6	-0.035915000	-0.300628000	-0.119378000
1	0.862358000	-0.297715000	-0.746062000
1	0.284470000	-0.555961000	0.900348000
1	-0.681518000	-1.110393000	-0.473409000
6	-3.203004000	0.183885000	0.130037000
1	-2.909646000	-0.770443000	-0.318777000
1	-3.398630000	-0.002535000	1.196584000
1	-4.151954000	0.480839000	-0.327175000

κ-O

6	-0.071626000	2.271821000	-0.067164000
6	-1.023980000	3.320165000	-0.038440000
6	-2.336191000	2.703245000	-0.084577000
6	-2.179513000	1.266046000	-0.017440000
6	-0.786450000	1.005353000	-0.065645000
27	-1.345900000	2.150877000	-1.730132000
7	-0.038324000	1.366127000	-4.196503000
8	-0.022247000	1.303081000	-2.992207000

7	-0.028523000	1.398923000	-5.328154000
6	-2.320837000	2.917457000	-2.948759000
7	-2.910075000	3.575056000	-3.780685000
6	-4.084433000	3.368338000	-4.596887000
1	-4.526996000	2.373904000	-4.449204000
1	-4.834114000	4.129642000	-4.355401000
1	-3.822153000	3.487994000	-5.653552000
6	-3.640553000	3.443462000	0.009808000
1	-4.463202000	2.865824000	-0.423314000
1	-3.898139000	3.652468000	1.057600000
1	-3.598700000	4.400923000	-0.518474000
6	-0.754869000	4.792843000	0.077849000
1	-1.475460000	5.380645000	-0.499123000
1	-0.820057000	5.126694000	1.124015000
1	0.243680000	5.052884000	-0.287639000
6	1.424773000	2.408724000	-0.033286000
1	1.745553000	3.412136000	-0.330473000
1	1.819782000	2.221939000	0.975640000
1	1.915134000	1.695739000	-0.706019000
6	-0.124975000	-0.344676000	-0.041300000
1	0.736667000	-0.388998000	-0.717252000

1	0.244094000	-0.588197000	0.964994000
1	-0.816464000	-1.139371000	-0.338553000
6	-3.285444000	0.262676000	0.145151000
1	-3.010888000	-0.715346000	-0.263051000
1	-3.536385000	0.115980000	1.206531000
1	-4.199677000	0.582713000	-0.364071000

η-NN

6	-0.071626000	2.271821000	-0.067164000
6	-1.023980000	3.320165000	-0.038440000
6	-2.336191000	2.703245000	-0.084577000
6	-2.179513000	1.266046000	-0.017440000
6	-0.786450000	1.005353000	-0.065645000
27	-1.345900000	2.150877000	-1.730132000
7	-0.038324000	1.366127000	-4.196503000
8	-0.022247000	1.303081000	-2.992207000
7	-0.028523000	1.398923000	-5.328154000
6	-2.320837000	2.917457000	-2.948759000
7	-2.910075000	3.575056000	-3.780685000
6	-4.084433000	3.368338000	-4.596887000
1	-4.526996000	2.373904000	-4.449204000
1	-4.834114000	4.129642000	-4.355401000

1	-3.822153000	3.487994000	-5.653552000
6	-3.640553000	3.443462000	0.009808000
1	-4.463202000	2.865824000	-0.423314000
1	-3.898139000	3.652468000	1.057600000
1	-3.598700000	4.400923000	-0.518474000
6	-0.754869000	4.792843000	0.077849000
1	-1.475460000	5.380645000	-0.499123000
1	-0.820057000	5.126694000	1.124015000
1	0.243680000	5.052884000	-0.287639000
6	1.424773000	2.408724000	-0.033286000
1	1.745553000	3.412136000	-0.330473000
1	1.819782000	2.221939000	0.975640000
1	1.915134000	1.695739000	-0.706019000
6	-0.124975000	-0.344676000	-0.041300000
1	0.736667000	-0.388998000	-0.717252000
1	0.244094000	-0.588197000	0.964994000
1	-0.816464000	-1.139371000	-0.338553000
6	-3.285444000	0.262676000	0.145151000
1	-3.010888000	-0.715346000	-0.263051000
1	-3.536385000	0.115980000	1.206531000
1	-4.199677000	0.582713000	-0.364071000

η-NO

6	-0.206415000	2.205115000	-0.293455000
6	-1.256052000	3.170844000	-0.327489000
6	-2.494454000	2.514154000	0.084340000
6	-2.207281000	1.148116000	0.291923000
6	-0.806532000	0.938717000	0.001689000
27	-1.695078000	1.701598000	-1.714658000
7	-0.633644000	0.781237000	-2.947822000
7	0.369447000	0.667593000	-3.532603000
8	-1.786635000	0.055307000	-2.719890000
6	-2.588840000	2.677794000	-2.945360000
7	-3.192731000	3.299870000	-3.735808000
6	-3.902933000	3.991085000	-4.747761000
1	-4.969935000	3.751530000	-4.691455000
1	-3.773165000	5.071023000	-4.625591000
1	-3.523419000	3.696714000	-5.731229000
6	-3.803485000	3.214785000	0.311874000
1	-4.644741000	2.515663000	0.296023000
1	-3.811949000	3.721560000	1.286818000
1	-3.995155000	3.976377000	-0.451151000
6	-1.102123000	4.649440000	-0.551800000

1	-1.987258000	5.079586000	-1.031274000
1	-0.958729000	5.177636000	0.400954000
1	-0.242067000	4.873768000	-1.189245000
6	1.239646000	2.427102000	-0.633467000
1	1.477209000	3.493501000	-0.684449000
1	1.891847000	1.979825000	0.125708000
1	1.497078000	1.978641000	-1.603152000
6	-0.102934000	-0.385215000	0.084281000
1	0.910198000	-0.322643000	-0.321498000
1	-0.031500000	-0.730817000	1.124035000
1	-0.639423000	-1.147921000	-0.490126000
6	-3.159907000	0.055798000	0.680131000
1	-3.085206000	-0.792876000	-0.009186000
1	-2.939783000	-0.319140000	1.688633000
1	-4.198114000	0.399820000	0.673971000

[Co(η^5-Cp)(CNMe)(N_2O)]

κ-N

6	-0.093369000	2.479841000	-0.126377000
6	-1.182112000	3.379455000	-0.057993000
6	-2.373031000	2.583820000	-0.059454000
6	-2.009422000	1.192812000	-0.011744000

6	-0.602174000	1.131470000	-0.082658000
1	0.953347000	2.749725000	-0.188328000
1	-1.130620000	4.459294000	-0.041850000
1	-3.385121000	2.966136000	-0.032016000
1	-2.693298000	0.357006000	0.042708000
1	0.001168000	0.233098000	-0.103189000
27	-1.359610000	2.146679000	-1.772495000
7	-0.150475000	1.768099000	-3.056423000
7	0.624982000	1.489695000	-3.841953000
8	1.459713000	1.226704000	-4.674874000
6	-2.694157000	2.448849000	-2.884057000
7	-3.636769000	2.561003000	-3.601345000
6	-4.515865000	3.309937000	-4.436248000
1	-4.499212000	2.902598000	-5.452377000
1	-5.540710000	3.235619000	-4.058195000
1	-4.225925000	4.367696000	-4.472514000

κ-O

6	-0.136658000	2.433255000	0.070499000
6	-1.248850000	3.301506000	0.090653000
6	-2.431587000	2.483503000	-0.009520000
6	-2.042490000	1.102160000	0.001117000

6	-0.628952000	1.080607000	-0.006762000
1	0.906019000	2.721967000	0.104913000
1	-1.227073000	4.380914000	0.153498000
1	-3.448165000	2.853650000	-0.023483000
1	-2.703431000	0.246469000	-0.007181000
1	-0.008228000	0.194149000	-0.056641000
27	-1.322377000	2.182878000	-1.657110000
7	0.060456000	1.644459000	-4.138658000
8	0.079083000	1.536488000	-2.937740000
7	0.076949000	1.722719000	-5.267774000
6	-2.372350000	2.883818000	-2.853747000
7	-3.042311000	3.483304000	-3.660498000
6	-4.190259000	3.226335000	-4.493470000
1	-4.552700000	2.194705000	-4.393123000
1	-4.997663000	3.914711000	-4.222302000
1	-3.932847000	3.414327000	-5.541117000

η-NN

6	-0.418612000	2.885047000	-0.997074000
6	-1.464705000	3.835662000	-1.043295000
6	-2.704325000	3.157151000	-0.727623000
6	-2.410532000	1.796867000	-0.508598000

6	-1.008386000	1.614215000	-0.723844000
1	0.626221000	3.070130000	-1.207206000
1	-1.360420000	4.891763000	-1.253964000
1	-3.679228000	3.622277000	-0.668146000
1	-3.124935000	1.012870000	-0.296398000
1	-0.482326000	0.669602000	-0.678595000
27	-1.837529000	2.379974000	-2.484840000
7	-1.952998000	0.731013000	-3.546228000
7	-0.922911000	1.334959000	-3.745181000
8	0.146450000	1.293414000	-4.361531000
6	-2.659971000	3.397779000	-3.726398000
7	-3.206738000	4.049414000	-4.532901000
6	-3.841246000	4.800407000	-5.552426000
1	-3.116111000	5.064915000	-6.328873000
1	-4.647845000	4.212614000	-6.002074000
1	-4.262227000	5.718202000	-5.130467000

η-NO

6	-0.218644000	2.449515000	-0.423533000
6	-1.413723000	3.211422000	-0.372034000
6	-2.463278000	2.370903000	0.163547000
6	-1.921809000	1.093163000	0.373523000

6	-0.544709000	1.121928000	-0.030867000
1	0.739609000	2.788196000	-0.794509000
1	-1.514434000	4.256833000	-0.632309000
1	-3.486140000	2.675038000	0.341649000
1	-2.461371000	0.216020000	0.705702000
1	0.131562000	0.277448000	-0.021683000
27	-1.694392000	1.641904000	-1.704783000
7	-0.645515000	0.841550000	-3.060222000
7	0.272213000	0.887075000	-3.773695000
8	-1.635711000	-0.012290000	-2.680916000
6	-2.812148000	2.441203000	-2.876694000
7	-3.558046000	2.937808000	-3.631253000
6	-4.442487000	3.499591000	-4.584699000
1	-5.396970000	2.963579000	-4.573102000
1	-4.621572000	4.553431000	-4.350442000
1	-4.003439000	3.426104000	-5.584502000

[Co(η^5-Cp)(PMe_3)(N_2O)]

κ-N

6	0.132163000	1.490694000	-0.220354000
6	-0.336195000	2.750451000	0.286965000
6	-1.748236000	2.707170000	0.370961000

6	-2.152881000	1.428089000	-0.139056000
6	-0.988665000	0.655061000	-0.453262000
1	1.168056000	1.235310000	-0.401539000
1	0.293281000	3.592455000	0.545074000
1	-2.400640000	3.484255000	0.744933000
1	-3.174462000	1.073091000	-0.201460000
1	-0.973636000	-0.364387000	-0.813580000
27	-1.124517000	2.403428000	-1.620540000
15	-2.767377000	2.463014000	-3.033363000
7	0.008673000	3.177957000	-2.709994000
7	0.750375000	3.863418000	-3.295045000
8	1.650194000	3.995510000	-4.124713000
6	-4.306100000	3.321002000	-2.462562000
1	-5.097172000	3.285978000	-3.220793000
1	-4.676606000	2.854960000	-1.544226000
1	-4.071821000	4.366658000	-2.240064000
6	-2.439973000	3.320101000	-4.634893000
1	-1.613849000	2.829115000	-5.157365000
1	-3.325975000	3.309826000	-5.279352000
1	-2.150712000	4.358138000	-4.445081000
6	-3.430599000	0.832118000	-3.607209000

1	-3.755574000	0.237636000	-2.747523000
1	-4.276737000	0.954195000	-4.293748000
1	-2.633720000	0.281692000	-4.116817000

κ-O

6	0.171251000	1.930410000	0.067940000
6	-0.492095000	3.179709000	-0.035579000
6	-1.889443000	2.901485000	0.122991000
6	-2.064936000	1.502596000	0.439437000
6	-0.788322000	0.903323000	0.389710000
1	1.236893000	1.768252000	-0.046751000
1	-0.035931000	4.149688000	-0.178597000
1	-2.681680000	3.640618000	0.106902000
1	-2.999720000	1.019584000	0.691239000
1	-0.557567000	-0.139695000	0.566384000
27	-1.248421000	1.812542000	-1.450253000
15	-2.805020000	2.350724000	-2.817150000
7	0.355934000	1.003477000	-3.690835000
8	-0.154415000	0.661885000	-2.649041000
7	0.839805000	1.239700000	-4.689830000
6	-4.537024000	2.027068000	-2.231582000
1	-5.288538000	2.381027000	-2.947780000

1	-4.669586000	0.952396000	-2.073310000
1	-4.699665000	2.530269000	-1.273246000
6	-2.960539000	4.130632000	-3.332222000
1	-2.058456000	4.431254000	-3.874775000
1	-3.837602000	4.311288000	-3.966440000
1	-3.034756000	4.757915000	-2.437938000
6	-2.851965000	1.517480000	-4.478095000
1	-2.859340000	0.430271000	-4.348292000
1	-3.746373000	1.807216000	-5.041560000
1	-1.974849000	1.791212000	-5.074065000

η-NN

6	-0.194517000	2.651509000	-0.460765000
6	-1.501707000	3.210892000	-0.266835000
6	-2.374380000	2.199505000	0.236907000
6	-1.618979000	0.998097000	0.290731000
6	-0.280638000	1.276241000	-0.120663000
1	0.684033000	3.179132000	-0.805804000
1	-1.766972000	4.249431000	-0.423430000
1	-3.414940000	2.321907000	0.503696000
1	-2.001093000	0.020784000	0.555291000
1	0.515200000	0.548023000	-0.207460000

27	-1.619923000	1.723531000	-1.691736000
15	-2.276014000	3.052404000	-3.309605000
7	-2.290576000	0.101451000	-2.564670000
7	-1.143448000	0.377945000	-2.861336000
8	-0.195806000	-0.032481000	-3.553246000
6	-1.127131000	4.431905000	-3.744395000
1	-0.955681000	5.071365000	-2.872789000
1	-0.165286000	4.011143000	-4.053501000
1	-1.526022000	5.045920000	-4.559874000
6	-3.884090000	3.923208000	-3.045976000
1	-4.147901000	4.552171000	-3.903947000
1	-4.671850000	3.178821000	-2.894216000
1	-3.831452000	4.550579000	-2.150699000
6	-2.530016000	2.205242000	-4.923753000
1	-1.607287000	1.693592000	-5.212450000
1	-3.311785000	1.448760000	-4.812856000
1	-2.816154000	2.917766000	-5.704700000

η-NO

6	-0.111594000	2.541751000	-0.350930000
6	-1.390242000	3.145631000	-0.228314000
6	-2.303833000	2.170899000	0.323941000

6	-1.592973000	0.968007000	0.471225000
6	-0.245427000	1.177089000	0.030485000
1	0.780933000	3.011225000	-0.743037000
1	-1.622053000	4.181755000	-0.440670000
1	-3.344933000	2.338408000	0.564822000
1	-2.006688000	0.019280000	0.787678000
1	0.530783000	0.424662000	-0.005916000
27	-1.511120000	1.575199000	-1.590347000
15	-2.861415000	2.528323000	-3.043997000
7	-0.532291000	0.843911000	-2.968411000
7	0.312097000	0.881767000	-3.771471000
8	-1.504669000	-0.085671000	-2.529003000
6	-4.384560000	3.340646000	-2.389027000
1	-4.118246000	4.119069000	-1.667553000
1	-4.969986000	3.794726000	-3.196350000
1	-5.004174000	2.596652000	-1.878791000
6	-3.520113000	1.371895000	-4.313393000
1	-4.177513000	1.893483000	-5.017731000
1	-2.687229000	0.918099000	-4.855694000
1	-4.070938000	0.567402000	-3.819343000
6	-2.068571000	3.858480000	-4.046724000

1	-2.743215000	4.246314000	-4.818278000
1	-1.760319000	4.682521000	-3.395272000
1	-1.172760000	3.446293000	-4.521945000

[Co(η^5-Cp)(PH_3)(N_2O)]

κ-N

6	0.037099000	2.061459000	-0.001231000
6	-0.719276000	3.276183000	0.044009000
6	-2.083063000	2.912006000	-0.048934000
6	-2.170314000	1.467709000	-0.083320000
6	-0.858846000	0.943215000	-0.014288000
1	1.118094000	1.995954000	0.004752000
1	-0.318985000	4.278355000	0.114481000
1	-2.927436000	3.589319000	-0.050650000
1	-3.088755000	0.896173000	-0.116991000
1	-0.578186000	-0.101040000	0.000102000
27	-1.095239000	2.169042000	-1.711318000
1	-2.902586000	1.398114000	-4.171266000
1	-3.994395000	2.448572000	-2.690541000
1	-2.738789000	3.499201000	-4.036663000
15	-2.663141000	2.375655000	-3.167437000
7	0.213898000	2.060855000	-2.904669000

7	1.124791000	2.159799000	-3.603230000
8	2.030883000	1.865463000	-4.362051000

κ-O

6	-0.015762000	2.375164000	0.160805000
6	-1.009690000	3.374634000	0.067106000
6	-2.266566000	2.688822000	-0.084956000
6	-2.054499000	1.269677000	0.035963000
6	-0.658721000	1.079721000	0.141847000
1	1.050880000	2.539697000	0.251674000
1	-0.863445000	4.445437000	0.106768000
1	-3.233108000	3.169796000	-0.176397000
1	-2.819469000	0.505307000	0.048518000
1	-0.145893000	0.128693000	0.216585000
27	-1.076476000	2.120312000	-1.606486000
1	-1.921822000	2.586059000	-4.539941000
1	-3.648441000	2.244835000	-3.378057000
1	-2.719776000	4.130549000	-3.345331000
15	-2.335113000	2.766625000	-3.187713000
7	0.655661000	1.299375000	-3.841457000
8	0.432158000	1.389023000	-2.660206000
7	0.905065000	1.194700000	-4.945037000

η-NN

6	-0.111233000	2.446441000	-0.292399000
6	-1.323385000	3.193571000	-0.244997000
6	-2.396775000	2.325416000	0.165477000
6	-1.849358000	1.032425000	0.303494000
6	-0.448132000	1.095953000	0.007965000
1	0.868290000	2.825531000	-0.549214000
1	-1.413180000	4.256832000	-0.432338000
1	-3.427827000	2.612997000	0.319165000
1	-2.398784000	0.128340000	0.530689000
1	0.232275000	0.254502000	0.003902000
27	-1.510584000	1.709500000	-1.663477000
1	-2.468159000	2.414083000	-4.506305000
1	-3.495791000	3.676921000	-3.118275000
1	-1.506793000	4.147527000	-3.694541000
15	-2.246299000	3.022821000	-3.251847000
7	-1.987071000	0.084280000	-2.647991000
7	-0.847664000	0.451996000	-2.855782000
8	0.186993000	0.140713000	-3.459082000

η-NO

6	0.153826000	2.239560000	-0.223368000

6	-0.782992000	3.301837000	-0.244490000
6	-2.053879000	2.791077000	0.225459000
6	-1.900112000	1.417109000	0.477562000
6	-0.546933000	1.057650000	0.158642000
1	1.189434000	2.294523000	-0.532133000
1	-0.574807000	4.329919000	-0.510995000
1	-2.958898000	3.370884000	0.353442000
1	-2.677043000	0.732096000	0.790485000
1	-0.129133000	0.061324000	0.216381000
27	-1.399864000	1.815668000	-1.559307000
1	-2.084184000	2.873952000	-4.421432000
1	-3.862395000	2.728559000	-3.252780000
1	-2.551619000	4.391395000	-2.992821000
15	-2.481996000	2.980547000	-3.069026000
8	-1.746389000	0.233201000	-2.530502000
7	-0.534191000	0.726666000	-2.905080000
7	0.358632000	0.452494000	-3.600604000

