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# A Computational Study of High Energy Density Materials and Their Detection Using Surface-Enhanced Raman Spectroscopy

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# A COMPUTATIONAL STUDY OF HIGH ENERGY DENSITY MATERIALS AND THEIR DETECTION USING SURFACE-ENHANCED RAMAN SPECTROSCOPY

By: Emily Nicole Hugo

A thesis submitted to the faculty of The University of Mississippi in partial fulfillment of the requirements of the Sally McDonnell Barksdale Honors College.

Oxford

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# ABSTRACT

EMILY NICOLE HUGO: A Computational Study of High Energy Density Materials and Their Detection Using Surface-Enhanced Raman Spectroscopy
(Under the direction of Dr. Gregory Tschumper)

The purpose of this thesis is to theoretically predict the vibrational spectra of select high energy density materials (HEDMs) as well as some of their byproducts and to determine if using surface-enhanced Raman spectroscopy (SERS) could be a viable detection method for these compounds. Studying the vibrational patterns of these compounds will help in identifying them in the environment for remediation purposes. Because the byproducts are smaller and easier to model than the parent compounds, these were studied more in depth through analyzing their Infrared and Raman spectra. $Ag_2$ was used to model the interactions between the Ag nanoparticles used in SERS spectroscopy and the N atoms of the byproducts to investigate any changes in the spectra of the isolated molecules. Two molecules (1,2,4,5-tetrazine and 1,2,3,5-tetrazine) displayed significant increases in the Raman activity (on the order of $10^2$-$10^4$) when $Ag_2$ interacted with the N atoms. In most cases, however, adding $Ag_2$ only slightly enhanced the Raman activities. These results suggest that larger Ag clusters may be required to adequately model the SERS effect for these compounds.

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# LIST OF ABBREVIATIONS

| | |
|---|---|
| $D_e$ | dissociation energy |
| DFT | density functional theory |
| ECP | effective core potential |
| FOX-7 | 1,1-diamino-2,2-dinitroethylene |
| HEDM | high energy density material |
| HMX | high melting explosive (octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine) |
| IR | infrared |
| MDHAR6 | monodehydroascorbate reductase 6 |
| PES | potential energy surface |
| RDX | royal demolition explosive (1,3,5-trinitro-1,3,5-triazine) |
| SERS | surfaced-enhanced Raman spectroscopy |
| SP | surface plasmon |
| TNT | 2,4,6-trinitrotoluene |

# Chapter 1: Introduction

## 1.1 High Energy Density Materials Background

High Energy Density Materials (HEDMs), which typically contain N atoms, are commonly found in explosives and propellants. They have military and industrial uses as bombs and for demolition purposes.[1] HEDMs also contain other elements of low molecular weight, such as C, O, and H. These compounds are chosen as explosives because they have a large energy density, which is a high ratio of energy output per unit volume.[2] HEDMs contain many bonds between N, C, and O atoms, which store a large amount of potential chemical energy. During an explosion, these bonds are rapidly breaking and forming new bonds in a short amount of time, which releases most of this energy. The parent compounds will form more stable, lower energy byproducts, such as $N_2$, $CO_2$, $O_2$, $H_2O$, and nitrogen oxides. HEDMs that release a great deal of energy per unit volume are considered to be powerful.[3]

Another characteristic of a powerful HEDM is a large detonation velocity. This describes how far the particles in the explosive and the propellants travel over a period of time.[1] Because HEDMs can form molecules with lower molecular weights, these smaller particles can travel farther in the air during the explosion because they have less momentum. The faster these molecules move in the air, the more damage that can be caused from these explosives.

There is a delicate balance between the kinetic stability and the thermal instability of these compounds. Figure 1.1.1 shows a reaction coordinate diagram, which will be used to explain this concept.