[Co(η^5-Cp)(CO)(N_2O)]

κ-N

6	-0.064953000	2.386073000	-0.009504000
6	-1.096342000	3.346363000	0.014675000

6	-2.331176000	2.634944000	-0.171935000
6	-2.061337000	1.223532000	-0.191325000
6	-0.660634000	1.075670000	-0.136947000
1	0.996697000	2.585140000	0.060766000
1	-0.984543000	4.417028000	0.114917000
1	-3.314486000	3.085649000	-0.210062000
1	-2.795060000	0.433538000	-0.271495000
1	-0.113622000	0.142461000	-0.176751000
27	-1.171488000	2.266005000	-1.799663000
7	0.120060000	1.790620000	-2.980695000
7	0.947984000	1.481125000	-3.695650000
8	1.826290000	1.152681000	-4.449561000
6	-2.286549000	2.889971000	-2.970099000
8	-3.063764000	3.318105000	-3.714482000

κ-O

6	-0.120110000	2.351463000	0.182866000
6	-1.112757000	3.343010000	0.055884000
6	-2.344035000	2.661602000	-0.250816000
6	-2.121607000	1.240461000	-0.188169000
6	-0.742190000	1.055105000	0.031028000
1	0.933161000	2.520179000	0.368934000

1	-0.978431000	4.412303000	0.143460000
1	-3.300663000	3.139922000	-0.416013000
1	-2.869315000	0.469575000	-0.313606000
1	-0.225139000	0.105203000	0.085172000
27	-1.036784000	2.205589000	-1.709016000
7	0.760923000	1.568877000	-3.889155000
8	0.565860000	1.539833000	-2.698578000
7	0.988282000	1.574755000	-4.997429000
6	-1.949746000	2.812630000	-3.036266000
8	-2.611139000	3.240788000	-3.893174000

η-NN

6	-0.436746000	2.950379000	-1.064778000
6	-1.543699000	3.831626000	-1.079163000
6	-2.720692000	3.086639000	-0.676680000
6	-2.330217000	1.754099000	-0.441814000
6	-0.931495000	1.654610000	-0.729630000
1	0.581827000	3.194287000	-1.334579000
1	-1.519086000	4.886181000	-1.320127000
1	-3.717953000	3.493446000	-0.575347000
1	-2.980344000	0.932895000	-0.172200000
1	-0.345677000	0.745379000	-0.691794000

27	-1.900196000	2.319050000	-2.454645000
7	-1.967433000	0.620570000	-3.447321000
7	-0.977323000	1.252276000	-3.721915000
8	0.070859000	1.259555000	-4.361656000
6	-2.817149000	3.250293000	-3.634706000
8	-3.440967000	3.885289000	-4.362080000

η-NO

6	-0.137221000	2.240481000	-0.215817000
6	-1.151518000	3.229921000	-0.308479000
6	-2.430129000	2.596322000	-0.056049000
6	-2.198183000	1.223026000	0.113823000
6	-0.786556000	0.990772000	-0.028409000
1	0.923025000	2.395469000	-0.364604000
1	-0.995933000	4.288015000	-0.473228000
1	-3.388482000	3.097719000	-0.034599000
1	-2.950359000	0.458135000	0.254277000
1	-0.302760000	0.023829000	0.016122000
27	-1.467607000	1.846490000	-1.812269000
7	-0.329939000	0.854633000	-3.031001000
7	0.714661000	0.750264000	-3.523799000
8	-1.515982000	0.260408000	-2.910227000

6	-2.106864000	2.939933000	-3.033807000
8	-2.567415000	3.684374000	-3.779186000

[Co(η^5-Cp)py(N_2O)]

κ-N

6	-0.112042000	2.814938000	-0.109584000
6	-1.322855000	3.548891000	-0.080292000
6	-2.391874000	2.593993000	0.023529000
6	-1.846116000	1.284234000	0.132478000
6	-0.436779000	1.421471000	-0.011786000
1	0.884802000	3.222468000	-0.213373000
1	-1.425271000	4.625676000	-0.114993000
1	-3.447623000	2.836533000	0.048179000
1	-2.398229000	0.364718000	0.270049000
1	0.281451000	0.611997000	-0.038639000
27	-1.324578000	2.209627000	-1.708416000
7	-0.230645000	1.635681000	-2.958138000
7	0.463944000	1.052180000	-3.699882000
8	1.405311000	1.077960000	-4.493035000
7	-2.698622000	2.687175000	-2.972212000
6	-3.388567000	3.847627000	-2.876662000
6	-3.036742000	1.849527000	-3.980043000

6	-4.411045000	4.197467000	-3.749085000
1	-3.088886000	4.509650000	-2.073945000
6	-4.039239000	2.134646000	-4.898897000
1	-2.469727000	0.928977000	-4.039197000
6	-4.750028000	3.329193000	-4.787029000
1	-4.922357000	5.145420000	-3.615623000
1	-4.256583000	1.419323000	-5.685526000
1	-5.540506000	3.577845000	-5.488567000

κ-O

6	-0.198368000	2.243019000	0.159723000
6	-1.316367000	3.083007000	0.404551000
6	-2.472431000	2.331196000	0.017066000
6	-2.072584000	0.992140000	-0.340770000
6	-0.660392000	0.948173000	-0.265702000
1	0.841801000	2.518277000	0.288549000
1	-1.301025000	4.088068000	0.803635000
1	-3.494065000	2.691227000	0.052743000
1	-2.733165000	0.169944000	-0.585565000
1	-0.029211000	0.094931000	-0.480340000
27	-1.279559000	2.448498000	-1.603117000
7	0.421212000	2.303840000	-3.982662000

8	0.302798000	2.545468000	-2.804758000
7	0.579522000	2.116553000	-5.092081000
7	-2.479460000	3.016584000	-2.919096000
6	-3.735216000	2.489782000	-3.034036000
6	-2.165190000	3.998318000	-3.816765000
6	-4.650468000	2.893765000	-3.991636000
1	-3.977159000	1.707714000	-2.326085000
6	-3.020570000	4.427826000	-4.819153000
1	-1.196412000	4.466630000	-3.681951000
6	-4.299971000	3.876223000	-4.922887000
1	-5.629045000	2.423479000	-4.013049000
1	-2.687770000	5.209695000	-5.495288000
1	-4.995234000	4.202174000	-5.689600000

η-NN

6	-0.542964000	3.391957000	-1.116383000
6	-1.890574000	3.840649000	-0.895820000
6	-2.674170000	2.757933000	-0.419818000
6	-1.831958000	1.608060000	-0.428252000
6	-0.517969000	2.004094000	-0.824962000
1	0.295529000	4.000529000	-1.428002000
1	-2.247589000	4.850795000	-1.056860000

1	-3.721971000	2.789071000	-0.154705000
1	-2.137130000	0.596057000	-0.196841000
1	0.331611000	1.342947000	-0.935979000
27	-1.892981000	2.359800000	-2.368811000
7	-2.628503000	0.782767000	-3.249238000
7	-1.461701000	0.992588000	-3.529462000
8	-0.523870000	0.526995000	-4.192711000
7	-2.426061000	3.522655000	-3.843207000
6	-1.706406000	4.615143000	-4.175166000
6	-3.552420000	3.270774000	-4.542885000
6	-2.084180000	5.486878000	-5.189193000
1	-0.798173000	4.775246000	-3.606848000
6	-3.993589000	4.094338000	-5.573582000
1	-4.082023000	2.366917000	-4.266779000
6	-3.252608000	5.227072000	-5.905309000
1	-1.462243000	6.347220000	-5.413594000
1	-4.906952000	3.841803000	-6.102092000
1	-3.572579000	5.887406000	-6.705904000

η-NO

NA

[Co(η^5-Cp)py(p-NMe)$_2$(N$_2$O)]

κ-N

6	-0.135729000	2.903356000	-0.041238000
6	-1.455361000	3.414694000	0.052361000
6	-2.339023000	2.284397000	0.096290000
6	-1.573871000	1.083999000	0.105997000
6	-0.211586000	1.472134000	-0.035889000
1	0.773237000	3.483677000	-0.128805000
1	-1.743058000	4.456968000	0.094965000
1	-3.420359000	2.337470000	0.139785000
1	-1.957563000	0.075817000	0.181867000
1	0.635188000	0.803723000	-0.124668000
27	-1.250336000	2.214142000	-1.666826000
7	-0.119231000	1.976138000	-2.978423000
7	0.620030000	1.585509000	-3.808803000
8	1.472701000	1.920082000	-4.640601000
7	-2.745893000	2.468117000	-2.878144000
6	-3.608721000	3.501095000	-2.766155000
6	-2.987654000	1.599185000	-3.884176000
6	-4.695099000	3.698486000	-3.597748000
1	-3.400490000	4.204918000	-1.968806000
6	-4.042651000	1.714558000	-4.770016000

1	-2.284296000	0.780559000	-3.979590000
6	-4.956497000	2.789113000	-4.651417000
1	-5.322609000	4.564192000	-3.428372000
1	-4.145131000	0.967672000	-5.546804000
7	-6.020874000	2.940460000	-5.500161000
6	-6.894777000	4.097609000	-5.371907000
1	-7.692165000	4.027393000	-6.112862000
1	-7.360688000	4.137924000	-4.379002000
1	-6.355955000	5.041176000	-5.537626000
6	-6.201605000	2.016512000	-6.611124000
1	-5.353170000	2.042508000	-7.308990000
1	-6.323796000	0.984879000	-6.257125000
1	-7.102674000	2.290872000	-7.161189000

κ-O

NA

η-NN

6	-0.797917000	3.511710000	-0.921590000
6	-2.222496000	3.609550000	-0.774122000
6	-2.751848000	2.333336000	-0.446370000
6	-1.660246000	1.418241000	-0.476417000
6	-0.459491000	2.144578000	-0.740598000

1	-0.113451000	4.325410000	-1.121030000
1	-2.801560000	4.518096000	-0.887735000
1	-3.790083000	2.095557000	-0.260062000
1	-1.726572000	0.345743000	-0.348628000
1	0.528365000	1.713134000	-0.836990000
27	-1.783192000	2.318260000	-2.355668000
7	-2.014179000	0.709979000	-3.433054000
7	-0.938572000	1.257048000	-3.601941000
8	0.120413000	1.133482000	-4.237335000
7	-2.548322000	3.446435000	-3.754908000
6	-2.108010000	4.699614000	-3.992282000
6	-3.565648000	3.008348000	-4.527245000
6	-2.643505000	5.537522000	-4.951846000
1	-1.277010000	5.033120000	-3.381228000
6	-4.165169000	3.771425000	-5.511828000
1	-3.880827000	1.986950000	-4.349184000
6	-3.719050000	5.092255000	-5.759400000
1	-2.213474000	6.523304000	-5.073852000
1	-4.971094000	3.330078000	-6.083911000
7	-4.286371000	5.886003000	-6.719094000
6	-3.744202000	7.211882000	-6.981808000

1	-4.340985000	7.694905000	-7.756518000
1	-3.782388000	7.843163000	-6.085007000
1	-2.702493000	7.168902000	-7.329095000
6	-5.342597000	5.355718000	-7.570729000
1	-6.207956000	5.032982000	-6.978297000
1	-5.676933000	6.137541000	-8.253839000
1	-4.997151000	4.501768000	-8.169647000

η-NO

NA

[Co(η^5-Cp)py(p-NO)$_2$(N$_2$O)]

κ-N

6	0.117234000	2.454012000	-0.249454000
6	-0.455147000	3.742124000	-0.431233000
6	-1.852524000	3.598753000	-0.197352000
6	-2.120843000	2.252685000	0.237507000
6	-0.899880000	1.544248000	0.199645000
1	1.157404000	2.196951000	-0.406716000
1	0.061377000	4.645078000	-0.725942000
1	-2.586848000	4.390000000	-0.285266000
1	-3.081792000	1.858745000	0.542498000
1	-0.750891000	0.502152000	0.449860000

27	-1.347110000	2.310844000	-1.717114000
7	-0.395046000	1.272019000	-2.853507000
7	0.252907000	0.510510000	-3.404191000
8	0.968989000	-0.235802000	-4.023321000
7	-2.740221000	2.655647000	-2.932176000
6	-4.019363000	2.898730000	-2.510326000
6	-2.542775000	2.695741000	-4.285669000
6	-5.072819000	3.172062000	-3.359381000
1	-4.182399000	2.849802000	-1.442857000
6	-3.542210000	2.945406000	-5.204613000
1	-1.527646000	2.530614000	-4.620807000
6	-4.833804000	3.193540000	-4.734905000
1	-6.067768000	3.353490000	-2.973294000
1	-3.331141000	2.965329000	-6.266176000
7	-5.912186000	3.470833000	-5.662750000
8	-5.640970000	3.480509000	-6.868512000
8	-7.034776000	3.679508000	-5.189273000

κ-O

6	1.293616000	-0.333188000	-4.979509000
6	1.716987000	1.017507000	-4.965327000
6	2.077696000	1.351906000	-3.608387000

6	1.926805000	0.191883000	-2.792676000
6	1.376953000	-0.817723000	-3.630894000
1	0.966115000	-0.898943000	-5.842002000
1	1.778720000	1.677051000	-5.821620000
1	2.446223000	2.313413000	-3.273026000
1	2.165880000	0.101776000	-1.742024000
1	1.097858000	-1.815039000	-3.308799000
27	0.124275000	0.841613000	-3.674857000
7	-1.811482000	-1.335338000	-3.459221000
8	-1.611219000	-0.146811000	-3.433617000
7	-2.038174000	-2.445489000	-3.490427000
7	-0.740537000	2.476588000	-3.518651000
6	-1.940634000	2.634572000	-2.866370000
6	-0.203832000	3.628171000	-4.044569000
6	-2.602620000	3.836056000	-2.744549000
1	-2.360314000	1.742303000	-2.421568000
6	-0.794484000	4.868806000	-3.952847000
1	0.733848000	3.513461000	-4.569598000
6	-2.023536000	4.985777000	-3.294213000
1	-3.546759000	3.899467000	-2.218660000
1	-0.326344000	5.740795000	-4.391697000

7	-2.677918000	6.263406000	-3.181160000
8	-2.117028000	7.246036000	-3.686820000
8	-3.763980000	6.304347000	-2.585404000

η-NN

6	-0.491622000	3.423074000	-1.222266000
6	-1.818699000	3.895974000	-0.928790000
6	-2.575948000	2.838254000	-0.365425000
6	-1.745552000	1.679671000	-0.389466000
6	-0.455604000	2.048739000	-0.881499000
1	0.329988000	4.009945000	-1.611267000
1	-2.176618000	4.904628000	-1.096682000
1	-3.605346000	2.886680000	-0.038258000
1	-2.044066000	0.679914000	-0.102938000
1	0.380712000	1.376665000	-1.022700000
27	-1.935035000	2.361708000	-2.342282000
7	-2.801851000	0.769287000	-3.067558000
7	-1.643833000	0.885017000	-3.421790000
8	-0.763735000	0.328568000	-4.088143000
7	-2.477579000	3.454630000	-3.850036000
6	-1.804212000	4.582208000	-4.180381000
6	-3.571091000	3.136463000	-4.582378000

6	-2.188957000	5.422124000	-5.214537000
1	-0.921223000	4.799796000	-3.594036000
6	-4.025206000	3.914750000	-5.639039000
1	-4.069614000	2.215900000	-4.304965000
6	-3.319539000	5.072134000	-5.945033000
1	-1.626888000	6.315058000	-5.455744000
1	-4.904467000	3.634695000	-6.204828000
7	-3.767507000	5.933128000	-7.051603000
8	-3.103535000	6.941757000	-7.282774000
8	-4.774285000	5.584083000	-7.663599000

η-NO

6	0.407591000	2.190583000	-0.306625000
6	-0.538463000	3.233266000	-0.146158000
6	-1.770514000	2.635861000	0.309266000
6	-1.583947000	1.244893000	0.415997000
6	-0.250716000	0.959667000	-0.024394000
1	1.420101000	2.298262000	-0.672980000
1	-0.350469000	4.290133000	-0.283905000
1	-2.689471000	3.170011000	0.517261000
1	-2.332695000	0.515680000	0.694176000
1	0.181338000	-0.026085000	-0.131438000

27	-1.220928000	1.883782000	-1.609143000
7	-0.289088000	1.335245000	-3.109097000
8	-1.281339000	0.371276000	-2.764262000
7	0.534855000	1.463147000	-3.916844000
7	-2.508543000	2.857133000	-2.695532000
6	-3.230761000	2.198789000	-3.633680000
6	-2.749898000	4.178326000	-2.524090000
6	-4.206249000	2.818708000	-4.403937000
1	-2.974822000	1.152435000	-3.752225000
6	-3.704149000	4.876727000	-3.248107000
1	-2.145717000	4.685055000	-1.783496000
6	-4.438529000	4.172742000	-4.196796000
1	-4.769540000	2.265857000	-5.144770000
1	-3.871067000	5.934222000	-3.089387000
7	-5.463743000	4.871809000	-4.988696000
8	-5.626406000	6.069927000	-4.764568000
8	-6.085910000	4.208244000	-5.814798000

[Ir(η^5-Cp)(CNMe)(N_2O)]

κ-N

6	-0.093967000	2.589535000	0.067010000
6	-1.264010000	3.379523000	0.085722000

6	-2.388995000	2.467922000	0.091287000
6	-1.878770000	1.119902000	0.246581000
6	-0.473380000	1.197856000	0.175192000
1	0.921238000	2.958820000	0.003311000
1	-1.315596000	4.458107000	0.043001000
1	-3.428718000	2.755782000	0.173535000
1	-2.471981000	0.221389000	0.339929000
1	0.212728000	0.361382000	0.198115000
77	-1.447239000	2.080628000	-1.851968000
7	-0.227007000	1.659526000	-3.352526000
7	0.496203000	1.402765000	-4.191780000
8	1.273259000	1.136577000	-5.076791000
6	-2.849350000	2.331669000	-3.043497000
7	-3.780778000	2.419806000	-3.800721000
6	-4.445136000	3.421695000	-4.593940000
1	-4.439269000	3.118401000	-5.645745000
1	-5.489642000	3.505930000	-4.276693000
1	-3.962250000	4.402320000	-4.501405000

κ-O

6	-0.170134000	2.674510000	0.247111000
6	-1.405013000	3.343292000	0.265901000

6	-2.438325000	2.325138000	0.104756000
6	-1.792293000	1.016609000	0.187770000
6	-0.405650000	1.244397000	0.211741000
1	0.805000000	3.144435000	0.257614000
1	-1.563669000	4.410990000	0.317185000
1	-3.504036000	2.498854000	0.179188000
1	-2.292827000	0.058784000	0.184967000
1	0.364770000	0.484531000	0.202596000
7	-0.049844000	1.214483000	-4.313529000
8	0.155562000	2.053041000	-3.468634000
7	-0.206529000	0.444067000	-5.124039000
6	-2.718021000	2.388740000	-3.069201000
7	-3.536709000	2.430710000	-3.970355000
6	-4.117624000	3.555334000	-4.677458000
1	-3.939869000	3.442134000	-5.752227000
1	-5.201967000	3.559303000	-4.522085000
1	-3.704951000	4.516579000	-4.345296000
77	-1.441304000	2.195998000	-1.764455000