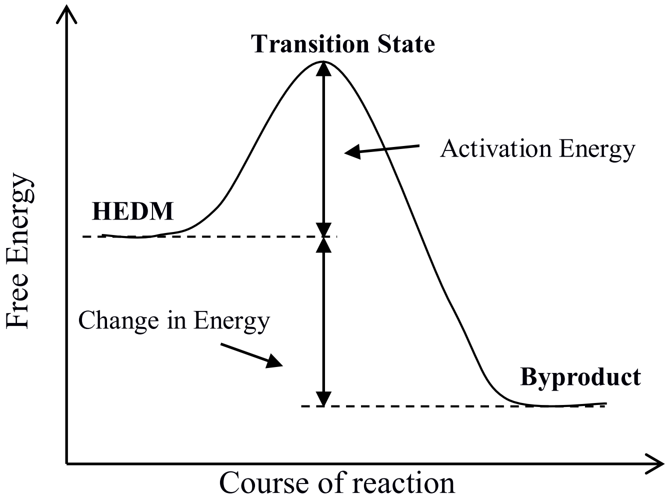


**Figure 1.1.1:** Reaction Coordinate Diagram

HEDMs require a certain amount of activation energy (shown in Figure 1.1.1) to react, which forms the byproducts. The activation energy is the minimum amount of energy needed to start a reaction. A large activation energy gives stability to HEDMs because the parent compounds will not begin to break down during storage and transportation. However, the activation energy cannot be too large to overcome when an outside energy is applied to initiate an explosion.[4,5]

As seen in Figure 1.1.1, HEDMs are higher in energy, and the byproducts are much lower in energy, as discussed previously. Because the products are significantly lower in energy, they are strongly favored to form. As the reaction occurs, the decomposition of the parent compound to the byproduct leads to a large change in energy. The released free energy causes a chain reaction as the parent compound overcomes the activation energy for conversion to the products. Once the parent compound overcomes this activation energy and forms an initial byproduct, that byproduct must overcome another activation energy barrier to form the next byproduct. This can continue until the simplest byproducts ($O_2$, $N_2$, $CO_2$, etc.) are formed or until the energy is depleted. All of this energy is released during the explosion. The more energy released results in a larger force produced, which causes more destruction.[5]

## 1.2 Motivation for Studying HEDMs

Interest in HEDMs has increased because of the need to perform environmental remediation in areas where explosives have been used. Polluted areas have become a domestic and an international problem. Hundreds of explosive-contaminated sites are in the United States, and even more are in Europe and Asia. The unreacted parent compounds that come from military and industrial uses and manufacturing operations can be persistent and mobile in the environment. This leads to pollution of water and soil, harmful effects on wildlife (most plants cannot grow in these contaminated conditions), and developmental issues in humans.[6] Further, the byproducts can be more harmful than the initial HEDM, such as the increased toxicity of the reduced forms of RDX (1,3,5-trinitro-1,3,5-triazine).[7] Some military agencies have started identifying contaminated areas and creating solutions to clean up these environments.[8,9] When detecting and identifying these compounds in the environment, it is important to know which parent compounds and byproducts are present and at what concentration. This can help determine how much remediation needs to be done and if the site is safe for wildlife and humans.

A recently discovered environmental remediation method involves a genetically modified antioxidant enzyme in plants. The plants can take up TNT (2,4,6-trinitrotoluene) from the soil and store it in their tissues. The enzyme monodehydroascorbate reductase 6 (MDHAR6) normally regenerates ascorbate (vitamin C) to help remove reactive oxygen, which can be harmful to the plant due to the free radical.[10] However, when the enzyme is mutated, the plant can tolerate the effects of TNT. The mutated MDHAR6 enzyme can detoxify TNT by reducing it in the mitochondria. Plants with this mutated enzyme can be put in areas with TNT-contaminated soil to help clean up the site. Further research on this enzyme may reveal that it can detoxify other HEDMs or if other mutated enzymes can do this as well.[11]

Interest in detecting HEDMs goes beyond identifying these compounds in the environment. The Department of Homeland Security has worked with the National Institute of Standards and Technology to improve the methods and requirements of testing for explosives. Due to the increase in national security threats on public transportation, security personnel are required to test all individuals, cargo, and checked baggage. Accurate and rapid testing for HEDMs can help ensure proper detection of explosives in order to avoid potential harm. Currently, bomb sniffing dogs are used to detect trace explosives on people. Chemical tests are conducted on checked baggage and cargo to test for HEDMs.[12] Improving detection limits, accuracy, and efficiency of detection methods will increase the ability to find trace explosives on packages, baggage, or individuals on public transportation. This can help reduce the number of explosives that might get through security.

## 1.3 HEDMs Studied

The compounds studied in this research mainly came from the article "Theoretical Study of Ionization and One-Electron Oxidation Potentials of *N*-Heterocyclic Compounds."[13] The EPA publication SW-846 *Test Methods for Evaluating Solid Waste, Physical/Chemical Methods*, which is a compilation of documents describing methods for testing environmental wastes, was also used when choosing which compounds to study. Specifically, Method 8095: *Explosives by Gas Chromatography* contained a list of nitrogen-containing compounds that "are used as explosives, are byproducts of the manufacture of explosives, or are the transformation products of explosives."[14] All of these compounds were chosen because they would likely appear in areas in which explosives have been used.

To help organize the results from this study, the compounds were sorted into three groups based on size and complexity. Group 1 (Figure A-1 in the appendix) is comprised of mainly the parent compounds, including TNT (2,4,6-trinitrotoluene), RDX (1,3,5-trinitroperhydro-1,3,5-triazine), and HMX (octahydro-1,3,5,7-tetrazocine), which are depicted in Figure 1.3.1. These molecules can have multiple conformations, which is more complex to model than the remaining compounds.

Group 2 (Figure A-2 in the appendix) contains the remaining parent compounds that are smaller or lower in energy than the Group 1 parent compounds, and the larger byproducts. A few representative molecules from this group are shown in Figure 1.3.2. Some of these molecules have aromatic ring structures, and almost all of them contain oxygen atoms. These compounds will continue to break down into smaller byproducts, which are the final group.

Group 3, which contains the simpler byproducts (i.e. smallest molecules), was the main focus of this preliminary research because they are easier to model than the Group 1 and 2 compounds. This can give insight on the effectiveness of SERS detection of HEDMs and byproducts. These Group 3 compounds were further broken down into three subgroups. Group 3A (Figure 1.3.3) contains single-ringed compounds with only one unique N environment, with the exception of 1H-pyrazole, which will be discussed later. Group 3B (Figure 1.3.4) is comprised of the remaining single-ringed compounds that have multiple unique N environments. Group 3C (Figure 1.3.5) contains the multi-ringed compounds. Some of these compounds are bigger than some of the Group 1 and 2 compounds. When the parent compounds break down, some of the initial byproducts may react to form these more stable molecules.