η-NN

6	-0.482830000	3.162765000	-0.975043000
6	-1.750093000	3.834716000	-0.863193000

6	-2.722394000	2.898248000	-0.340271000
6	-2.076025000	1.645601000	-0.229336000
6	-0.708111000	1.794251000	-0.634561000
1	0.453918000	3.605592000	-1.281289000
1	-1.915652000	4.893279000	-1.013710000
1	-3.756919000	3.112669000	-0.113385000
1	-2.545326000	0.714185000	0.059189000
1	0.032430000	1.005788000	-0.653633000
77	-1.985819000	2.384074000	-2.520998000
7	-2.497559000	0.619421000	-3.671103000
7	-1.378585000	1.003786000	-3.955532000
8	-0.399374000	0.720382000	-4.642395000
6	-2.714814000	3.473841000	-3.880393000
7	-3.185952000	4.154231000	-4.718043000
6	-3.590750000	4.967016000	-5.804217000
1	-2.722324000	5.271669000	-6.399063000
1	-4.283751000	4.413674000	-6.446214000
1	-4.098444000	5.863089000	-5.432472000

η-NO

6	-0.268540000	2.598996000	-0.406976000
6	-1.557163000	3.209339000	-0.209293000

6	-2.389147000	2.280290000	0.536102000
6	-1.666755000	1.085969000	0.667922000
6	-0.368130000	1.254735000	0.061866000
1	0.595939000	3.062674000	-0.861088000
1	-1.800666000	4.242453000	-0.418782000
1	-3.405887000	2.457923000	0.857768000
1	-2.040841000	0.161759000	1.089415000
1	0.418182000	0.512505000	0.038352000
77	-1.811614000	1.629589000	-1.734211000
8	-1.970753000	-0.205792000	-2.828568000
7	-0.024257000	0.383379000	-4.036680000
7	-0.901892000	0.478155000	-3.283138000
6	-2.913060000	2.473689000	-3.019818000
7	-3.605756000	3.003193000	-3.810506000
6	-4.350782000	3.634212000	-4.835080000
1	-5.019271000	2.909665000	-5.311465000
1	-4.954524000	4.445272000	-4.414743000
1	-3.678948000	4.049041000	-5.594648000

[Rh(η^5-Cp)(CNMe)(N_2O)]

κ-N

6	-0.057319000	2.497305000	0.163245000

6	-1.167598000	3.353025000	0.176587000
6	-2.340077000	2.512863000	0.076871000
6	-1.929294000	1.132473000	0.218139000
6	-0.528898000	1.123804000	0.193221000
1	0.982878000	2.798465000	0.164513000
1	-1.154585000	4.434136000	0.175613000
1	-3.363551000	2.864497000	0.117318000
1	-2.583890000	0.272614000	0.252265000
1	0.106867000	0.247523000	0.217165000
45	-1.347633000	2.139013000	-1.852000000
7	-0.083328000	1.684445000	-3.369429000
7	0.640124000	1.420410000	-4.205509000
8	1.408336000	1.141453000	-5.089746000
6	-2.752064000	2.582496000	-3.046210000
7	-3.644780000	2.834091000	-3.777981000
6	-4.613088000	3.380498000	-4.654862000
1	-4.607213000	2.838668000	-5.606551000
1	-5.611539000	3.292231000	-4.213661000
1	-4.406009000	4.439527000	-4.850370000

κ-O

6	-0.039780000	2.244592000	0.255359000

6	-0.975289000	3.281949000	0.213005000
6	-2.282950000	2.660799000	0.073962000
6	-2.125473000	1.227582000	0.249815000
6	-0.749820000	0.976215000	0.268850000
1	1.037175000	2.354257000	0.290004000
1	-0.772077000	4.343901000	0.211713000
1	-3.227139000	3.190936000	0.091762000
1	-2.921735000	0.496673000	0.276679000
1	-0.279125000	0.001632000	0.312113000
45	-1.364916000	2.116689000	-1.795800000
7	0.388533000	2.013627000	-4.352281000
8	0.065412000	1.268250000	-3.465273000
7	0.707196000	2.688662000	-5.201488000
6	-2.566946000	2.788177000	-3.050444000
7	-3.289699000	3.275859000	-3.875431000
6	-4.459511000	3.053152000	-4.675606000
1	-4.864030000	2.044409000	-4.526479000
1	-5.228368000	3.787766000	-4.414613000
1	-4.214892000	3.186796000	-5.734292000

η-NN

6	-0.445608000	3.060338000	-0.896766000

6	-1.648773000	3.828269000	-0.879023000
6	-2.727854000	2.984283000	-0.391722000
6	-2.207755000	1.694928000	-0.229960000
6	-0.811832000	1.720962000	-0.595013000
1	0.538075000	3.413843000	-1.172639000
1	-1.720543000	4.894043000	-1.054785000
1	-3.748778000	3.297827000	-0.221488000
1	-2.763800000	0.811220000	0.055066000
1	-0.141437000	0.871456000	-0.563777000
45	-1.931108000	2.365935000	-2.543730000
7	-2.239187000	0.589795000	-3.763280000
7	-1.158902000	1.043160000	-4.009575000
8	-0.114076000	0.925367000	-4.638076000
6	-2.700302000	3.479013000	-3.908946000
7	-3.173059000	4.155988000	-4.743604000
6	-3.723952000	4.944112000	-5.784217000
1	-2.964976000	5.140709000	-6.548440000
1	-4.566727000	4.419026000	-6.244996000
1	-4.077780000	5.898001000	-5.380691000

η-NO

6	-0.265143000	2.589512000	-0.356299000

6	-1.564111000	3.189134000	-0.233718000
6	-2.418551000	2.278827000	0.518257000
6	-1.706852000	1.094952000	0.692552000
6	-0.390530000	1.260074000	0.104946000
1	0.607933000	3.039330000	-0.808592000
1	-1.805277000	4.218113000	-0.468999000
1	-3.439168000	2.473774000	0.818731000
1	-2.079882000	0.181717000	1.138726000
1	0.391241000	0.510898000	0.107529000
45	-1.839282000	1.596545000	-1.726017000
8	-1.787750000	-0.254077000	-2.922660000
7	0.108586000	0.494314000	-4.083019000
7	-0.800791000	0.402465000	-3.380691000
6	-2.921415000	2.474867000	-3.033962000
7	-3.595958000	3.018194000	-3.830324000
6	-4.392601000	3.648364000	-4.816667000
1	-5.238745000	3.006828000	-5.084387000
1	-4.777912000	4.598944000	-4.433858000
1	-3.797657000	3.844270000	-5.715118000

$[Co(PMe_3)_2(N_2O)Cl]$

κ-N

27	0.019077000	0.971266000	-0.103737000
17	-2.234571000	0.972509000	-0.098511000
15	-0.070658000	-1.265603000	-0.106052000
15	-0.068312000	3.208293000	-0.105789000
7	1.736872000	0.970407000	-0.163260000
7	2.878847000	0.969826000	0.072156000
8	4.059521000	0.969277000	-0.269910000
6	-0.940679000	3.932620000	-1.558950000
1	-1.941971000	3.498707000	-1.620066000
1	-1.014367000	5.023421000	-1.481563000
1	-0.396217000	3.676590000	-2.473589000
6	-0.946305000	3.941477000	1.339878000
1	-1.016926000	5.032050000	1.256672000
1	-1.949050000	3.510777000	1.398875000
1	-0.407007000	3.689402000	2.258771000
6	1.536143000	4.121589000	-0.102536000
1	2.115203000	3.857614000	0.788040000
1	2.126162000	3.847816000	-0.982707000
1	1.377157000	5.205623000	-0.108789000
6	-0.945198000	-1.989670000	-1.558000000
1	-1.020750000	-3.080267000	-1.479563000

1	-1.945775000	-1.554059000	-1.618786000
1	-0.400935000	-1.735438000	-2.473259000
6	-0.948103000	-1.997216000	1.340788000
1	-1.950305000	-1.565364000	1.400607000
1	-1.020049000	-3.087744000	1.258102000
1	-0.407606000	-1.745391000	2.259046000
6	1.532824000	-2.180598000	-0.103642000
1	2.122805000	-1.907386000	-0.984011000
1	2.112482000	-1.917286000	0.786743000
1	1.372702000	-3.264464000	-0.109901000

κ-O

NA

η-NN

27	2.844993000	0.291472000	0.084508000
17	1.103553000	-0.933013000	-0.630246000
15	1.444323000	1.250215000	1.599775000
15	4.129110000	-0.783969000	-1.455599000
7	4.312756000	0.788565000	1.043573000
8	5.043255000	0.378709000	1.959036000
7	4.143814000	1.716082000	0.276934000
6	4.163287000	-2.615444000	-1.276410000

1	3.138067000	-2.993057000	-1.309714000
1	4.755888000	-3.085591000	-2.069187000
1	4.597248000	-2.875636000	-0.305620000
6	3.594184000	-0.513464000	-3.196364000
1	4.219180000	-1.074258000	-3.900399000
1	2.552437000	-0.828783000	-3.299142000
1	3.659069000	0.553154000	-3.434369000
6	5.909184000	-0.311486000	-1.463441000
1	5.999849000	0.758172000	-1.673121000
1	6.338980000	-0.498082000	-0.474462000
1	6.470687000	-0.877925000	-2.214108000
6	0.042643000	2.174097000	0.843893000
1	-0.521334000	1.495178000	0.198742000
1	-0.621957000	2.591752000	1.608502000
1	0.435571000	2.990500000	0.229375000
6	0.631799000	0.061582000	2.746315000
1	-0.067172000	0.568166000	3.421244000
1	0.097084000	-0.688133000	2.157426000
1	1.396851000	-0.446571000	3.342069000
6	2.226177000	2.480136000	2.725774000
1	3.044158000	2.002485000	3.273849000

1	2.649665000	3.296543000	2.133750000
1	1.501908000	2.886669000	3.439784000

η-NO

27	2.863525000	0.197721000	0.163472000
17	1.171095000	-1.180304000	-0.405560000
15	1.457054000	1.244726000	1.609286000
15	4.137723000	-0.786958000	-1.440576000
7	4.278444000	0.414516000	1.262574000
7	4.980243000	0.058812000	2.113347000
8	4.150492000	1.559659000	0.387455000
6	4.246652000	-2.621672000	-1.366420000
1	3.235923000	-3.036970000	-1.386161000
1	4.829838000	-3.024032000	-2.202188000
1	4.722417000	-2.916315000	-0.425469000
6	3.510125000	-0.438588000	-3.136731000
1	4.119373000	-0.935895000	-3.899786000
1	2.476188000	-0.786805000	-3.211283000
1	3.528199000	0.641146000	-3.316924000
6	5.890769000	-0.233350000	-1.494726000
1	5.918469000	0.856685000	-1.565537000
1	6.391481000	-0.519933000	-0.565097000

1	6.425117000	-0.677172000	-2.341599000
6	0.097785000	2.131865000	0.738996000
1	-0.455952000	1.417308000	0.123735000
1	-0.586404000	2.611447000	1.447981000
1	0.524419000	2.898594000	0.084202000
6	0.590217000	0.157097000	2.813062000
1	-0.108491000	0.724638000	3.437708000
1	0.050166000	-0.618243000	2.263790000
1	1.330490000	-0.328482000	3.457087000
6	2.235057000	2.543332000	2.653700000
1	2.979032000	2.083999000	3.311398000
1	2.755333000	3.255480000	2.008693000
1	1.490478000	3.065761000	3.263937000

$[Co(PH_3)_2(N_2O)Cl]$

κ-N

27	0.054392000	0.971255000	-0.107864000
17	-2.185955000	0.971249000	-0.107694000
15	-0.094164000	-1.224692000	-0.107973000
1	1.062679000	-2.046727000	-0.108369000
1	-0.772403000	-1.842765000	0.965276000
1	-0.773051000	-1.842594000	-1.180905000

15	-0.094173000	3.167201000	-0.107899000
1	1.062665000	3.989241000	-0.106543000
1	-0.771455000	3.785235000	-1.181788000
1	-0.774023000	3.785134000	0.964392000
7	1.801590000	0.971259000	-0.108253000
7	2.943067000	0.971253000	-0.107053000
8	4.151792000	0.971211000	-0.107206000

κ-O

NA

η-NN

27	0.272378000	0.967190000	-0.168560000
17	-1.846231000	0.942413000	0.507523000
15	0.188388000	-1.290168000	-0.117982000
1	1.354566000	-2.038568000	-0.399406000
1	-0.218641000	-1.921027000	1.074572000
1	-0.699844000	-1.907329000	-1.022696000
15	0.117574000	3.221240000	-0.175862000
1	1.259850000	3.998385000	-0.476710000
1	-0.789099000	3.786801000	-1.095889000
1	-0.309721000	3.869421000	1.000199000
7	2.101323000	0.997218000	-0.064327000

7	1.870917000	0.978191000	-1.255372000
8	2.986465000	1.022493000	0.792628000

η-NO

27	-1.627068000	-1.829945000	-1.258606000
17	-2.870952000	-0.064626000	-1.801707000
15	-2.567676000	-2.951885000	-2.975633000
15	-0.941845000	-0.711750000	0.577346000
1	-3.886615000	-3.403328000	-2.756830000
1	-2.744252000	-2.310402000	-4.217431000
1	-1.985439000	-4.167087000	-3.399242000
1	-0.590226000	0.648788000	0.477106000
1	-1.881746000	-0.632904000	1.626918000
1	0.162778000	-1.205430000	1.306233000
7	0.001406000	-2.609185000	-1.512662000
8	-0.774163000	-3.406249000	-0.655960000
7	1.052577000	-2.597645000	-2.000508000

$[Co(CNMe)_2(N_2O)Cl]$

κ-N

27	0.212497000	0.970937000	0.472719000
17	-2.022510000	0.971696000	0.511015000
6	0.095686000	-0.850292000	0.598652000

6	0.096921000	2.792019000	0.601618000
7	1.983040000	0.970486000	0.290753000
7	3.081621000	0.970120000	-0.008765000
8	4.269261000	0.969475000	-0.222523000
7	-0.055529000	3.942556000	0.756159000
7	-0.057573000	-2.000973000	0.751316000
6	-0.391060000	5.305679000	0.939544000
1	-1.475362000	5.403731000	1.050112000
1	0.098954000	5.694668000	1.837792000
1	-0.063688000	5.891487000	0.074664000
6	-0.394018000	-3.364168000	0.932473000
1	-1.478544000	-3.461865000	1.041146000
1	-0.065484000	-3.949068000	0.067421000
1	0.094339000	-3.754473000	1.831055000

κ-O

NA

η-NN

27	2.828345000	0.870235000	-0.314997000
17	1.056469000	-0.126364000	-1.209740000
6	1.659412000	1.658631000	0.900420000
6	3.855025000	0.002815000	-1.603041000

7	4.303727000	1.116604000	0.816051000
8	4.869702000	0.504297000	1.717015000
7	4.272439000	2.107393000	0.133537000
7	0.886194000	2.133562000	1.631264000
7	4.451301000	-0.555046000	-2.434184000
6	-0.104766000	2.670313000	2.491327000
1	-1.090631000	2.318151000	2.174565000
1	0.084627000	2.344841000	3.518332000
1	-0.077395000	3.762966000	2.448792000
6	5.116667000	-1.267428000	-3.463561000
1	5.815174000	-1.984167000	-3.022073000
1	4.380427000	-1.803554000	-4.069208000
1	5.670110000	-0.568543000	-4.097366000

η-NO

27	2.827851000	0.731959000	-0.223431000
17	1.105981000	-0.494328000	-0.923495000
6	1.656656000	1.580322000	0.949320000
6	3.852021000	-0.073707000	-1.553356000
7	4.224533000	0.679465000	1.036554000
7	4.729196000	0.069482000	1.882652000
8	4.301765000	1.826990000	0.345936000

7	0.880382000	2.109548000	1.638206000
7	4.442940000	-0.574937000	-2.423322000
6	-0.112414000	2.702704000	2.458351000
1	-1.093595000	2.300508000	2.190476000
1	0.097422000	2.478762000	3.508252000
1	-0.110980000	3.786944000	2.313972000
6	5.106037000	-1.230255000	-3.491487000
1	5.882852000	-1.888664000	-3.092068000
1	4.383485000	-1.823860000	-4.058756000
1	5.566242000	-0.488610000	-4.150719000

$[Co(CO)_2(N_2O)Cl]$

κ-N

27	0.014461000	0.971202000	-0.004102000
17	-2.092752000	0.973105000	-0.601396000
6	-0.159900000	-0.751940000	0.477618000
6	-0.157735000	2.693635000	0.480875000
7	1.841228000	0.970151000	-0.016237000
7	2.960942000	0.970270000	-0.199156000
8	4.140262000	0.970566000	-0.373991000
8	-0.350198000	3.715196000	0.962109000
8	-0.353416000	-1.774233000	0.956706000

κ-O

27	0.085324000	0.762574000	0.238954000
17	-1.882163000	0.965326000	1.160963000
6	-0.387900000	-0.783396000	-0.528139000
6	0.127670000	2.491025000	-0.175848000
8	2.041523000	0.365789000	0.160762000
7	2.944723000	1.165036000	0.041539000
7	3.819063000	1.868803000	-0.058166000
8	-0.804765000	-1.629251000	-1.183509000
8	-0.003264000	3.531848000	-0.649374000

η-NN

27	2.804875000	0.524838000	-0.106244000
17	1.087863000	-0.609659000	-0.858982000
6	1.629126000	1.272615000	1.092735000
6	3.794867000	-0.367865000	-1.371687000
7	4.339589000	0.949524000	0.959955000
8	4.949110000	0.402794000	1.858622000
7	4.186006000	1.871616000	0.211770000
8	4.358889000	-0.943184000	-2.174150000
8	0.859452000	1.708535000	1.807489000

η-NO

27	2.814518000	0.425073000	-0.030937000
17	1.191058000	-0.971576000	-0.527032000
6	1.619484000	1.259512000	1.084091000
6	3.776963000	-0.375791000	-1.372535000
7	4.324310000	0.595257000	1.181628000
7	4.881216000	0.051934000	2.032152000
8	4.240617000	1.650109000	0.406224000
8	0.823911000	1.775332000	1.712578000
8	4.306405000	-0.864273000	-2.252906000

$[Co(C_4N_2H_5)_2(NC_4H_8)(N_2O)]$

κ-N

6	2.427590000	-2.186447000	0.855929000
6	1.407993000	-0.077524000	1.690586000
1	1.818689000	0.938773000	1.692726000
27	0.878962000	-2.930446000	-0.051012000
7	2.520395000	-1.010838000	1.535999000
6	-2.368888000	-2.738607000	0.604097000
1	-2.230542000	-2.897497000	1.681123000
7	-1.907652000	-3.918980000	-0.119594000
1	-3.438560000	-2.622811000	0.399872000
6	-0.613172000	-4.095923000	-0.513561000

7	-0.634840000	-5.338756000	-1.099966000
6	-2.706902000	-5.003666000	-0.431316000
6	-1.902486000	-5.898206000	-1.055805000
1	-2.116433000	-6.867751000	-1.478253000
6	0.486084000	-6.029307000	-1.733489000
1	0.713734000	-5.596016000	-2.709285000
1	1.372817000	-5.951392000	-1.106983000
1	0.211424000	-7.080326000	-1.854098000
1	-3.758021000	-5.038265000	-0.189628000
7	3.642574000	-2.780271000	1.081467000
6	4.453126000	-1.987243000	1.878950000
6	3.741930000	-0.870772000	2.172138000
1	5.453455000	-2.282820000	2.155284000
1	3.992182000	-0.001718000	2.761024000
1	0.927584000	-0.263641000	2.659807000
6	4.069563000	-4.083518000	0.579625000
1	3.221390000	-4.766572000	0.591779000
1	4.441953000	-4.008836000	-0.444384000
1	4.857259000	-4.464297000	1.235146000
7	-0.211542000	-1.560046000	0.552555000
6	0.382314000	-0.230005000	0.578317000