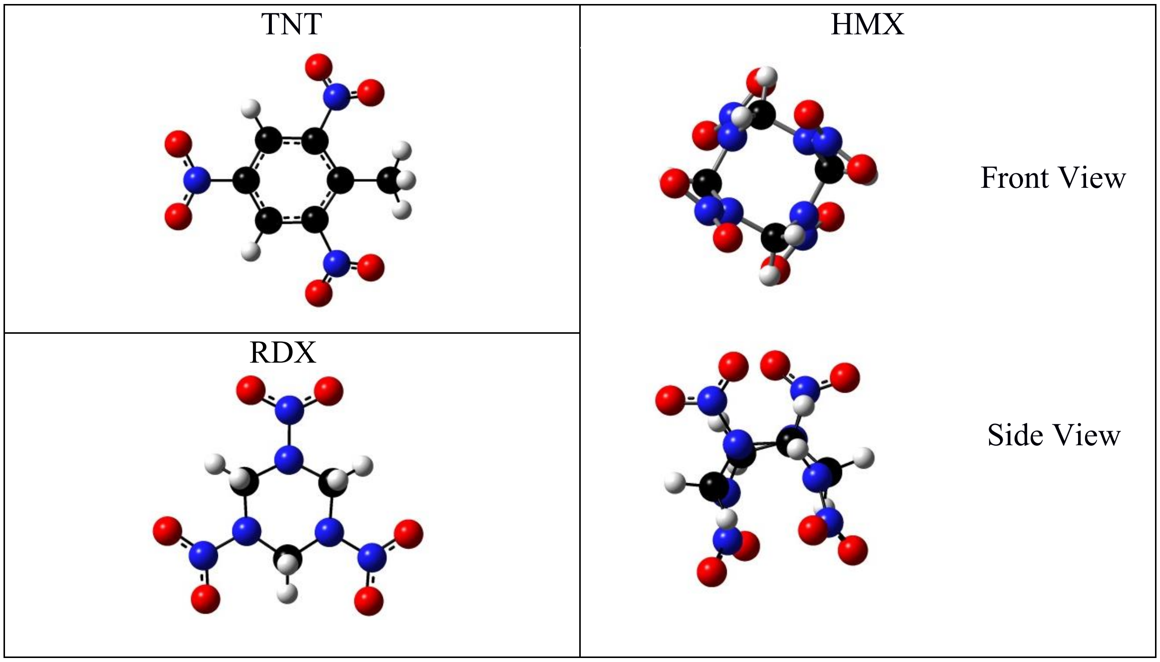


**Figure 1.3.1:** Group 1 Molecules (Mainly Parent Compounds)

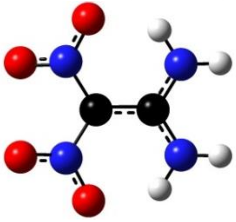
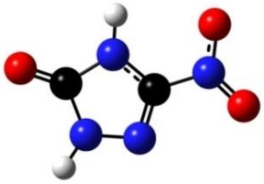
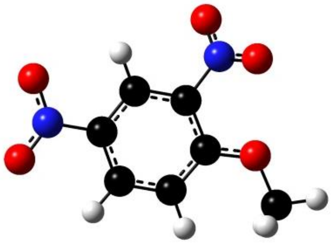
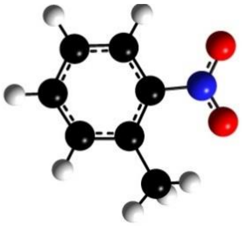
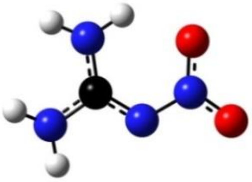
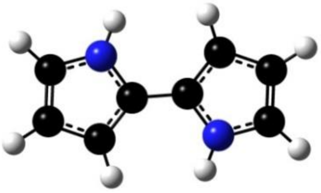
| | | |
|---|---|---|
| 2,2-Dintroethene-1,1-diamine (FOX-7)<br> | Nitrotriazolone<br> | 2,4-Dinitroanisole<br> |
| 2-Nitrotoluene<br> | Nitroguanidine<br> | 2,2'-Bipyrrol<br> |

**Figure 1.3.2:** Group 2 Molecules (Remaining Parent Compounds and Larger Byproducts)

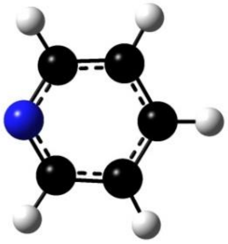
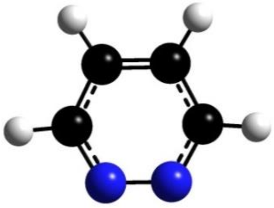
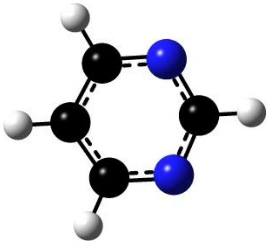
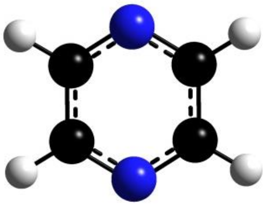
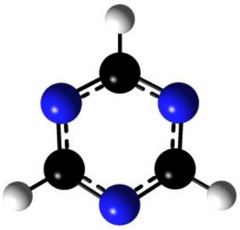
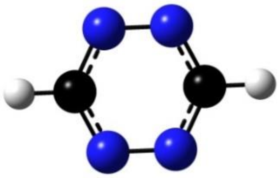
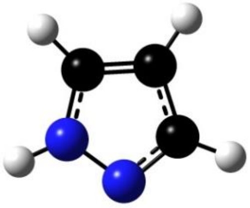
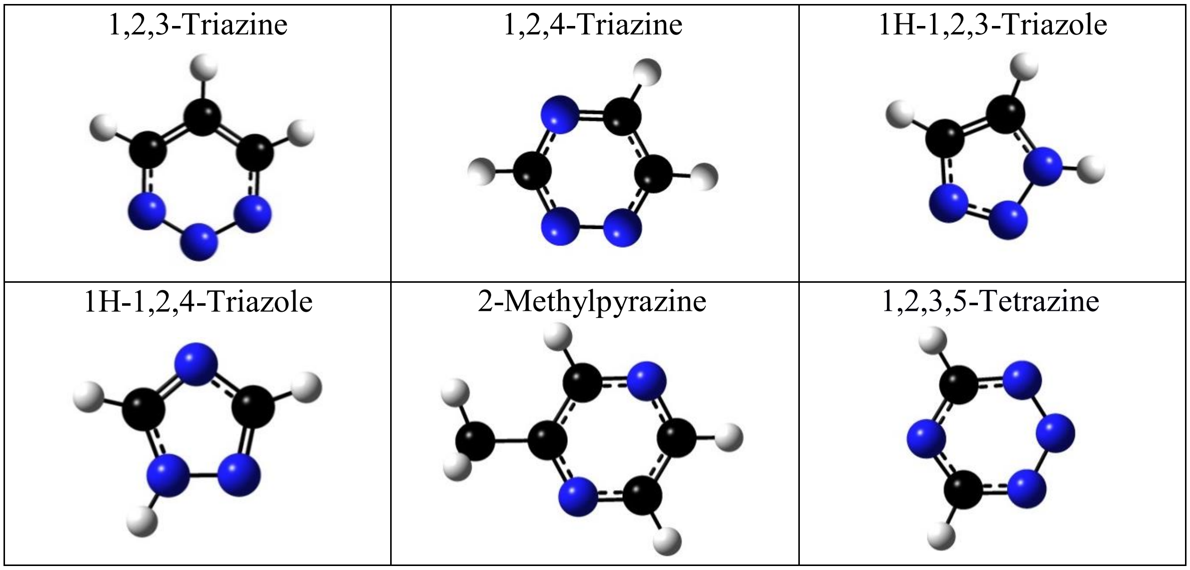
| | | |
|---|---|---|
| Pyridine<br> | Pyridazine<br> | Pyrimidine<br> |
| Pyrazine<br> | 1,3,5-Triazine<br> | 1,2,4,5-Tetrazine<br> |
| 1H-Pyrazole<br> | | |