6	-1.610275000	-1.495751000	0.174013000
1	0.847044000	0.057655000	-0.380811000
1	-0.389895000	0.529383000	0.782514000
1	-1.773889000	-1.340683000	-0.910799000
1	-2.101637000	-0.648312000	0.682055000
7	1.875249000	-3.486669000	-1.365454000
7	2.546382000	-3.500937000	-2.359300000
8	2.697345000	-2.745187000	-3.353153000

κ-O

NA

η-NN

6	2.442198000	-2.152986000	0.947665000
6	1.208086000	-0.386202000	2.110282000
1	1.465759000	0.602006000	2.505490000
27	0.831313000	-3.121469000	0.400599000
7	2.452686000	-1.057277000	1.749232000
6	-2.386028000	-2.680852000	0.511037000
1	-2.237676000	-2.827335000	1.586628000
7	-1.956612000	-3.876149000	-0.207843000
1	-3.453922000	-2.540162000	0.313612000
6	-0.638250000	-4.123282000	-0.418282000

7	-0.643130000	-5.215311000	-1.240664000
6	-2.771060000	-4.786441000	-0.855783000
6	-1.937887000	-5.637616000	-1.507050000
1	-2.145972000	-6.488054000	-2.137666000
6	0.528355000	-5.857900000	-1.831050000
1	1.288801000	-5.102724000	-2.020040000
1	0.947302000	-6.606432000	-1.156313000
1	0.226288000	-6.323444000	-2.773503000
1	-3.848050000	-4.744757000	-0.803473000
7	3.767401000	-2.392060000	0.712368000
6	4.568826000	-1.473562000	1.375592000
6	3.735604000	-0.624631000	2.029770000
1	5.645651000	-1.500538000	1.312813000
1	3.937881000	0.234540000	2.650487000
1	0.695589000	-0.960553000	2.889893000
6	4.317269000	-3.430184000	-0.155788000
1	4.440333000	-4.369904000	0.385406000
1	3.631770000	-3.598734000	-0.984027000
1	5.281620000	-3.083333000	-0.537769000
7	-0.173894000	-1.541220000	0.388775000
6	0.317082000	-0.258995000	0.876601000

6	-1.583790000	-1.474957000	0.026918000
1	0.882221000	0.309133000	0.113745000
1	-0.521923000	0.389069000	1.174611000
1	-1.749024000	-1.379705000	-1.062839000
1	-2.059461000	-0.592176000	0.481991000
7	1.894764000	-4.850403000	0.496726000
7	1.253931000	-4.527360000	1.474824000
8	0.988480000	-4.913008000	2.628742000

η-NO

6	2.446707000	-2.137544000	0.907789000
6	1.220411000	-0.390280000	2.113085000
1	1.481077000	0.593756000	2.516597000
27	0.835663000	-3.093116000	0.349857000
7	2.461654000	-1.049415000	1.718235000
6	-2.387785000	-2.693095000	0.507070000
1	-2.237563000	-2.865707000	1.578686000
7	-1.948167000	-3.868429000	-0.238960000
1	-3.457560000	-2.559514000	0.315058000
6	-0.629787000	-4.105348000	-0.455881000
7	-0.626019000	-5.208460000	-1.261161000
6	-2.756560000	-4.796451000	-0.869329000

6	-1.917630000	-5.646370000	-1.515403000
1	-2.120509000	-6.506396000	-2.134586000
6	0.552308000	-5.868275000	-1.819215000
1	1.295271000	-5.115896000	-2.078164000
1	0.994479000	-6.550574000	-1.092885000
1	0.246460000	-6.409032000	-2.719379000
1	-3.833599000	-4.765301000	-0.811530000
7	3.769225000	-2.394773000	0.684397000
6	4.575561000	-1.490948000	1.360917000
6	3.747520000	-0.636421000	2.014970000
1	5.652470000	-1.530717000	1.307281000
1	3.955109000	0.215519000	2.643798000
1	0.730721000	-0.978194000	2.897467000
6	4.313302000	-3.458192000	-0.157155000
1	4.347584000	-4.402675000	0.386334000
1	3.673902000	-3.588002000	-1.028657000
1	5.316073000	-3.161041000	-0.477130000
7	-0.190810000	-1.520440000	0.396958000
6	0.297873000	-0.247856000	0.904490000
6	-1.603199000	-1.463815000	0.053723000
1	0.838296000	0.347919000	0.143478000

1	-0.540562000	0.383888000	1.239195000
1	-1.784609000	-1.336435000	-1.031099000
1	-2.086474000	-0.601982000	0.541256000
8	1.878550000	-4.762045000	0.405380000
7	1.156855000	-4.425324000	1.547716000
7	0.976297000	-4.877987000	2.608514000

$[Co(C_6N_2H_{11})_2(NC_4H_8)(N_2O)]$

κ-N

6	2.574284000	-2.185951000	0.845504000
6	1.176236000	-0.264735000	1.623859000
1	1.440048000	0.791724000	1.750161000
27	0.985220000	-3.303423000	0.321292000
7	2.432108000	-1.014024000	1.529075000
6	-1.852887000	-3.273948000	1.440458000
1	-1.198601000	-3.550571000	2.277381000
7	-1.704027000	-4.293729000	0.405655000
1	-2.894542000	-3.281692000	1.777023000
6	-0.522765000	-4.430673000	-0.236079000
7	-0.763150000	-5.387880000	-1.186452000
6	-2.674421000	-5.132401000	-0.103107000
6	-2.082597000	-5.830478000	-1.104541000

1	-2.489361000	-6.588083000	-1.750771000
6	0.249803000	-5.917668000	-2.149938000
1	-3.679541000	-5.166264000	0.287597000
7	3.927527000	-2.435333000	0.919727000
6	4.567790000	-1.459190000	1.675860000
6	3.626677000	-0.563691000	2.053672000
1	5.626019000	-1.467187000	1.869457000
1	3.701993000	0.346504000	2.628447000
1	0.618730000	-0.592235000	2.508904000
6	4.697578000	-3.581148000	0.330248000
7	-0.161332000	-1.846629000	0.262260000
6	0.358323000	-0.492971000	0.352409000
6	-1.492560000	-1.907845000	0.863174000
1	0.998258000	-0.262035000	-0.509265000
1	-0.464102000	0.238148000	0.333635000
1	-2.269724000	-1.617533000	0.130877000
1	-1.586003000	-1.197140000	1.703934000
6	1.259804000	-6.777940000	-1.368758000
1	0.759129000	-7.654156000	-0.941945000
1	2.055097000	-7.128332000	-2.036554000
1	1.704777000	-6.217322000	-0.544413000

6	-0.436740000	-6.787127000	-3.216098000
1	0.318200000	-7.105062000	-3.941973000
1	-0.879994000	-7.693317000	-2.789886000
1	-1.210221000	-6.233012000	-3.759004000
6	0.919317000	-4.723424000	-2.851054000
1	1.329295000	-4.020954000	-2.122102000
1	1.730147000	-5.073097000	-3.499182000
1	0.191110000	-4.180441000	-3.463548000
6	4.823771000	-4.694199000	1.386014000
1	3.837901000	-5.056105000	1.683927000
1	5.405359000	-5.529525000	0.978982000
1	5.343044000	-4.322643000	2.276993000
6	3.983444000	-4.087133000	-0.925115000
1	4.537103000	-4.936905000	-1.338302000
1	2.975798000	-4.418159000	-0.683087000
1	3.924772000	-3.304337000	-1.689361000
6	6.099926000	-3.090527000	-0.085954000
1	6.742215000	-2.861074000	0.770194000
1	6.594845000	-3.888335000	-0.648662000
1	6.041166000	-2.206173000	-0.729787000
7	1.494004000	-4.550834000	1.457939000

7	1.185000000	-5.174689000	2.451238000
8	0.322728000	-4.890491000	3.344451000

κ-O

NA

η-NN

6	2.489315000	-2.127448000	0.685239000
6	1.048299000	-0.192023000	1.373517000
1	1.326709000	0.858643000	1.517597000
27	0.860017000	-3.264547000	0.179654000
7	2.296388000	-0.963568000	1.376536000
6	-2.007058000	-3.037373000	1.186486000
1	-1.366958000	-3.245967000	2.048856000
7	-1.874176000	-4.139087000	0.238307000
1	-3.050217000	-2.995996000	1.515758000
6	-0.692571000	-4.337289000	-0.392187000
7	-0.971867000	-5.288305000	-1.338817000
6	-2.880221000	-4.934364000	-0.272508000
6	-2.310714000	-5.668866000	-1.259719000
1	-2.746104000	-6.414960000	-1.900711000
6	-0.009499000	-5.868817000	-2.330789000
1	-3.890182000	-4.915618000	0.106857000

7	3.849914000	-2.338298000	0.797565000
6	4.433172000	-1.360289000	1.596350000
6	3.457988000	-0.494104000	1.951969000
1	5.482271000	-1.345188000	1.832491000
1	3.489879000	0.408062000	2.543207000
1	0.417792000	-0.501397000	2.214803000
6	4.722017000	-3.373063000	0.131732000
7	-0.243750000	-1.748884000	-0.036979000
6	0.322267000	-0.415482000	0.044245000
6	-1.601545000	-1.732676000	0.503232000
1	1.039435000	-0.240746000	-0.768363000
1	-0.457436000	0.355386000	-0.061491000
1	-2.354038000	-1.498742000	-0.274959000
1	-1.716580000	-0.950676000	1.276297000
7	1.810400000	-4.986982000	0.753360000
7	1.169879000	-4.365419000	1.575435000
8	0.840323000	-4.410032000	2.780425000
6	0.813630000	-6.971930000	-1.642378000
1	0.153299000	-7.771365000	-1.286126000
1	1.520841000	-7.409426000	-2.356916000
1	1.366167000	-6.574219000	-0.788409000

6	-0.784943000	-6.470438000	-3.516928000
1	-0.063432000	-6.774451000	-4.281731000
1	-1.352057000	-7.364809000	-3.237699000
1	-1.467898000	-5.742355000	-3.968048000
6	0.881307000	-4.736550000	-2.859722000
1	1.375182000	-4.221754000	-2.035144000
1	1.647516000	-5.146909000	-3.526026000
1	0.288749000	-4.001100000	-3.414720000
6	4.959965000	-4.539822000	1.106220000
1	4.020947000	-5.049179000	1.332707000
1	5.652983000	-5.260493000	0.656314000
1	5.407016000	-4.178525000	2.039785000
6	4.071147000	-3.849380000	-1.169952000
1	4.737603000	-4.570078000	-1.656394000
1	3.122248000	-4.336199000	-0.968135000
1	3.910504000	-3.010614000	-1.856843000
6	6.075390000	-2.723937000	-0.236292000
1	6.700723000	-2.508958000	0.635930000
1	6.635285000	-3.427131000	-0.860637000
1	5.936458000	-1.799436000	-0.807132000

η-NO

6	2.505081000	-2.103868000	0.694039000
6	1.049349000	-0.164232000	1.344387000
1	1.314814000	0.892420000	1.465999000
27	0.889705000	-3.254279000	0.189420000
7	2.306822000	-0.919642000	1.347718000
6	-1.992954000	-3.074294000	1.188282000
1	-1.370674000	-3.296218000	2.060084000
7	-1.837209000	-4.155729000	0.221242000
1	-3.041165000	-3.046368000	1.501670000
6	-0.645133000	-4.346566000	-0.392547000
7	-0.903638000	-5.300533000	-1.341494000
6	-2.830090000	-4.957988000	-0.304688000
6	-2.241294000	-5.688313000	-1.283461000
1	-2.663036000	-6.435448000	-1.932120000
6	0.083284000	-5.881666000	-2.309122000
1	-3.845754000	-4.945334000	0.059348000
7	3.866389000	-2.305246000	0.811071000
6	4.446609000	-1.295578000	1.571102000
6	3.467861000	-0.423280000	1.901047000
1	5.496374000	-1.264470000	1.801342000
1	3.496924000	0.499847000	2.459093000

1	0.434006000	-0.465496000	2.199928000
6	4.733950000	-3.384652000	0.212353000
7	-0.242737000	-1.761110000	-0.025088000
6	0.310132000	-0.421208000	0.029291000
6	-1.585756000	-1.748539000	0.549970000
1	1.014889000	-0.251867000	-0.795426000
1	-0.482154000	0.336172000	-0.080191000
1	-2.346252000	-1.471040000	-0.205382000
1	-1.678726000	-0.997973000	1.358117000
8	1.854522000	-4.911486000	0.692941000
7	1.115319000	-4.263501000	1.676733000
7	0.878343000	-4.431088000	2.809837000
6	0.935941000	-6.931648000	-1.575416000
1	0.302828000	-7.757035000	-1.228553000
1	1.688397000	-7.344879000	-2.257440000
1	1.431357000	-6.488835000	-0.708201000
6	-0.663096000	-6.548732000	-3.478253000
1	0.075373000	-6.867151000	-4.220634000
1	-1.212484000	-7.443908000	-3.168056000
1	-1.356658000	-5.856820000	-3.968744000
6	0.938760000	-4.738373000	-2.873999000

1	1.424814000	-4.184381000	-2.070666000
1	1.712217000	-5.144779000	-3.534335000
1	0.321477000	-4.036844000	-3.445861000
6	4.882106000	-4.531184000	1.227086000
1	3.908118000	-4.982399000	1.424238000
1	5.557101000	-5.295786000	0.824446000
1	5.311222000	-4.161843000	2.165999000
6	4.126676000	-3.871183000	-1.107147000
1	4.796187000	-4.614633000	-1.553471000
1	3.161254000	-4.335568000	-0.933112000
1	4.012554000	-3.042207000	-1.815247000
6	6.125030000	-2.793133000	-0.106776000
1	6.716031000	-2.577703000	0.789091000
1	6.687095000	-3.533906000	-0.683708000
1	6.049832000	-1.881064000	-0.709045000

[N_2]

7	-0.319166000	0.170807000	0.000000000
7	0.786135000	0.170807000	0.000000000

[$Ni(CNMe)_2(N_2)$]

κ-N

1	-3.067619000	-2.796576000	2.352720000

1	-1.777659000	-2.374548000	3.506156000
1	-3.286025000	-1.433661000	3.477587000
6	-1.309765000	-0.581469000	-4.328026000
1	-0.335717000	-0.778595000	-4.789807000
1	-1.904278000	-1.502249000	-4.355695000
1	-1.824217000	0.185314000	-4.918122000
7	0.530281000	1.774414000	0.278894000
7	1.395373000	2.435666000	0.556655000
28	-0.756409000	0.632125000	-0.164808000
6	-1.558949000	-0.333741000	1.104676000
6	-1.039478000	0.242196000	-1.884225000
7	-1.993123000	-1.082405000	1.908697000
7	-1.140227000	-0.136802000	-2.998525000
6	-2.558136000	-1.965582000	2.854638000

η-NN

1	-5.276784000	2.124601000	-3.573808000
1	-5.555319000	1.006984000	-2.217517000
1	-5.329496000	2.745654000	-1.905393000
6	0.618279000	-1.919686000	-4.816958000
1	0.086812000	-2.849330000	-4.585524000
1	0.418246000	-1.653333000	-5.860652000

1	1.693897000	-2.089918000	-4.697170000
7	-0.052391000	2.550887000	-0.842384000
7	0.858268000	1.932556000	-1.210387000
28	-0.697648000	1.290499000	-2.149369000
6	-2.456954000	1.561183000	-2.288977000
6	-0.135616000	-0.015777000	-3.229381000
7	-3.620058000	1.700450000	-2.415191000
7	0.185998000	-0.883867000	-3.958125000
6	-5.013439000	1.905285000	-2.533224000

$[Ni(CO)_2(N_2)]$

κ-N

28	0.128013000	0.727116000	0.049862000
6	-0.560578000	2.290369000	0.460522000
8	-0.924584000	3.360950000	0.676862000
6	1.876279000	0.588940000	-0.055120000
8	3.022801000	0.604796000	-0.158484000
7	-0.938543000	-0.650178000	-0.446600000
7	-1.594481000	-1.485301000	-0.791266000

η-NN

28	-0.379237000	0.117093000	0.297372000
6	-1.035240000	1.745710000	0.419761000

8	-1.361110000	2.844725000	0.488127000
6	1.363273000	0.120211000	0.056606000
8	2.495874000	0.234273000	-0.095683000
7	-1.893658000	-1.118783000	0.488345000
7	-0.952246000	-1.760170000	0.345718000

$[Ni(C_{10}N_4H_{16})(N_2)]$

κ-N

6	-2.349724000	-1.693255000	-1.220263000
6	-0.659911000	-0.495157000	-0.226771000
1	-2.837568000	-2.247710000	-2.007734000
6	4.780324000	-1.150869000	-0.005701000
6	4.371247000	-1.613214000	1.200613000
6	2.619656000	-0.431546000	0.298661000
7	3.715906000	-0.432290000	-0.537355000
1	5.719588000	-1.267479000	-0.525078000
1	4.888833000	-2.200323000	1.944207000
7	3.063418000	-1.175479000	1.370058000
6	2.245918000	-1.428527000	2.539185000
6	3.735479000	0.247774000	-1.817435000
1	3.596306000	-0.453437000	-2.650132000
1	2.917425000	0.971381000	-1.816881000

1	4.685200000	0.775516000	-1.952853000
7	-1.753241000	-0.616236000	0.604239000
7	-1.066492000	-1.176948000	-1.352846000
6	-2.780064000	-1.346029000	0.016884000
1	-3.711176000	-1.550253000	0.523734000
6	-1.805723000	-0.037602000	1.932359000
1	-2.779915000	0.431689000	2.104312000
1	-1.632480000	-0.792760000	2.709637000
1	-1.023783000	0.722712000	1.989806000
6	-0.238896000	-1.297698000	-2.535932000
28	0.957542000	0.412245000	0.069589000
1	0.782247000	-1.052341000	-2.234721000
1	-0.272816000	-2.321374000	-2.924440000
1	-0.557559000	-0.603970000	-3.323336000
1	2.528680000	-0.779640000	3.376931000
1	1.212432000	-1.216330000	2.255389000
1	2.335468000	-2.475116000	2.850009000
7	0.912707000	2.160590000	0.136705000
7	0.883482000	3.292148000	0.180317000

η-NN

6	-2.445756000	-0.714753000	-1.284826000

6	-0.923526000	0.816244000	-0.505332000
1	-2.817879000	-1.499368000	-1.926099000
6	4.301892000	0.079805000	-0.284518000
6	3.741272000	-0.547631000	0.778172000
6	2.163462000	0.886735000	-0.071449000
7	3.338123000	0.942778000	-0.787645000
1	5.284138000	-0.013786000	-0.722523000
1	4.141425000	-1.287692000	1.454566000
7	2.446528000	-0.057329000	0.889257000
6	1.508250000	-0.452200000	1.924805000
6	3.548453000	1.827819000	-1.920815000
1	3.692236000	1.254654000	-2.844444000
1	2.663484000	2.457000000	-2.010457000
1	4.424292000	2.463224000	-1.753028000
7	-2.098045000	0.858230000	0.212021000
7	-1.171294000	-0.179892000	-1.422192000
6	-3.028419000	-0.062991000	-0.248972000
1	-4.005381000	-0.175266000	0.196408000
6	-2.340641000	1.784528000	1.305043000
1	-3.237703000	2.381271000	1.109638000
1	-2.465635000	1.247945000	2.253043000

1	-1.478093000	2.447351000	1.366583000
6	-0.220349000	-0.583559000	-2.442653000
28	0.599531000	1.900046000	-0.313577000
1	0.786821000	-0.493968000	-2.031957000
1	-0.410433000	-1.622719000	-2.727659000
1	-0.298417000	0.050840000	-3.333042000
1	1.551347000	0.229432000	2.782027000
1	0.500539000	-0.430383000	1.506278000
1	1.744298000	-1.465588000	2.263126000
7	-0.023317000	3.684787000	-0.403656000
7	1.150760000	3.710574000	-0.307841000

$[Ni(PH_3)_2(N_2)]$

κ-N

28	-0.637634000	0.122652000	-0.004112000
15	-1.743755000	1.926980000	-0.043699000
15	-1.784025000	-1.649505000	0.157007000
1	-1.217690000	-2.955935000	0.202127000
1	-2.640629000	-1.851078000	1.273217000
1	-2.748982000	-1.970630000	-0.835971000
1	-2.702610000	2.156470000	-1.067519000
1	-1.148201000	3.217207000	-0.144510000

1	-2.594136000	2.271479000	1.041889000
7	1.101292000	0.097725000	-0.099778000
7	2.225683000	0.081568000	-0.162318000

η-NN

28	-1.016684000	0.339390000	0.049245000
15	-2.182667000	2.117417000	-0.092399000
15	-2.231995000	-1.408928000	0.133844000
1	-1.634605000	-2.693479000	0.230652000
1	-3.164921000	-1.607617000	1.186292000
1	-3.116029000	-1.744096000	-0.926166000
1	-3.057726000	2.339285000	-1.188979000
1	-1.549502000	3.386701000	-0.158144000
1	-3.108871000	2.474280000	0.923595000
7	0.784000000	0.899068000	0.055049000
7	0.767815000	-0.264785000	0.129633000

$[Ni(PMe_3)_2(N_2)]$

κ-N

28	2.444886000	0.038579000	-0.258946000
15	1.357183000	1.876515000	-0.139250000
15	1.324090000	-1.754729000	0.063738000
6	0.852717000	2.406297000	1.565957000

1	0.280297000	3.341945000	1.553622000
1	0.246482000	1.623746000	2.033215000
1	1.747961000	2.550306000	2.179770000
6	2.155705000	3.437416000	-0.752968000
1	2.401963000	3.323694000	-1.814015000
1	1.511726000	4.318128000	-0.632202000
1	3.091845000	3.605436000	-0.210474000
6	-0.255568000	1.978403000	-1.054242000
1	-0.935975000	1.199478000	-0.694677000
1	-0.740741000	2.955634000	-0.938271000
1	-0.076302000	1.801278000	-2.120225000
6	-0.008328000	-1.744598000	1.358384000
1	-0.750759000	-0.975622000	1.119800000
1	-0.516547000	-2.713105000	1.446663000
1	0.435208000	-1.492977000	2.327969000
6	2.233792000	-3.288619000	0.581753000
1	1.569588000	-4.154468000	0.699715000
1	3.000703000	-3.527500000	-0.162177000
1	2.740642000	-3.101755000	1.534492000
6	0.392240000	-2.383005000	-1.412181000
1	1.097132000	-2.606049000	-2.219622000

1	-0.178288000	-3.290854000	-1.180915000
1	-0.296949000	-1.611519000	-1.770205000
7	4.145121000	-0.004094000	-0.621168000
7	5.248959000	-0.029848000	-0.861752000

η-NN

28	5.471816000	0.244961000	-0.158130000
15	4.271011000	2.023985000	-0.075999000
15	4.298526000	-1.533653000	0.116041000
6	3.765329000	2.604604000	1.609896000
1	3.149677000	3.511312000	1.568774000
1	3.204096000	1.816405000	2.122171000
1	4.663618000	2.814656000	2.199748000
6	5.035084000	3.560422000	-0.769759000
1	5.252836000	3.405591000	-1.831557000
1	4.384341000	4.437218000	-0.664614000
1	5.985109000	3.754695000	-0.262683000
6	2.653061000	2.027708000	-0.982960000
1	2.003290000	1.233490000	-0.599996000
1	2.127540000	2.986222000	-0.893245000
1	2.838904000	1.827754000	-2.043746000
6	2.974736000	-1.518545000	1.415131000

1	2.241985000	-0.733861000	1.198362000
1	2.450464000	-2.479224000	1.487318000
1	3.430495000	-1.294174000	2.385586000
6	5.226859000	-3.054410000	0.617067000
1	4.577160000	-3.934129000	0.702195000
1	6.013644000	-3.257596000	-0.115792000
1	5.711975000	-2.877263000	1.582556000
6	3.371193000	-2.148518000	-1.365985000
1	4.084358000	-2.372369000	-2.166123000
1	2.790977000	-3.052919000	-1.146363000
1	2.692752000	-1.369786000	-1.729243000
7	7.238757000	0.828274000	-0.461905000
7	7.249482000	-0.341475000	-0.385486000

[Co(η^5-Cp*)(CNMe)(N_2)]

κ-N

6	-0.072529000	2.319197000	-0.159871000
6	-1.060180000	3.333187000	-0.090989000
6	-2.348106000	2.672340000	-0.099162000
6	-2.144912000	1.246063000	-0.057334000
6	-0.743893000	1.028639000	-0.152500000
27	-1.362999000	2.146636000	-1.808500000

7	-0.278611000	1.481449000	-3.033450000
7	0.454184000	1.044645000	-3.766151000
6	-2.489583000	2.892168000	-2.940718000
7	-3.201279000	3.500302000	-3.679481000
6	-4.345984000	3.563899000	-4.529790000
1	-4.901837000	2.617635000	-4.524985000
1	-5.010983000	4.368132000	-4.198494000
1	-4.032754000	3.785298000	-5.555287000
6	-3.673392000	3.368175000	0.041409000
1	-4.489937000	2.770090000	-0.374975000
1	-3.905025000	3.552765000	1.099320000
1	-3.678638000	4.335050000	-0.471018000
6	-0.835693000	4.813978000	0.021869000
1	-1.603774000	5.381313000	-0.513155000
1	-0.859176000	5.141046000	1.071702000
1	0.133849000	5.108829000	-0.391395000
6	1.418057000	2.509639000	-0.158709000
1	1.695529000	3.521666000	-0.468737000
1	1.836416000	2.344132000	0.844037000
1	1.918723000	1.811043000	-0.837602000
6	-0.042158000	-0.300484000	-0.138462000

1	0.830190000	-0.307942000	-0.800405000
1	0.314621000	-0.545994000	0.871473000
1	-0.704446000	-1.110111000	-0.459970000
6	-3.211454000	0.201517000	0.110381000
1	-2.921764000	-0.750808000	-0.344816000
1	-3.415369000	0.007722000	1.173922000
1	-4.155455000	0.509069000	-0.350192000

η-NN

6	-0.201862000	2.192422000	-0.302669000
6	-1.243053000	3.155830000	-0.324582000
6	-2.498313000	2.474078000	-0.016659000
6	-2.215735000	1.098985000	0.197369000
6	-0.811389000	0.912651000	-0.051001000
27	-1.675570000	1.721874000	-1.761285000
7	-0.695538000	0.634475000	-3.099177000
6	-2.544483000	2.725602000	-2.955163000
7	-3.090249000	3.440181000	-3.721055000
6	-3.953201000	4.106496000	-4.623928000
1	-4.944451000	3.637074000	-4.633448000
1	-4.063018000	5.156569000	-4.333225000
1	-3.536454000	4.070290000	-5.636061000

7	-1.673669000	0.067669000	-2.858618000
6	-3.819126000	3.163292000	0.181301000
1	-4.657655000	2.468054000	0.076206000
1	-3.882779000	3.610434000	1.183355000
1	-3.967914000	3.969064000	-0.544718000
6	-1.094731000	4.641674000	-0.493450000
1	-1.925597000	5.069421000	-1.063815000
1	-1.071630000	5.148603000	0.481573000
1	-0.170750000	4.897727000	-1.020723000
6	1.266342000	2.437650000	-0.502217000
1	1.450482000	3.389648000	-1.009368000
1	1.799887000	2.467343000	0.458564000
1	1.728989000	1.651680000	-1.108319000
6	-0.076338000	-0.393938000	0.050722000
1	0.800370000	-0.416485000	-0.604447000
1	0.274451000	-0.568572000	1.077061000
1	-0.714186000	-1.239106000	-0.227236000
6	-3.183410000	0.027108000	0.610190000
1	-2.988862000	-0.916203000	0.089257000
1	-3.118261000	-0.175247000	1.688946000
1	-4.217378000	0.311723000	0.392235000

[Co(η^5-Cp)(CNMe)(N_2)]

κ-N

6	-0.086412000	2.479188000	-0.130028000
6	-1.180195000	3.370908000	-0.046964000
6	-2.366419000	2.568042000	-0.038093000
6	-1.996575000	1.180561000	0.002413000
6	-0.589614000	1.127489000	-0.089866000
1	0.958224000	2.753949000	-0.201255000
1	-1.136288000	4.451097000	-0.031231000
1	-3.379999000	2.945850000	-0.001697000
1	-2.675134000	0.340608000	0.058898000
1	0.018092000	0.232605000	-0.125500000
27	-1.352015000	2.141935000	-1.766585000
7	-0.184543000	1.742458000	-3.029084000
7	0.586627000	1.475121000	-3.800807000
6	-2.679931000	2.499905000	-2.880743000
7	-3.606022000	2.668959000	-3.599352000
6	-4.524139000	3.319882000	-4.464591000
1	-4.492938000	2.857233000	-5.456460000
1	-5.541760000	3.221280000	-4.072646000
1	-4.283334000	4.385762000	-4.562919000

η-NN

6	-0.421015000	2.901867000	-1.001206000
6	-1.474819000	3.841404000	-1.068066000
6	-2.713699000	3.156225000	-0.758517000
6	-2.413228000	1.799106000	-0.510436000
6	-1.009358000	1.630705000	-0.721492000
1	0.627518000	3.093647000	-1.184396000
1	-1.379771000	4.897568000	-1.283266000
1	-3.690663000	3.618283000	-0.706932000
1	-3.118340000	1.016650000	-0.264405000
1	-0.474436000	0.691243000	-0.660043000
27	-1.855770000	2.377918000	-2.484651000
7	-1.909860000	0.697375000	-3.542827000
7	-0.906140000	1.212579000	-3.782546000
6	-2.666559000	3.371209000	-3.729784000
7	-3.206465000	4.042096000	-4.532309000
6	-3.838236000	4.817608000	-5.531353000
1	-3.119917000	5.092384000	-6.311900000
1	-4.658415000	4.253341000	-5.988970000
1	-4.245650000	5.733652000	-5.091031000

[Co(η^5-Cp)(CO)(N_2)]

κ-N

6	-0.062374000	2.386134000	-0.018165000
6	-1.095189000	3.345326000	0.013745000
6	-2.329790000	2.633914000	-0.167374000
6	-2.059790000	1.223520000	-0.192163000
6	-0.658427000	1.075032000	-0.145676000
1	0.999506000	2.585449000	0.045479000
1	-0.983495000	4.416261000	0.111123000
1	-3.313225000	3.084490000	-0.203181000
1	-2.793647000	0.433960000	-0.275245000
1	-0.111006000	0.142524000	-0.192006000
27	-1.164691000	2.263063000	-1.801566000
7	0.100722000	1.797155000	-2.957654000
7	0.922906000	1.488849000	-3.653385000
6	-2.278714000	2.887011000	-2.977532000
8	-3.051999000	3.313537000	-3.724648000

η-NN

6	-0.434322000	2.956498000	-1.060620000
6	-1.541587000	3.835146000	-1.079532000
6	-2.722137000	3.087104000	-0.688747000
6	-2.332886000	1.753022000	-0.441003000

6	-0.935571000	1.660609000	-0.730769000
1	0.589271000	3.201874000	-1.308168000
1	-1.519517000	4.891171000	-1.314032000
1	-3.718578000	3.496317000	-0.588441000
1	-2.977720000	0.936480000	-0.146201000
1	-0.347280000	0.752353000	-0.692118000
27	-1.920914000	2.334346000	-2.446115000
7	-1.931798000	0.614556000	-3.471992000
7	-0.975774000	1.173998000	-3.775243000
6	-2.832851000	3.257242000	-3.615983000
8	-3.445485000	3.906305000	-4.347814000

[Co(η^5-Cp)(PH_3)(N_2)]

κ-N

6	0.056532000	2.321211000	-0.048574000
6	-0.894397000	3.365887000	-0.074570000
6	-2.188498000	2.744921000	-0.067270000
6	-2.035032000	1.325571000	0.082628000
6	-0.647388000	1.062092000	0.048535000
1	1.132617000	2.433005000	-0.083071000
1	-0.693316000	4.427529000	-0.116426000
1	-3.134548000	3.272635000	-0.082583000

1	-2.832456000	0.601546000	0.178448000
1	-0.178604000	0.087700000	0.097907000
27	-1.165638000	2.047214000	-1.700536000
1	-2.290237000	2.450832000	-4.532936000
1	-3.912320000	2.253819000	-3.177312000
1	-2.882279000	4.093142000	-3.324959000
15	-2.567562000	2.715355000	-3.169225000
7	-0.069523000	1.345056000	-2.870904000
7	0.657521000	0.883056000	-3.596344000

η-NN

6	-0.153565000	2.518367000	-0.335051000
6	-1.426094000	3.178890000	-0.254480000
6	-2.417569000	2.248828000	0.209212000
6	-1.776167000	0.992610000	0.305100000
6	-0.387392000	1.157817000	-0.029268000
1	0.790880000	2.972892000	-0.600814000
1	-1.593242000	4.235666000	-0.426377000
1	-3.455297000	2.467785000	0.419916000
1	-2.246910000	0.053777000	0.567485000
1	0.346290000	0.362298000	-0.056315000
27	-1.587214000	1.710201000	-1.650924000

1	-2.383258000	2.479407000	-4.531742000
1	-3.317309000	3.847497000	-3.191068000
1	-1.279739000	4.095714000	-3.688619000
15	-2.142632000	3.052499000	-3.259838000
7	-2.209570000	0.083779000	-2.566324000
7	-1.091683000	0.221109000	-2.837368000

[Co(η^5-Cp)(PMe_3)(N_2)]

κ-N

6	0.127576000	1.478267000	-0.260538000
6	-0.325617000	2.732139000	0.288966000
6	-1.734331000	2.690609000	0.402625000
6	-2.153410000	1.430431000	-0.141009000
6	-0.998232000	0.653902000	-0.489393000
1	1.160410000	1.220121000	-0.456970000
1	0.314996000	3.558956000	0.568150000
1	-2.376815000	3.459390000	0.809569000
1	-3.178328000	1.083275000	-0.194086000
1	-0.995940000	-0.360502000	-0.864040000
27	-1.138098000	2.441402000	-1.611016000
15	-2.762487000	2.477753000	-3.027387000
7	-0.017334000	3.293643000	-2.641056000

7	0.743065000	3.840877000	-3.269988000
6	-4.315036000	3.333370000	-2.486946000
1	-5.102357000	3.273444000	-3.247886000
1	-4.684035000	2.883129000	-1.560066000
1	-4.092549000	4.385723000	-2.285080000
6	-2.438218000	3.302971000	-4.648468000
1	-1.605242000	2.807950000	-5.156668000
1	-3.321052000	3.269260000	-5.296510000
1	-2.158438000	4.347756000	-4.483127000
6	-3.418091000	0.834590000	-3.579633000
1	-3.739050000	0.251294000	-2.710899000
1	-4.265521000	0.941459000	-4.267337000
1	-2.618765000	0.280217000	-4.081097000

η-NN

6	-0.175566000	2.639076000	-0.418735000
6	-1.487384000	3.210498000	-0.300697000
6	-2.396285000	2.216897000	0.195837000
6	-1.662010000	1.010247000	0.286966000
6	-0.302640000	1.268884000	-0.088389000
1	0.727526000	3.156550000	-0.712045000
1	-1.732181000	4.252545000	-0.468924000

1	-3.439124000	2.363967000	0.441207000
1	-2.058385000	0.042855000	0.568403000
1	0.484184000	0.526615000	-0.134154000
27	-1.591355000	1.730652000	-1.695363000
15	-2.271802000	3.039115000	-3.298321000
7	-2.137360000	0.064789000	-2.573734000
7	-1.035044000	0.267741000	-2.876621000
6	-1.146826000	4.432556000	-3.768379000
1	-0.952783000	5.065280000	-2.896511000
1	-0.190313000	4.022713000	-4.107539000
1	-1.573352000	5.051764000	-4.566304000
6	-3.873954000	3.926037000	-3.025006000
1	-4.131385000	4.576219000	-3.869415000
1	-4.671902000	3.190055000	-2.885271000
1	-3.813254000	4.534505000	-2.117145000
6	-2.564307000	2.221232000	-4.927152000
1	-1.640336000	1.748774000	-5.273477000
1	-3.320365000	1.438378000	-4.815787000
1	-2.902405000	2.943377000	-5.678279000

[Co(η^5-Cp)py(N_2)]

κ-N

6	-0.062364000	2.670255000	-0.196270000
6	-1.176338000	3.538890000	-0.192656000
6	-2.342228000	2.724303000	0.019374000
6	-1.944802000	1.374623000	0.247308000
6	-0.538659000	1.333594000	0.047103000
1	0.971159000	2.948857000	-0.356169000
1	-1.158230000	4.613841000	-0.317488000
1	-3.362224000	3.088677000	0.053882000
1	-2.591380000	0.544169000	0.495227000
1	0.085440000	0.449921000	0.091522000
27	-1.394312000	2.051377000	-1.695022000
7	-0.395745000	1.229475000	-2.876405000
7	0.282336000	0.702146000	-3.608033000
7	-2.726640000	2.555612000	-2.972847000
6	-3.313481000	3.778806000	-2.940877000
6	-3.152042000	1.702321000	-3.938207000
6	-4.308101000	4.171219000	-3.825939000
1	-2.949544000	4.454325000	-2.177473000
6	-4.128508000	2.030461000	-4.869519000
1	-2.681526000	0.727139000	-3.949193000
6	-4.731852000	3.287113000	-4.818913000

1	-4.732036000	5.166598000	-3.738034000
1	-4.413792000	1.296508000	-5.616509000
1	-5.502546000	3.568918000	-5.529681000

η-NN

6	-0.409911000	3.192603000	-1.267874000
6	-1.665175000	3.841309000	-0.994945000
6	-2.555184000	2.914599000	-0.377811000
6	-1.890177000	1.657765000	-0.382430000
6	-0.568150000	1.834894000	-0.906328000
1	0.484292000	3.657548000	-1.662011000
1	-1.883453000	4.886250000	-1.181964000
1	-3.550681000	3.122383000	-0.010063000
1	-2.307227000	0.716020000	-0.048660000
1	0.166112000	1.049080000	-1.029549000
27	-2.026733000	2.337854000	-2.349498000
7	-2.988075000	0.804764000	-3.087157000
7	-1.899283000	0.762540000	-3.491200000
7	-2.532241000	3.481777000	-3.826004000
6	-1.739729000	4.505814000	-4.220184000
6	-3.702956000	3.319189000	-4.483946000
6	-2.079228000	5.378322000	-5.246023000

1	-0.801692000	4.606813000	-3.688649000
6	-4.105657000	4.142066000	-5.529827000
1	-4.320598000	2.493332000	-4.152505000
6	-3.286046000	5.198908000	-5.922703000
1	-1.395873000	6.178446000	-5.511918000
1	-5.056737000	3.953287000	-6.017284000
1	-3.576465000	5.861030000	-6.732833000

[Co(η^5-Cp)py(p-NMe)$_2$(N_2)]