**Figure 1.3.3:** Group 3A Molecules (Single-Ringed Compounds with One Unique N Environment)



1,2,3-Triazine

1,2,4-Triazine

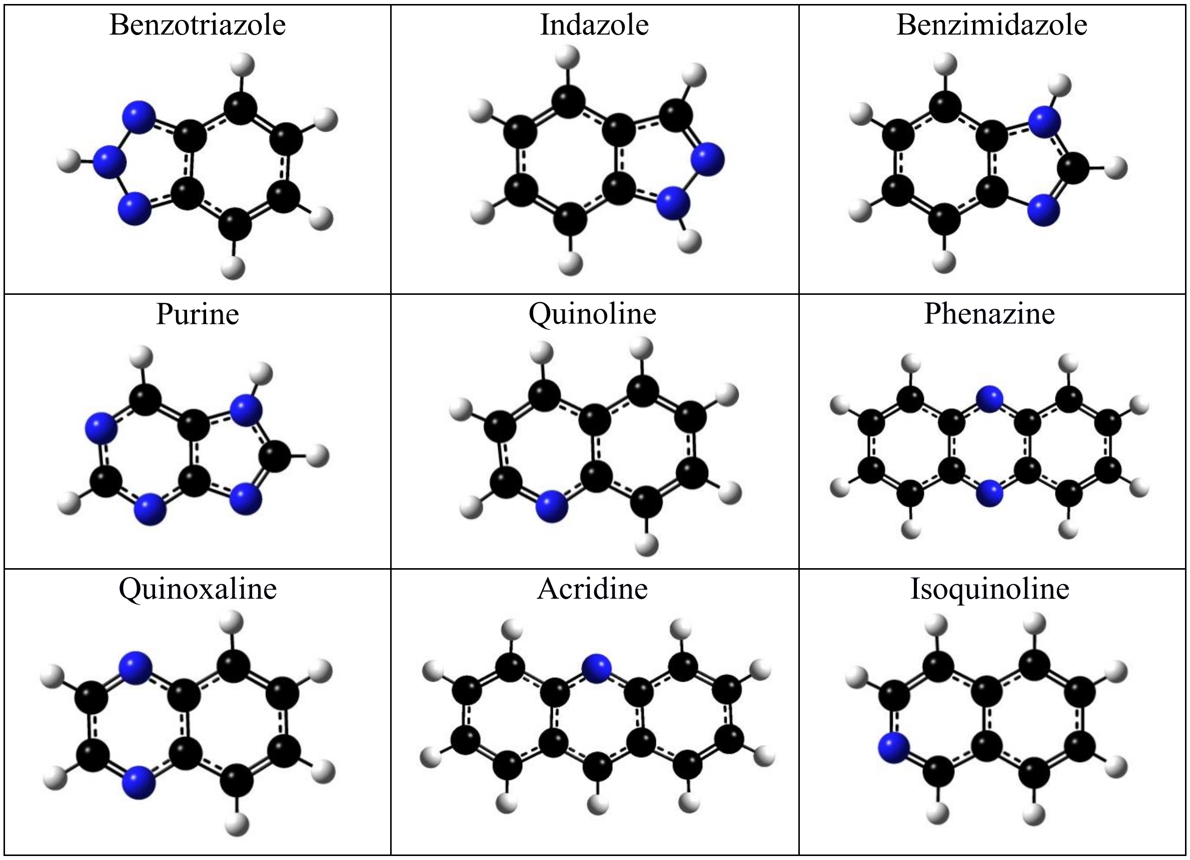
1H-1,2,3-Triazole

1H-1,2,4-Triazole

2-Methylpyrazine

1,2,3,5-Tetrazine

**Figure 1.3.4:** Group 3B Molecules (Single-Ringed Compounds with Multiple Unique N Environments)



Benzotriazole

Indazole

Benzimidazole

Purine

Quinoline

Phenazine

Quinoxaline

Acridine

Isoquinoline

**Figure 1.3.5:** Group 3C Molecules (Multi-Ringed Compounds)

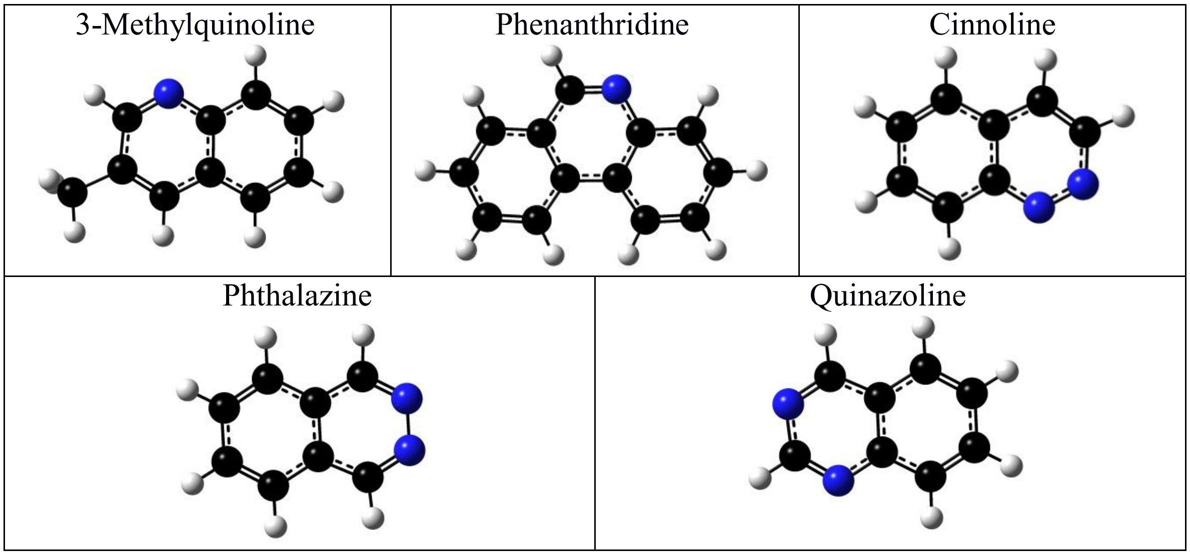

3-Methylquinoline
Phenanthridine
Cinnoline
Phthalazine
Quinazoline

**Figure 1.3.5 Continued**

## 1.4 Spectroscopy

Spectroscopy is the study of matter interacting with electromagnetic radiation. Most atoms and molecules have distinct energy levels based on the types of chemicals bonds present, so they will absorb different wavelengths of light. The presence of a peak indicates at which frequency the radiation is absorbed. The peaks of the spectrum will create a distinct pattern or “fingerprint” that can help in identifying a specific compound or a family of compounds. The frequency at which the peak is located on the spectra suggests that certain bonds or functional groups are present, which can correspond to a particular molecular structure.[5,15]

Various forms of spectroscopy can be used to study the energy transitions occurring in a molecule.[5] In this thesis, two types of vibrational spectra were modeled, infrared (IR) and Raman spectroscopy.

### 1.4.1 Infrared Spectroscopy

Infrared (IR) spectroscopy is an analysis of molecules as they interact with the infrared region of the electromagnetic spectrum. In order for a vibrational mode in a molecule to be IR active, a net change in dipole moment must occur when a particular molecular vibrational motion occurs. A dipole moment is the separation of charge due to an uneven distribution of electrons within a bond between two atoms with different electronegativities. When the electron density is shifted toward the more electronegative atom, it is partially negative, and the other atom is partially positive. A net change in dipole moment occurs when the overall direction and magnitude of the dipole is altered during certain molecular vibrations. Each molecule will absorb IR light of different frequencies based on the types of bonds and atoms in the compound.[15]