κ-N

6	0.166623000	2.555159000	-0.344154000
6	-0.786245000	3.600868000	-0.355610000
6	-2.034038000	3.025936000	0.063467000
6	-1.834089000	1.663605000	0.437936000
6	-0.482498000	1.358822000	0.125434000
1	1.207298000	2.630099000	-0.632642000
1	-0.610193000	4.636213000	-0.616917000
1	-2.975232000	3.558883000	0.133380000
1	-2.573265000	0.994832000	0.857242000
1	-0.002239000	0.395043000	0.238972000
27	-1.391107000	2.002530000	-1.620281000
7	-0.651247000	0.959263000	-2.809274000

7	-0.149396000	0.281585000	-3.561433000
7	-2.833033000	2.517135000	-2.796698000
6	-3.203471000	3.808424000	-2.957187000
6	-3.552206000	1.609379000	-3.496042000
6	-4.247720000	4.224640000	-3.761665000
1	-2.615555000	4.536014000	-2.410678000
6	-4.603820000	1.929315000	-4.335177000
1	-3.255224000	0.574690000	-3.371632000
6	-5.003084000	3.277411000	-4.493730000
1	-4.457695000	5.284982000	-3.823179000
1	-5.108618000	1.124627000	-4.854533000
7	-6.049703000	3.641679000	-5.302150000
6	-6.376456000	5.048585000	-5.477720000
1	-7.250420000	5.134947000	-6.124895000
1	-6.619920000	5.524364000	-4.519051000
1	-5.551814000	5.610261000	-5.939651000
6	-6.740671000	2.634044000	-6.092753000
1	-7.543723000	3.110497000	-6.656823000
1	-6.068232000	2.138103000	-6.807074000
1	-7.189970000	1.863044000	-5.453570000

η-NN

6	-0.626728000	3.411282000	-1.017728000
6	-2.026590000	3.681469000	-0.841619000
6	-2.694398000	2.494497000	-0.413346000
6	-1.723198000	1.457404000	-0.443044000
6	-0.455512000	2.022150000	-0.799202000
1	0.144644000	4.130346000	-1.260249000
1	-2.497045000	4.649790000	-0.967048000
1	-3.737776000	2.402726000	-0.143942000
1	-1.902760000	0.409379000	-0.238615000
1	0.467890000	1.466747000	-0.904382000
27	-1.847731000	2.299302000	-2.351572000
7	-2.213178000	0.674011000	-3.363267000
7	-1.139721000	1.027135000	-3.642091000
7	-2.602830000	3.425686000	-3.747499000
6	-2.088397000	4.640497000	-4.038697000
6	-3.688538000	3.055572000	-4.460904000
6	-2.606999000	5.495115000	-4.993522000
1	-1.209734000	4.926985000	-3.472405000
6	-4.274206000	3.835597000	-5.441801000
1	-4.090997000	2.075635000	-4.231557000
6	-3.745738000	5.113087000	-5.743475000

1	-2.115582000	6.446058000	-5.155466000
1	-5.139935000	3.444445000	-5.960899000
7	-4.298056000	5.926222000	-6.698488000
6	-5.431526000	5.459199000	-7.483435000
1	-6.292636000	5.225311000	-6.844082000
1	-5.733245000	6.244128000	-8.178247000
1	-5.184177000	4.561924000	-8.067723000
6	-3.684075000	7.209679000	-7.005047000
1	-2.660643000	7.095154000	-7.389190000
1	-4.277323000	7.717256000	-7.766847000
1	-3.647432000	7.857551000	-6.119691000

$[Co(\eta^5\text{-}Cp)py(p\text{-}NO)_2(N_2)]$

κ-N

6	0.072810000	2.179465000	-0.250997000
6	-0.298635000	3.506575000	-0.598769000
6	-1.688708000	3.623512000	-0.315282000
6	-2.145851000	2.413230000	0.313565000
6	-1.056333000	1.516171000	0.343821000
1	1.051142000	1.737568000	-0.391797000
1	0.337659000	4.265204000	-1.033002000
1	-2.292940000	4.503186000	-0.500273000

1	-3.142906000	2.225053000	0.690377000
1	-1.062811000	0.505862000	0.730829000
27	-1.445726000	2.063280000	-1.652932000
7	-0.732610000	0.768167000	-2.619664000
7	-0.243811000	-0.083354000	-3.167934000
7	-2.800439000	2.476272000	-2.899937000
6	-4.005474000	2.984570000	-2.502106000
6	-2.635886000	2.310770000	-4.246587000
6	-5.021216000	3.329638000	-3.372039000
1	-4.143468000	3.095359000	-1.435699000
6	-3.604415000	2.615580000	-5.183709000
1	-1.678084000	1.922922000	-4.565935000
6	-4.818478000	3.140232000	-4.739433000
1	-5.959519000	3.726190000	-3.005741000
1	-3.423946000	2.465082000	-6.240386000
7	-5.861985000	3.484706000	-5.689990000
8	-6.916680000	3.941434000	-5.238231000
8	-5.626544000	3.298789000	-6.887604000

η-NN

6	-0.818069000	3.244438000	-0.644468000
6	-2.183146000	3.611977000	-0.808700000

6	-2.996868000	2.422632000	-0.803421000
6	-2.119051000	1.320425000	-0.720864000
6	-0.778959000	1.822763000	-0.656322000
1	0.026945000	3.915363000	-0.573838000
1	-2.554403000	4.627524000	-0.875382000
1	-4.077452000	2.382223000	-0.848548000
1	-2.397586000	0.274944000	-0.743152000
1	0.115115000	1.213193000	-0.623804000
27	-1.641285000	2.478188000	-2.435289000
7	-1.228705000	1.012717000	-3.680640000
7	-0.284336000	1.677270000	-3.618155000
7	-2.353532000	3.598764000	-3.806261000
6	-1.653888000	3.912739000	-4.931037000
6	-3.589706000	4.157652000	-3.682879000
6	-2.139241000	4.741058000	-5.928964000
1	-0.666685000	3.478055000	-5.015595000
6	-4.146338000	5.006479000	-4.622605000
1	-4.145552000	3.888131000	-2.795414000
6	-3.405008000	5.298562000	-5.765800000
1	-1.547035000	4.963742000	-6.807272000
1	-5.135147000	5.424671000	-4.484747000

7	-3.953878000	6.186097000	-6.787107000
8	-3.253923000	6.415605000	-7.775091000
8	-5.080551000	6.646837000	-6.591881000

[Ir(η^5-Cp)(CNMe)(N_2)]

κ-N

6	-0.623417000	0.952156000	0.064891000
6	-1.648540000	1.918751000	0.177376000
6	-2.904343000	1.219246000	0.035703000
6	-2.633990000	-0.201290000	0.003891000
6	-1.232237000	-0.356038000	-0.032915000
1	0.440529000	1.149032000	0.074317000
1	-1.519481000	2.986610000	0.281323000
1	-3.885270000	1.667234000	0.123276000
1	-3.371684000	-0.989326000	-0.048307000
1	-0.696197000	-1.292206000	-0.116307000
77	-1.922292000	0.931709000	-1.937404000
7	-0.744338000	0.529337000	-3.410571000
7	-0.033704000	0.278271000	-4.244430000
6	-3.205713000	1.576308000	-3.129523000
7	-4.068075000	1.921837000	-3.887367000
6	-4.568064000	3.072248000	-4.588170000

1	-4.558952000	2.876342000	-5.664914000
1	-5.604379000	3.260768000	-4.289969000
1	-3.966277000	3.965381000	-4.381109000

η-NN

6	-0.558621000	3.301271000	-1.089939000
6	-1.898119000	3.821496000	-0.882593000
6	-2.697428000	2.781745000	-0.256752000
6	-1.903748000	1.614799000	-0.231382000
6	-0.595913000	1.930646000	-0.747168000
1	0.289122000	3.849540000	-1.474924000
1	-2.187636000	4.860058000	-0.975850000
1	-3.719075000	2.877945000	0.081622000
1	-2.223749000	0.636684000	0.103537000
1	0.219899000	1.227691000	-0.854918000
77	-2.180799000	2.414254000	-2.496377000
7	-2.785779000	0.573322000	-3.590589000
7	-1.745207000	0.831022000	-4.006392000
6	-2.975190000	3.464323000	-3.809576000
7	-3.556308000	4.120389000	-4.626168000
6	-3.378098000	4.960653000	-5.775527000
1	-2.318793000	5.062704000	-6.040154000

1	-3.919403000	4.536472000	-6.626995000
1	-3.794155000	5.952881000	-5.573122000

[Rh(η^5-Cp)(CNMe)(N_2)]

κ-N

6	-0.048025000	2.473421000	0.158771000
6	-1.147454000	3.343990000	0.202568000
6	-2.330753000	2.522837000	0.105046000
6	-1.940441000	1.136280000	0.212848000
6	-0.539159000	1.106607000	0.167742000
1	0.996163000	2.759799000	0.152842000
1	-1.119245000	4.424713000	0.215442000
1	-3.348876000	2.888753000	0.152386000
1	-2.607187000	0.285425000	0.234402000
1	0.083683000	0.220949000	0.167491000
45	-1.331174000	2.155872000	-1.846325000
7	-0.111641000	1.719944000	-3.333765000
7	0.598056000	1.465968000	-4.161237000
6	-2.728864000	2.640571000	-3.050348000
7	-3.603436000	2.935044000	-3.783131000
6	-4.616515000	3.358683000	-4.675218000
1	-4.597326000	2.747248000	-5.583575000

1	-5.599560000	3.253407000	-4.204209000
1	-4.469247000	4.408572000	-4.953365000

η-NN

6	-0.523334000	3.222110000	-0.973450000
6	-1.850522000	3.795337000	-0.897819000
6	-2.741158000	2.819776000	-0.304837000
6	-2.017361000	1.621874000	-0.210906000
6	-0.651228000	1.869432000	-0.623841000
1	0.372556000	3.726302000	-1.307791000
1	-2.087321000	4.840470000	-1.054600000
1	-3.781727000	2.973042000	-0.055100000
1	-2.402404000	0.667031000	0.124675000
1	0.137069000	1.127229000	-0.642469000
45	-2.075379000	2.347549000	-2.518143000
7	-2.675899000	0.485484000	-3.648791000
7	-1.602610000	0.682496000	-3.970089000
6	-2.703026000	3.488344000	-3.904197000
7	-3.094345000	4.196082000	-4.761175000
6	-3.539520000	5.021171000	-5.820802000
1	-2.776307000	5.080777000	-6.604715000
1	-4.460699000	4.617165000	-6.254573000

1	-3.741082000	6.031237000	-5.448963000

$[Co(PH_3)_2Cl(N_2)]$

κ-N

27	0.051770000	0.971254000	-0.107797000
17	-2.189051000	0.971249000	-0.107883000
15	-0.085506000	-1.225934000	-0.107939000
1	1.079859000	-2.032696000	-0.108129000
1	-0.761471000	-1.842447000	0.966852000
1	-0.761721000	-1.842280000	-1.182667000
15	-0.085515000	3.168442000	-0.107864000
1	1.079846000	3.975209000	-0.106629000
1	-0.760428000	3.784888000	-1.183367000
1	-0.762786000	3.784849000	0.966151000
7	1.763388000	0.971258000	-0.107814000
7	2.890784000	0.971257000	-0.107587000

η-NN

27	0.299674000	0.967286000	-0.189382000
17	-1.857397000	0.940731000	0.380729000
15	0.174699000	-1.277997000	-0.118107000
1	1.310629000	-2.074958000	-0.404591000
1	-0.205855000	-1.877226000	1.101123000

1	-0.753203000	-1.912631000	-0.970545000
15	0.104278000	3.208629000	-0.175655000
1	1.214743000	4.033258000	-0.482910000
1	-0.842708000	3.791691000	-1.043799000
1	-0.295481000	3.826728000	1.027906000
7	2.224205000	0.998647000	-0.099294000
7	1.927876000	0.979608000	-1.219985000

$[Co(PMe_3)_2Cl(N_2)]$

κ-N

27	0.040432000	0.971286000	-0.102759000
17	-2.225782000	0.972489000	-0.115072000
15	-0.063383000	-1.255499000	-0.102731000
15	-0.061000000	3.198168000	-0.103077000
7	1.741111000	0.970373000	-0.093567000
7	2.872664000	0.969836000	-0.087467000
6	-0.934931000	3.920292000	-1.556814000
1	-1.931180000	3.476020000	-1.623400000
1	-1.019750000	5.009977000	-1.474169000
1	-0.384343000	3.674444000	-2.470588000
6	-0.950463000	3.919491000	1.341635000
1	-1.034033000	5.009266000	1.258899000

1	-1.947487000	3.475446000	1.397127000
1	-0.409851000	3.672779000	2.261116000
6	1.532226000	4.131807000	-0.094160000
1	2.115901000	3.868260000	0.793282000
1	2.125535000	3.868856000	-0.975366000
1	1.359267000	5.213688000	-0.094737000
6	-0.938026000	-1.976904000	-1.556396000
1	-1.024085000	-3.066476000	-1.473557000
1	-1.933769000	-1.531517000	-1.623130000
1	-0.387096000	-1.731847000	-2.470176000
6	-0.953688000	-1.975625000	1.342062000
1	-1.950229000	-1.530486000	1.397450000
1	-1.038437000	-3.065322000	1.259494000
1	-0.412835000	-1.729355000	2.261519000
6	1.528826000	-2.190867000	-0.093569000
1	2.122498000	-1.928684000	-0.974759000
1	2.112712000	-1.927837000	0.793888000
1	1.354686000	-3.272559000	-0.094012000

η-NN

27	2.890640000	0.303502000	0.116527000
17	1.127445000	-0.876814000	-0.647371000

15	1.459623000	1.253230000	1.596410000
15	4.133403000	-0.772746000	-1.444609000
7	4.438921000	0.840161000	1.120663000
7	4.206933000	1.683448000	0.353681000
6	4.153759000	-2.607996000	-1.277454000
1	3.122895000	-2.971270000	-1.289113000
1	4.721359000	-3.081867000	-2.086459000
1	4.605719000	-2.881640000	-0.318452000
6	3.577558000	-0.509765000	-3.181948000
1	4.175182000	-1.093882000	-3.891088000
1	2.526507000	-0.799618000	-3.259930000
1	3.662831000	0.552035000	-3.435211000
6	5.927713000	-0.345373000	-1.516413000
1	6.045878000	0.723932000	-1.717183000
1	6.398021000	-0.559148000	-0.551650000
1	6.443262000	-0.913969000	-2.298072000
6	0.049492000	2.157713000	0.828314000
1	-0.483554000	1.473485000	0.163137000
1	-0.640118000	2.549582000	1.584682000
1	0.433158000	2.991329000	0.231049000
6	0.632447000	0.062326000	2.734003000

1	-0.089043000	0.563088000	3.389681000
1	0.121088000	-0.695420000	2.134734000
1	1.386995000	-0.436451000	3.351020000
6	2.169856000	2.503572000	2.753735000
1	2.966302000	2.046667000	3.349194000
1	2.608610000	3.328395000	2.183805000
1	1.405131000	2.903666000	3.428436000

$[Co(CO)_2Cl(N_2)]$

κ-N

27	0.087111000	0.971093000	0.046472000
17	-1.994192000	0.973384000	-0.640422000
6	-0.110507000	-0.775739000	0.447401000
6	-0.108853000	2.717543000	0.450005000
7	1.860401000	0.970391000	0.211999000
7	2.976155000	0.970200000	0.217802000
8	-0.321725000	3.766936000	0.851042000
8	-0.324316000	-1.825487000	0.847016000

η-NN

27	2.807859000	0.519946000	-0.099790000
17	1.098990000	-0.635379000	-0.833207000
6	1.629866000	1.266328000	1.080893000

6	3.782120000	-0.364885000	-1.367765000
7	4.415015000	1.114354000	0.915854000
7	4.180634000	1.939652000	0.160998000
8	4.342090000	-0.944192000	-2.173438000
8	0.854136000	1.699337000	1.794412000

$[Co(CNMe)_2Cl(N_2)]$

κ-N

27	0.226988000	0.970642000	0.749114000
17	-2.005246000	0.971234000	0.888445000
6	0.109214000	-0.856117000	0.756775000
6	0.110341000	2.797627000	0.760149000
7	1.965129000	0.970218000	0.638249000
7	3.085230000	0.969917000	0.566141000
7	-0.035210000	3.957952000	0.772696000
7	-0.037118000	-2.016369000	0.767540000
6	-0.345750000	5.339265000	0.796045000
1	-1.429862000	5.468989000	0.867774000
1	0.132169000	5.814579000	1.658364000
1	0.014924000	5.818246000	-0.119611000
6	-0.348683000	-3.397480000	0.788885000
1	-1.432922000	-3.526504000	0.859972000

1	0.012016000	-3.875504000	-0.127263000
1	0.128512000	-3.874311000	1.650766000

η-NN

27	2.881178000	0.903027000	-0.290582000
17	1.092974000	0.036192000	-1.287084000
6	1.705587000	1.681356000	0.905308000
6	3.886294000	0.041474000	-1.581575000
7	4.432702000	1.174101000	0.891225000
7	4.359571000	2.101469000	0.215374000
7	0.908028000	2.141089000	1.624249000
7	4.457736000	-0.529009000	-2.425550000
6	-0.132379000	2.651083000	2.438641000
1	-1.096542000	2.294140000	2.064427000
1	0.002505000	2.312110000	3.470338000
1	-0.119302000	3.745095000	2.417269000
6	5.057937000	-1.253418000	-3.484223000
1	5.741086000	-2.006399000	-3.079472000
1	4.280773000	-1.750114000	-4.072751000
1	5.619611000	-0.571541000	-4.130010000

[Ti(η^5-Cp*)$_2$(N_2)] singlet

κ-N

6	-0.993559000	3.392063000	-2.638938000
6	-2.102514000	4.279052000	-2.833750000
6	-3.310222000	3.534478000	-2.608133000
6	-2.929203000	2.178837000	-2.289526000
6	-1.508843000	2.100095000	-2.331497000
22	-2.317154000	2.717126000	-4.540107000
7	-5.099653000	1.344012000	-4.874704000
7	-4.084343000	1.840293000	-4.747541000
6	-4.701715000	4.099323000	-2.503227000
1	-5.456922000	3.404680000	-2.886798000
1	-4.965452000	4.322633000	-1.458908000
1	-4.801791000	5.034210000	-3.065218000
6	-2.021705000	5.769073000	-3.044171000
1	-2.840887000	6.140705000	-3.669681000
1	-2.079706000	6.309224000	-2.088546000
1	-1.083822000	6.064601000	-3.525159000
6	0.454243000	3.785146000	-2.537677000
1	0.671989000	4.714145000	-3.069430000
1	0.728196000	3.945044000	-1.485015000
1	1.126447000	3.012660000	-2.926291000
6	-0.684002000	0.881540000	-2.011084000

1	0.272185000	0.883109000	-2.544425000
1	-0.454923000	0.828189000	-0.937482000
1	-1.206884000	-0.044348000	-2.273645000
6	-3.851636000	1.099818000	-1.794534000
1	-3.439231000	0.100116000	-1.966615000
1	-4.017654000	1.201794000	-0.712577000
1	-4.831441000	1.135635000	-2.278721000
1	-4.673031000	2.118303000	-7.326973000
1	-3.807570000	2.799825000	-8.707797000
6	-3.975699000	2.906150000	-7.626436000
1	-4.480790000	3.865289000	-7.470588000
6	-2.673444000	2.834154000	-6.877886000
6	-1.946577000	1.625539000	-6.559360000
6	-0.663725000	2.017842000	-6.052230000
6	-0.589778000	3.446576000	-6.082423000
6	-1.834850000	3.943975000	-6.561882000
6	-2.169580000	5.392405000	-6.803948000
1	-3.235244000	5.596530000	-6.651505000
1	-1.932399000	5.686382000	-7.836018000
1	-1.608543000	6.058760000	-6.141395000
1	0.418146000	5.248043000	-5.404983000

6	0.643242000	4.277245000	-5.859067000
1	1.375365000	3.773821000	-5.223319000
1	1.137538000	4.481888000	-6.819468000
6	0.463218000	1.079201000	-5.705781000
1	0.099226000	0.156185000	-5.240951000
1	1.025396000	0.784203000	-6.603004000
1	1.178086000	1.534820000	-5.012900000
6	-2.376517000	0.227237000	-6.912939000
1	-3.443798000	0.065266000	-6.727782000
1	-2.194219000	0.011664000	-7.976043000
1	-1.826437000	-0.522993000	-6.334743000

η-NN

6	-1.015583000	3.227333000	-2.654228000
6	-2.031624000	4.213793000	-2.881523000
6	-3.300798000	3.604119000	-2.599640000
6	-3.059119000	2.269123000	-2.169283000
6	-1.664886000	2.018717000	-2.244075000
22	-2.310619000	2.573931000	-4.543662000
7	-3.520396000	0.839970000	-4.605407000
7	-4.238014000	1.750465000	-4.800605000
6	-4.639008000	4.293183000	-2.634956000

1	-5.437466000	3.611850000	-2.945632000
1	-4.911255000	4.692606000	-1.647646000
1	-4.640779000	5.137317000	-3.333156000
6	-1.819203000	5.692593000	-3.073750000
1	-2.583471000	6.143200000	-3.715386000
1	-1.864712000	6.216539000	-2.108251000
1	-0.844139000	5.918145000	-3.513080000
6	0.464825000	3.474461000	-2.536001000
1	0.769964000	4.399762000	-3.028578000
1	0.748726000	3.564667000	-1.477694000
1	1.064886000	2.659191000	-2.954759000
6	-0.973173000	0.739262000	-1.856045000
1	-0.034666000	0.600805000	-2.404271000
1	-0.722504000	0.729387000	-0.785577000
1	-1.601912000	-0.135572000	-2.050365000
6	-4.098175000	1.292634000	-1.698656000
1	-3.860685000	0.266154000	-1.994830000
1	-4.170912000	1.313011000	-0.602451000
1	-5.088264000	1.527056000	-2.099169000
1	-4.508491000	1.813566000	-7.316221000
1	-3.779188000	2.630682000	-8.705279000

6	-3.921368000	2.686957000	-7.616758000
1	-4.531568000	3.572377000	-7.411822000
6	-2.597097000	2.747624000	-6.907900000
6	-1.726426000	1.635652000	-6.666635000
6	-0.511857000	2.142528000	-6.113932000
6	-0.613636000	3.564750000	-6.046247000
6	-1.912829000	3.934525000	-6.504747000
6	-2.418416000	5.340281000	-6.697819000
1	-3.488409000	5.426834000	-6.477020000
1	-2.281007000	5.667003000	-7.738204000
1	-1.890033000	6.056524000	-6.062369000
1	0.209527000	5.438498000	-5.304886000
6	0.524901000	4.515889000	-5.800746000
1	1.320597000	4.067401000	-5.201590000
1	0.974476000	4.810664000	-6.759913000
6	0.710538000	1.318912000	-5.802754000
1	0.449516000	0.351654000	-5.358970000
1	1.286349000	1.106685000	-6.714442000
1	1.384668000	1.829786000	-5.108832000
6	-1.987018000	0.213518000	-7.077846000
1	-3.026655000	-0.080573000	-6.903429000

1	-1.779345000	0.073168000	-8.148083000
1	-1.355517000	-0.490529000	-6.526743000

[Ti(η^5-Cp*)$_2$(N_2)] triplet

κ-N

6	-1.024090000	3.366662000	-2.629383000
6	-2.116508000	4.286480000	-2.751815000
6	-3.322586000	3.561388000	-2.531110000
6	-2.973768000	2.190600000	-2.278727000
6	-1.557034000	2.068795000	-2.359568000
22	-2.327525000	2.714133000	-4.546763000
7	-5.190789000	1.376949000	-4.940380000
7	-4.172853000	1.852539000	-4.800290000
6	-4.705414000	4.150063000	-2.444035000
1	-5.474961000	3.447612000	-2.780688000
1	-4.953666000	4.429383000	-1.409878000
1	-4.799630000	5.055304000	-3.053272000
6	-2.004545000	5.779192000	-2.916200000
1	-2.866369000	6.196953000	-3.447297000
1	-1.949902000	6.285093000	-1.941410000
1	-1.107079000	6.063807000	-3.475038000
6	0.431648000	3.730201000	-2.517350000

1	0.662050000	4.683121000	-2.999317000
1	0.714674000	3.828373000	-1.459377000
1	1.089059000	2.968941000	-2.950749000
6	-0.755473000	0.836052000	-2.035239000
1	0.192581000	0.809330000	-2.582270000
1	-0.511196000	0.787107000	-0.963813000
1	-1.302086000	-0.080305000	-2.282100000
6	-3.915839000	1.104805000	-1.833721000
1	-3.593899000	0.115755000	-2.177430000
1	-3.968434000	1.065674000	-0.736542000
1	-4.934376000	1.262951000	-2.199446000
1	-4.513521000	1.941942000	-7.552391000
1	-3.738372000	2.949756000	-8.775319000
6	-3.919746000	2.849154000	-7.695928000
1	-4.540682000	3.698833000	-7.391775000
6	-2.617395000	2.804714000	-6.943322000
6	-1.858815000	1.623859000	-6.635428000
6	-0.614682000	2.035995000	-6.077551000
6	-0.601437000	3.468916000	-6.047613000
6	-1.847935000	3.940935000	-6.562029000
6	-2.203716000	5.379772000	-6.828070000

1	-3.287048000	5.539852000	-6.814860000
1	-1.841937000	5.705732000	-7.814433000
1	-1.763809000	6.054102000	-6.086088000
1	0.340301000	5.286505000	-5.315648000
6	0.601031000	4.337527000	-5.796110000
1	1.350115000	3.843335000	-5.173117000
1	1.089730000	4.588289000	-6.748668000
6	0.541406000	1.131859000	-5.739950000
1	0.203598000	0.154583000	-5.379135000
1	1.175471000	0.949426000	-6.619637000
1	1.185170000	1.561290000	-4.965396000
6	-2.253806000	0.209806000	-6.968149000
1	-3.334201000	0.052329000	-6.885175000
1	-1.968024000	-0.050324000	-7.997604000
1	-1.765871000	-0.513583000	-6.306217000

η-NN

6	-1.010714000	3.331514000	-2.664429000
6	-2.077997000	4.278322000	-2.781829000
6	-3.299606000	3.592058000	-2.519808000
6	-2.986534000	2.223752000	-2.245776000
6	-1.577305000	2.054907000	-2.360095000

22	-2.369001000	2.668753000	-4.554979000
7	-4.145967000	1.215269000	-4.756429000
7	-4.606577000	2.254244000	-4.916460000
6	-4.660691000	4.227840000	-2.424264000
1	-5.459841000	3.535269000	-2.706145000
1	-4.868065000	4.565085000	-1.398655000
1	-4.745877000	5.103263000	-3.076664000
6	-1.937014000	5.766850000	-2.960150000
1	-2.770989000	6.192139000	-3.528854000
1	-1.914761000	6.281716000	-1.988804000
1	-1.013728000	6.032841000	-3.483677000
6	0.453845000	3.656635000	-2.545946000
1	0.707591000	4.615122000	-3.003055000
1	0.733596000	3.722963000	-1.484630000
1	1.096153000	2.890971000	-2.992986000
6	-0.808814000	0.803649000	-2.027233000
1	0.137317000	0.746788000	-2.575119000
1	-0.564297000	0.757712000	-0.955711000
1	-1.381414000	-0.099336000	-2.264597000
6	-3.953888000	1.169596000	-1.779955000
1	-3.690921000	0.173852000	-2.151872000

1	-3.963030000	1.116525000	-0.682169000
1	-4.978430000	1.378260000	-2.101045000
1	-4.372511000	1.739304000	-7.659086000
1	-3.638512000	2.831039000	-8.834736000
6	-3.842350000	2.690230000	-7.763930000
1	-4.530637000	3.484351000	-7.456339000
6	-2.558963000	2.714818000	-6.978908000
6	-1.763902000	1.578442000	-6.629759000
6	-0.561421000	2.052437000	-6.028534000
6	-0.615599000	3.482833000	-6.010183000
6	-1.864566000	3.889883000	-6.573282000
6	-2.282570000	5.307085000	-6.862974000
1	-3.372386000	5.415860000	-6.868472000
1	-1.920878000	5.637395000	-7.847934000
1	-1.885533000	6.009635000	-6.123077000
1	0.242354000	5.340825000	-5.267404000
6	0.542436000	4.411087000	-5.761602000
1	1.326343000	3.949007000	-5.158231000
1	1.000560000	4.696412000	-6.719594000
6	0.624097000	1.199670000	-5.661684000
1	0.320865000	0.223149000	-5.269234000

1	1.261176000	1.010076000	-6.537643000
1	1.255075000	1.675715000	-4.905075000
6	-2.078880000	0.142297000	-6.952739000
1	-3.154019000	-0.060328000	-6.923026000
1	-1.724428000	-0.123753000	-7.958816000
1	-1.600043000	-0.545951000	-6.248264000

[Zr(η^5-Cp*)$_2$(N_2)] singlet

κ-N

6	-1.096767000	3.666813000	-2.481442000
6	-2.315349000	4.405464000	-2.544057000
6	-3.407681000	3.484873000	-2.384566000
6	-2.845430000	2.161360000	-2.218511000
6	-1.423738000	2.283597000	-2.296228000
40	-2.394917000	2.914133000	-4.576685000
7	-5.331150000	1.459739000	-4.915334000
7	-4.320846000	1.970893000	-4.799489000
6	-4.848629000	3.856665000	-2.146990000
1	-5.539107000	3.107036000	-2.546205000
1	-5.059838000	3.954411000	-1.071587000
1	-5.103453000	4.815143000	-2.612221000
6	-2.443941000	5.904523000	-2.635614000

1	-3.311388000	6.209184000	-3.233621000
1	-2.575346000	6.353022000	-1.640364000
1	-1.557131000	6.363823000	-3.084190000
6	0.287757000	4.255190000	-2.454241000
1	0.365989000	5.160335000	-3.065319000
1	0.570177000	4.532689000	-1.428751000
1	1.043333000	3.550023000	-2.814095000
6	-0.437408000	1.167438000	-2.069522000
1	0.529797000	1.371861000	-2.539564000
1	-0.250731000	1.017766000	-0.996722000
1	-0.800303000	0.213581000	-2.467746000
6	-3.608563000	0.934543000	-1.797783000
1	-3.044833000	0.018848000	-2.003492000
1	-3.817810000	0.953024000	-0.717882000
1	-4.570281000	0.847699000	-2.313242000
1	-4.651829000	2.409475000	-7.532762000
1	-3.673661000	2.898006000	-8.920740000
6	-3.848423000	3.081577000	-7.850067000
1	-4.224562000	4.106223000	-7.757326000
6	-2.586277000	2.874481000	-7.053453000
6	-2.031812000	1.590309000	-6.680172000

6	-0.719587000	1.822346000	-6.161706000
6	-0.445172000	3.227848000	-6.234120000
6	-1.594775000	3.875652000	-6.773825000
6	-1.719130000	5.340898000	-7.104575000
1	-2.730312000	5.722020000	-6.916695000
1	-1.505373000	5.527393000	-8.166771000
1	-1.023050000	5.952160000	-6.521203000
1	0.761622000	4.916845000	-5.601341000
6	0.877444000	3.882614000	-5.941796000
1	1.443506000	3.346159000	-5.174351000
1	1.504404000	3.908458000	-6.844363000
6	0.262699000	0.752553000	-5.760293000
1	-0.230936000	-0.095700000	-5.273553000
1	0.793222000	0.355433000	-6.637258000
1	1.022156000	1.130781000	-5.068577000
6	-2.631410000	0.250509000	-7.012179000
1	-3.712321000	0.226469000	-6.840461000
1	-2.463281000	-0.005064000	-8.069010000
1	-2.187741000	-0.549558000	-6.410763000

η-NN

6	-1.035698000	3.238278000	-2.483465000

6	-2.038677000	4.241018000	-2.715173000
6	-3.321279000	3.643612000	-2.455623000
6	-3.102869000	2.293603000	-2.049458000
6	-1.705224000	2.033020000	-2.085687000
40	-2.325091000	2.563260000	-4.546986000
7	-3.643115000	0.722045000	-4.647204000
7	-4.366877000	1.637476000	-4.849005000
6	-4.647467000	4.358477000	-2.477405000
1	-5.466050000	3.687146000	-2.755184000
1	-4.889275000	4.782670000	-1.492171000
1	-4.651141000	5.190250000	-3.190996000
6	-1.793170000	5.713555000	-2.925533000
1	-2.569756000	6.179765000	-3.541844000
1	-1.783898000	6.249471000	-1.965347000
1	-0.830437000	5.905458000	-3.408502000
6	0.450656000	3.468129000	-2.394677000
1	0.769924000	4.330714000	-2.985178000
1	0.750248000	3.661143000	-1.354389000
1	1.027601000	2.600876000	-2.735042000
6	-1.030426000	0.751002000	-1.673368000
1	-0.100751000	0.578766000	-2.228200000

1	-0.765198000	0.766341000	-0.606409000
1	-1.676857000	-0.117246000	-1.835117000
6	-4.164454000	1.324769000	-1.610491000
1	-3.916373000	0.294853000	-1.884825000
1	-4.289027000	1.357898000	-0.519215000
1	-5.134144000	1.554364000	-2.060922000
1	-4.505876000	1.813458000	-7.386228000
1	-3.730638000	2.428557000	-8.853632000
6	-3.880773000	2.621144000	-7.781838000
1	-4.456204000	3.548251000	-7.695063000
6	-2.561145000	2.717002000	-7.065474000
6	-1.676576000	1.612130000	-6.811355000
6	-0.464344000	2.138410000	-6.266038000
6	-0.587512000	3.562171000	-6.194977000
6	-1.886137000	3.916591000	-6.676442000
6	-2.401177000	5.320301000	-6.866953000
1	-3.488289000	5.379195000	-6.744045000
1	-2.173979000	5.690027000	-7.876870000
1	-1.949681000	6.022288000	-6.158327000
1	0.159351000	5.447263000	-5.414247000
6	0.523546000	4.528499000	-5.885172000

1	1.278887000	4.092317000	-5.225607000
1	1.039324000	4.827648000	-6.808928000
6	0.774112000	1.341962000	-5.943030000
1	0.531610000	0.340144000	-5.571865000
1	1.402469000	1.208810000	-6.834937000
1	1.392638000	1.834046000	-5.185079000
6	-1.935622000	0.186849000	-7.217148000
1	-2.936127000	-0.148740000	-6.923515000
1	-1.853944000	0.069413000	-8.307073000
1	-1.216338000	-0.500372000	-6.760606000

[Zr(η^5-Cp*)$_2$(N_2)] triplet

κ-N

6	-1.049969000	3.395485000	-2.501405000
6	-2.135868000	4.327427000	-2.613175000
6	-3.347855000	3.612923000	-2.371675000
6	-3.012270000	2.240049000	-2.120741000
6	-1.592837000	2.102955000	-2.208867000
40	-2.391810000	2.701183000	-4.557564000
7	-5.444971000	1.378887000	-4.969552000
7	-4.410217000	1.826606000	-4.832685000
6	-4.721837000	4.219504000	-2.260664000

1	-5.507654000	3.514034000	-2.548827000
1	-4.931855000	4.533879000	-1.227871000
1	-4.827178000	5.104005000	-2.897465000
6	-2.007783000	5.819342000	-2.776997000
1	-2.886863000	6.250177000	-3.267075000
1	-1.899298000	6.319059000	-1.803077000
1	-1.132948000	6.092236000	-3.376727000
6	0.413034000	3.746683000	-2.448690000
1	0.636388000	4.672126000	-2.986080000
1	0.734359000	3.893409000	-1.407373000
1	1.046148000	2.956878000	-2.867876000
6	-0.798644000	0.872328000	-1.858263000
1	0.144756000	0.822139000	-2.412085000
1	-0.546433000	0.853456000	-0.787250000
1	-1.355204000	-0.044778000	-2.076372000
6	-3.966831000	1.162963000	-1.677927000
1	-3.649123000	0.171379000	-2.017508000
1	-4.031213000	1.127105000	-0.581050000
1	-4.980222000	1.328676000	-2.055169000
1	-4.454031000	1.875080000	-7.715510000
1	-3.680593000	2.876625000	-8.945511000

6	-3.865627000	2.784899000	-7.865786000
1	-4.492529000	3.632949000	-7.570240000
6	-2.566809000	2.754065000	-7.104271000
6	-1.808022000	1.579420000	-6.776399000
6	-0.572441000	2.001320000	-6.200188000
6	-0.564344000	3.436981000	-6.181972000
6	-1.802519000	3.901908000	-6.729652000
6	-2.145936000	5.334428000	-7.042528000
1	-3.228090000	5.499163000	-7.051325000
1	-1.763549000	5.628618000	-8.031659000
1	-1.715601000	6.027020000	-6.311638000
1	0.333332000	5.265997000	-5.427059000
6	0.623795000	4.309371000	-5.875433000
1	1.329864000	3.824478000	-5.196137000
1	1.174458000	4.544456000	-6.797770000
6	0.586517000	1.106052000	-5.847589000
1	0.250073000	0.116271000	-5.522399000
1	1.250212000	0.956918000	-6.711989000
1	1.199530000	1.524301000	-5.042072000
6	-2.189663000	0.160395000	-7.106259000
1	-3.273674000	0.010237000	-7.080967000

1	-1.847564000	-0.116861000	-8.114155000
1	-1.744777000	-0.552644000	-6.404301000

η-NN

6	-1.035280000	3.343269000	-2.547624000
6	-2.100749000	4.301102000	-2.629224000
6	-3.322634000	3.615060000	-2.355211000
6	-3.014959000	2.238076000	-2.113824000
6	-1.603129000	2.063218000	-2.242520000
40	-2.437101000	2.675029000	-4.569859000
7	-4.393515000	1.256370000	-4.823265000
7	-4.814453000	2.324737000	-4.942988000
6	-4.681366000	4.251042000	-2.228115000
1	-5.483497000	3.573280000	-2.536754000
1	-4.882753000	4.542567000	-1.187359000
1	-4.765014000	5.153716000	-2.841805000
6	-1.943669000	5.791185000	-2.784390000
1	-2.818105000	6.244219000	-3.262695000
1	-1.816587000	6.280631000	-1.807540000
1	-1.068646000	6.051311000	-3.388882000
6	0.434611000	3.663637000	-2.485173000
1	0.676479000	4.601573000	-2.990729000

1	0.754026000	3.770697000	-1.438432000
1	1.054949000	2.875934000	-2.925842000
6	-0.831675000	0.814180000	-1.906457000
1	0.099407000	0.741454000	-2.478068000
1	-0.559550000	0.790362000	-0.840412000
1	-1.414261000	-0.089643000	-2.111900000
6	-3.989439000	1.179177000	-1.671683000
1	-3.715068000	0.187479000	-2.046262000
1	-4.023958000	1.117188000	-0.574760000
1	-5.006721000	1.387751000	-2.015816000
1	-4.321254000	1.687246000	-7.790133000
1	-3.592804000	2.760665000	-8.987472000
6	-3.795939000	2.638731000	-7.914179000
1	-4.488183000	3.434924000	-7.620664000
6	-2.514924000	2.683107000	-7.124502000
6	-1.714329000	1.554405000	-6.758246000
6	-0.521391000	2.041717000	-6.144089000
6	-0.585161000	3.475075000	-6.137468000
6	-1.825746000	3.872186000	-6.732246000
6	-2.228411000	5.282153000	-7.075389000
1	-3.316607000	5.393690000	-7.118308000

1	-1.831789000	5.581104000	-8.057528000
1	-1.853149000	6.003995000	-6.342584000
1	0.216275000	5.340763000	-5.360190000
6	0.553355000	4.412415000	-5.834159000
1	1.302466000	3.957524000	-5.181879000
1	1.066370000	4.698601000	-6.763593000
6	0.666832000	1.204690000	-5.748917000
1	0.367148000	0.213725000	-5.392443000
1	1.343727000	1.051938000	-6.602128000
1	1.255198000	1.674829000	-4.954557000
6	-2.023143000	0.114049000	-7.070075000
1	-3.096183000	-0.096237000	-7.018849000
1	-1.686229000	-0.151420000	-8.082527000
1	-1.524723000	-0.566400000	-6.372152000

$[Re(\eta^5\text{-}Cp^*)(CO)_2(PMe_3)(N_2)]$

κ-N

6	-0.187299000	2.293131000	-0.434115000
6	-1.038935000	3.290488000	0.143014000
6	-2.338358000	2.684946000	0.374301000
6	-2.273529000	1.329479000	-0.069293000
6	-0.953849000	1.077793000	-0.596702000

6	-0.677874000	2.844025000	-3.400255000
8	0.136035000	2.874444000	-4.247657000
7	-2.661138000	4.492636000	-2.294548000
7	-3.097914000	5.533340000	-2.388758000
6	-3.486147000	3.347092000	1.086494000
1	-4.441383000	2.870054000	0.847787000
1	-3.355546000	3.297179000	2.177038000
1	-3.572150000	4.404648000	0.817693000
6	-0.632876000	4.668557000	0.587050000
1	-1.439775000	5.394040000	0.443239000
1	-0.369135000	4.676701000	1.654083000
1	0.234555000	5.029773000	0.027628000
6	1.284281000	2.434553000	-0.710053000
1	1.559671000	3.474731000	-0.904035000
1	1.871857000	2.087256000	0.151000000
1	1.590545000	1.846897000	-1.580076000
6	-0.396877000	-0.265931000	-0.981824000
1	0.411482000	-0.170702000	-1.712611000
1	0.009461000	-0.794015000	-0.106464000
1	-1.162598000	-0.909993000	-1.424865000
6	-3.335663000	0.284953000	0.131823000

1	-3.337907000	-0.458656000	-0.671016000
1	-3.162144000	-0.256258000	1.072420000
1	-4.335766000	0.723853000	0.189780000
75	-1.879265000	2.729854000	-1.939269000
15	-3.468189000	1.767187000	-3.416179000
6	-5.233619000	1.667902000	-2.849285000
6	-3.165827000	0.023846000	-3.970369000
6	-3.675646000	2.627025000	-5.043628000
1	-2.716179000	2.640546000	-5.569265000
1	-4.425783000	2.132791000	-5.671255000
1	-3.980939000	3.663473000	-4.869614000
1	-3.143228000	-0.644824000	-3.104340000
1	-3.942664000	-0.319737000	-4.663411000
1	-2.191559000	-0.029044000	-4.465629000
1	-5.301873000	1.063015000	-1.940563000
1	-5.879793000	1.227088000	-3.617331000
1	-5.592582000	2.675510000	-2.616635000

η-NN

6	-0.268622000	2.172075000	-0.213726000
6	-0.877605000	3.444083000	0.010797000
6	-2.306471000	3.245048000	0.164581000

6	-2.567300000	1.850734000	0.033790000
6	-1.317454000	1.171597000	-0.247645000
6	-0.381993000	1.922799000	-3.253260000
8	0.452828000	1.463960000	-3.947834000
7	-2.447234000	4.397552000	-3.156805000
7	-1.402885000	4.660263000	-2.742008000
6	-3.293362000	4.321833000	0.521488000
1	-4.316964000	4.035033000	0.262763000
1	-3.272765000	4.538372000	1.599210000
1	-3.073716000	5.258517000	-0.001116000
6	-0.168350000	4.756449000	0.186045000
1	-0.721226000	5.580521000	-0.275394000
1	-0.047760000	4.992216000	1.252372000
1	0.826108000	4.738144000	-0.267540000
6	1.205746000	1.887731000	-0.291363000
1	1.764680000	2.755574000	-0.651918000
1	1.600638000	1.621728000	0.698985000
1	1.418745000	1.056938000	-0.969659000
6	-1.096151000	-0.316728000	-0.225622000
1	-0.244764000	-0.602442000	-0.850137000
1	-0.895049000	-0.673052000	0.795293000

1	-1.969489000	-0.861970000	-0.595757000
6	-3.878154000	1.170576000	0.313276000
1	-4.015458000	0.272545000	-0.296088000
1	-3.922636000	0.855557000	1.365260000
1	-4.729580000	1.833928000	0.136462000
75	-1.647259000	2.552148000	-2.012395000
15	-3.282621000	1.544579000	-3.420981000
6	-3.379922000	-0.306100000	-3.425032000
6	-3.092019000	1.888574000	-5.229393000
6	-5.055601000	2.017816000	-3.155940000
1	-5.150459000	3.102951000	-3.258357000
1	-5.713326000	1.529235000	-3.884051000
1	-5.374114000	1.737215000	-2.148035000
1	-2.113471000	1.531175000	-5.563284000
1	-3.877368000	1.400608000	-5.817734000
1	-3.136171000	2.968878000	-5.394934000
1	-2.400669000	-0.712633000	-3.695322000
1	-4.129315000	-0.665833000	-4.139522000
1	-3.638643000	-0.674908000	-2.428045000

[Re(η^5-Cp*)$(CO)_2(N_2)$]

κ-N

6	-0.072276000	2.146637000	-0.173329000
6	-1.050516000	3.214303000	-0.201754000
6	-2.343400000	2.616152000	-0.006947000
6	-2.183230000	1.199317000	0.138798000
6	-0.766071000	0.907635000	0.030665000
6	-0.080995000	2.331668000	-3.259910000
8	0.793478000	2.696300000	-3.938281000
7	-2.888806000	2.518123000	-3.125044000
7	-3.753662000	2.979601000	-3.675817000
6	-3.641438000	3.366637000	0.106329000
1	-4.491643000	2.757477000	-0.212992000
1	-3.819525000	3.663387000	1.148501000
1	-3.637396000	4.277744000	-0.498665000
6	-0.747154000	4.687390000	-0.237011000
1	-1.567537000	5.259075000	-0.680423000
1	-0.583119000	5.078228000	0.777344000
1	0.153259000	4.899561000	-0.820416000
6	1.420003000	2.334038000	-0.193251000
1	1.715564000	3.161786000	-0.843961000
1	1.790625000	2.555882000	0.816686000
1	1.933782000	1.436547000	-0.547378000

6	-0.134276000	-0.435771000	0.273510000
1	0.844201000	-0.512559000	-0.207781000
1	0.007495000	-0.604983000	1.349695000
1	-0.754907000	-1.250183000	-0.110794000
6	-3.256127000	0.211131000	0.506543000
1	-3.047710000	-0.781660000	0.097689000
1	-3.334414000	0.108753000	1.598170000
1	-4.236642000	0.520729000	0.133832000
75	-1.420319000	1.764827000	-2.010531000
6	-1.549773000	0.047203000	-2.853388000
8	-1.606959000	-1.039879000	-3.269150000

η-NN

6	-0.027568000	2.257726000	-0.096484000
6	-1.036101000	3.265703000	-0.067660000
6	-2.325199000	2.609970000	0.070333000
6	-2.101992000	1.202443000	0.125650000
6	-0.678854000	0.961878000	-0.030324000
6	0.143213000	1.646150000	-3.115359000
8	1.116402000	1.472968000	-3.733605000
7	-2.839001000	3.295580000	-3.141026000
7	-1.826954000	3.810549000	-3.245646000

6	-3.638798000	3.320094000	0.243247000
1	-4.483754000	2.668166000	0.006654000
1	-3.760996000	3.663151000	1.279825000
1	-3.711823000	4.200967000	-0.402366000
6	-0.821474000	4.753447000	-0.059158000
1	-1.593388000	5.277729000	-0.631332000
1	-0.852903000	5.144160000	0.967217000
1	0.146715000	5.023618000	-0.488756000
6	1.458996000	2.481610000	-0.105013000
1	1.722934000	3.436122000	-0.568112000
1	1.847438000	2.489129000	0.922368000
1	1.982564000	1.692488000	-0.651269000
6	0.013980000	-0.359164000	0.164836000
1	0.966953000	-0.393385000	-0.370491000
1	0.220603000	-0.541042000	1.228906000
1	-0.596605000	-1.188560000	-0.202835000
6	-3.136468000	0.143637000	0.388213000
1	-2.899388000	-0.789421000	-0.129888000
1	-3.188981000	-0.076746000	1.462982000
1	-4.131706000	0.459152000	0.063866000
75	-1.360985000	1.896618000	-1.961764000

6	-2.223139000	0.446659000	-2.862158000
8	-2.750621000	-0.486940000	-3.319778000

$[Os(NH_3)_5(N_2)]$

κ-N

76	-0.773064000	-0.488455000	-0.001082000
7	-2.967755000	-0.426390000	0.005252000
1	-3.328960000	0.353383000	-0.553273000
1	-3.438865000	-1.259073000	-0.360704000
7	-0.782470000	-0.505467000	-2.197803000
1	-0.453193000	0.385331000	-2.583156000
1	-0.189556000	-1.217784000	-2.634578000
7	-0.823524000	-2.693694000	0.018489000
1	0.101880000	-3.133293000	0.028117000
1	-1.305795000	-3.092581000	0.829733000
7	1.423088000	-0.533986000	-0.011454000
1	1.815261000	0.398237000	0.154897000
1	1.856447000	-1.130289000	0.700391000
7	-0.763693000	-0.462022000	2.194706000
1	-0.852675000	0.492054000	2.558690000
1	-1.521038000	-0.986306000	2.643748000
1	-3.376576000	-0.279671000	0.933175000

1	-1.706456000	-0.641370000	-2.619030000
1	1.843137000	-0.836099000	-0.895768000
1	0.092219000	-0.824087000	2.625746000
1	-1.295402000	-3.108106000	-0.791274000
7	-0.725503000	1.448617000	-0.018225000
7	-0.691585000	2.571497000	-0.026595000

η-NN

76	0.758858000	0.171998000	0.107439000
7	-0.606200000	-1.554032000	0.144263000
1	-1.574687000	-1.247758000	0.010053000
1	-0.442570000	-2.257631000	-0.582210000
7	0.681307000	0.186843000	-2.081978000
1	-0.061197000	0.812554000	-2.413996000
1	1.527506000	0.520441000	-2.553774000
7	2.389264000	-1.234954000	0.119654000
1	3.210883000	-0.906297000	0.636920000
1	2.153150000	-2.129774000	0.560230000
7	2.269885000	1.771517000	0.066431000
1	1.825353000	2.681016000	-0.091741000
1	2.802305000	1.889603000	0.933938000
7	0.705966000	0.269197000	2.294814000

1	-0.038100000	0.900304000	2.613214000
1	0.516342000	-0.616327000	2.773920000
1	-0.619218000	-2.080538000	1.023252000
1	0.474872000	-0.714042000	-2.524340000
1	2.979322000	1.685979000	-0.667676000
1	1.555366000	0.625278000	2.743638000
1	2.745422000	-1.485729000	-0.808615000
7	-1.270425000	1.173547000	0.100787000
7	-0.525433000	2.034605000	0.080060000

$[Fe(NH_3)_5(N_2)]$

κ-N

26	-0.766144000	-0.498339000	-0.015562000
7	-2.832148000	-0.397267000	-0.045010000
1	-3.190995000	0.483280000	0.338267000
1	-3.252056000	-0.442386000	-0.978683000
7	-0.743848000	-0.664636000	-2.076296000
1	-1.044361000	0.190224000	-2.556051000
1	0.174546000	-0.863179000	-2.485200000
7	-0.849963000	-2.555337000	0.122162000
1	-0.222180000	-3.044129000	-0.523936000
1	-0.605364000	-2.935935000	1.041667000

7	1.299212000	-0.567547000	0.030537000
1	1.703424000	-0.140467000	0.869931000
1	1.730084000	-1.496269000	-0.011004000
7	-0.804887000	-0.356236000	2.047979000
1	-0.679405000	0.600988000	2.393175000
1	-1.680456000	-0.661473000	2.483952000
1	-3.326576000	-1.120622000	0.486718000
1	-1.348449000	-1.396768000	-2.461811000
1	1.741121000	-0.047275000	-0.734289000
1	-0.082970000	-0.893717000	2.538363000
1	-1.769077000	-2.962736000	-0.076598000
7	-0.680968000	1.345219000	-0.152996000
7	-0.632618000	2.455053000	-0.235315000

η-NN

26	0.766926000	0.161066000	0.103803000
7	-0.526037000	-1.465172000	0.099925000
1	-1.169957000	-1.487879000	0.896723000
1	-1.158595000	-1.474298000	-0.706147000
7	0.753921000	0.153320000	-1.956237000
1	-0.019827000	0.691541000	-2.361950000
1	1.586720000	0.558449000	-2.395080000

7	2.312783000	-1.165376000	0.181722000
1	3.217614000	-0.756347000	0.434906000
1	2.182621000	-1.912926000	0.870914000
7	2.170679000	1.694516000	0.073218000
1	1.842885000	2.526501000	-0.426641000
1	2.427207000	2.057844000	0.996495000
7	0.698976000	0.264983000	2.160366000
1	0.273740000	1.131027000	2.509691000
1	0.154705000	-0.472512000	2.619205000
1	-0.092365000	-2.393383000	0.093492000
1	0.667440000	-0.768913000	-2.395420000
1	3.068026000	1.469599000	-0.367691000
1	1.607758000	0.226096000	2.632805000
1	2.500630000	-1.659982000	-0.696360000
7	-1.261886000	1.131511000	0.103452000
7	-0.545993000	1.986137000	0.013092000

$[Ru(NH_3)_5(N_2)]$

κ-N

44	-0.767358000	-0.499650000	-0.013579000
7	-2.966439000	-0.395402000	-0.052411000
1	-3.308274000	0.512273000	0.275832000

1	-3.373104000	-0.503977000	-0.985492000
7	-0.735810000	-0.647935000	-2.209573000
1	-1.033973000	0.222071000	-2.659879000
1	0.189240000	-0.841897000	-2.602542000
7	-0.856356000	-2.679044000	0.126667000
1	-0.240803000	-3.157018000	-0.537428000
1	-0.591213000	-3.046959000	1.044549000
7	1.431567000	-0.565999000	0.030938000
1	1.823221000	-0.170351000	0.890036000
1	1.849377000	-1.496776000	-0.050221000
7	-0.806743000	-0.346594000	2.182849000
1	-0.695506000	0.619313000	2.504077000
1	-1.680453000	-0.666393000	2.609419000
1	-3.446397000	-1.087034000	0.530007000
1	-1.344575000	-1.373911000	-2.597054000
1	1.854796000	-0.012618000	-0.719444000
1	-0.069838000	-0.872090000	2.661258000
1	-1.786046000	-3.068031000	-0.053743000
7	-0.679288000	1.498810000	-0.149380000
7	-0.630102000	2.609657000	-0.224890000

η-NN

44	0.783301000	0.149730000	0.101354000
7	-0.637895000	-1.534556000	0.109533000
1	-1.329619000	-1.456927000	0.860091000
1	-1.200255000	-1.576454000	-0.744753000
7	0.794234000	0.127100000	-2.097688000
1	0.064083000	0.732028000	-2.486428000
1	1.662574000	0.462608000	-2.523373000
7	2.400119000	-1.239183000	0.178726000
1	3.315022000	-0.791017000	0.282689000
1	2.334951000	-1.895383000	0.962544000
7	2.246498000	1.801112000	0.089336000
1	1.793064000	2.689225000	-0.141905000
1	2.706029000	1.968699000	0.988607000
7	0.697482000	0.244039000	2.297087000
1	0.128766000	1.032530000	2.621078000
1	0.281130000	-0.578357000	2.742580000
1	-0.229706000	-2.467707000	0.210256000
1	0.629029000	-0.789593000	-2.522826000
1	3.009370000	1.705863000	-0.586738000
1	1.601713000	0.363910000	2.761850000
1	2.481138000	-1.822744000	-0.659126000

7	-1.399491000	1.260983000	0.047747000
7	-0.673565000	2.109897000	-0.006359000

[Rh(η^5-Cp)$Cl_2(N_2)$]

κ-N

6	-0.102973000	2.353803000	0.232030000
6	-1.151479000	3.295951000	0.139429000
6	-2.370518000	2.580086000	-0.159350000
6	-2.062650000	1.168584000	-0.132942000
6	-0.670591000	1.028576000	0.062319000
1	0.943420000	2.580113000	0.388410000
1	-1.046514000	4.371768000	0.163723000
1	-3.349158000	3.017132000	-0.298963000
1	-2.760049000	0.370962000	-0.348408000
1	-0.120049000	0.097206000	0.070394000
45	-1.079155000	2.240364000	-1.825796000
7	0.486045000	1.742426000	-3.175352000
7	1.273597000	1.499345000	-3.912675000
17	-1.198162000	4.318415000	-3.000749000
17	-2.539102000	1.191525000	-3.401044000

η-NN

NA

[Ir(η^5-Cp)Cl$_2$(N$_2$)]

κ-N

6	-0.086082000	2.350754000	0.208155000
6	-1.145717000	3.294711000	0.127472000
6	-2.373588000	2.579584000	-0.144690000
6	-2.056736000	1.167925000	-0.144780000
6	-0.654566000	1.023619000	0.038173000
1	0.959341000	2.581172000	0.361509000
1	-1.039095000	4.370473000	0.154116000
1	-3.356347000	3.014625000	-0.254500000
1	-2.753219000	0.368677000	-0.357985000
1	-0.107429000	0.090804000	0.042546000
77	-1.064863000	2.233713000	-1.821928000
7	0.422676000	1.759996000	-3.100310000
7	1.238083000	1.501202000	-3.807777000
17	-1.201700000	4.306379000	-3.051438000
17	-2.528097000	1.212625000	-3.447537000

η-NN

NA

[Co(η^5-Cp)Cl$_2$(N$_2$)]

κ-N

6	-0.080256000	2.361516000	0.052545000
6	-1.141706000	3.292746000	0.044385000
6	-2.362014000	2.579406000	-0.180036000
6	-2.045322000	1.184428000	-0.225519000
6	-0.644395000	1.045215000	-0.115966000
1	0.971864000	2.598330000	0.140829000
1	-1.040502000	4.367725000	0.076795000
1	-3.343455000	3.015366000	-0.299550000
1	-2.745896000	0.388693000	-0.432578000
1	-0.091582000	0.117017000	-0.176671000
27	-1.112721000	2.246266000	-1.760490000
7	0.363738000	1.751207000	-2.831146000
7	1.208645000	1.473914000	-3.490053000
17	-1.194595000	4.228829000	-2.807342000
17	-2.489142000	1.205601000	-3.194177000

η-NN

NA

VITA

Upon completing his studies at Carthage High School, Carthage Texas, in 2016, Cole B. Donald entered Panola College. He received an Associate of Science from this institution in 2018. Following this degree, he attended Stephen F. Austin State University to obtain a Bachelor of Science in Chemistry in 2020. He entered the Graduate Program of Natural and Applied Sciences in 2021 to receive the Master of Science in Natural and Applied Science with Chemistry Focus in 2022.

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