### 1.4.2 Raman Spectroscopy

Raman spectroscopy is a technique that observes how the frequency of photons in monochromatic light changes as it interacts with a molecule. Most of the photons that pass through the sample will undergo elastic scattering, which means their frequencies will not change as light interacts with the sample. However, a few of the photons will undergo inelastic scattering, meaning the photons are absorbed by the molecule and reemitted with a different frequency. This results in a change in energy, which can be measured by calculating the vibrational energy ($\Delta E = E_{vib}$).[16] This method complements IR absorption spectroscopy because Raman detects vibrational modes differently. Raman spectroscopy detects at which vibrational modes the scattering of light causes a change in polarization, or a "distortion of the electron cloud around the vibrating atoms."[15] A molecular vibration can be both IR and Raman active if both a change in dipole moment and a change in polarizability occur when the molecule interacts with electromagnetic radiation.[15] Observing both types of spectra gives a more complete picture of the molecule's vibrational motions.

### 1.4.3 Surface-Enhanced Raman Spectroscopy

Surface-enhanced Raman spectroscopy (SERS), or surface-enhanced Raman scattering, is a technique in which the molecule of interest is adsorbed onto a noble metal in order greatly increase certain Raman signals.[17] The first experiments using SERS were documented in the 1970s, in which this technique was tested on pyridine. In these experiments, the Raman spectrum of pyridine was observed when the molecule was adsorbed to an Ag electrode.[18,19] Since then, other metals have been used, including Au, Cu, Li, Na, and K. These metals must have rough surfaces at the atomic level. When a Raman excitation laser strikes the metal, surface plasmons (SP), which are electron oscillations, are produced on its surface, creating a strong electromagnetic field. These SPs then interact with the molecule of interest, and the electromagnetic field enhances the Raman signal produced. [16] SERS is an attractive technique because the SPs are tightly localized at the surface of the metal, which makes them highly sensitive.[20] The Raman signal can be enhanced by orders of up to $10^6$ and higher.[15]

In a study done by A.G. Brolo, D. E. Irish, and J. Lipkowski, they observed experimentally the ring-breathing vibrations of adsorbed pyridine and pyrazine on an Au electrode. As the pyridine interacted with the Au electrode, the frequency of the ring-breathing mode shifted from 1002 $cm^{-1}$ to 1010 $cm^{-1}$. In pyrazine, the frequency shifted from 1015 cm$^{-1}$ to 1019 cm$^{-1}$. They concluded that an increase in frequency for this mode indicates that the molecule had adsorbed on the electrode via their N lone pairs (i.e., an N···Ag configuration).[21] This N···Ag configuration is illustrated in Figure 1.4.1.

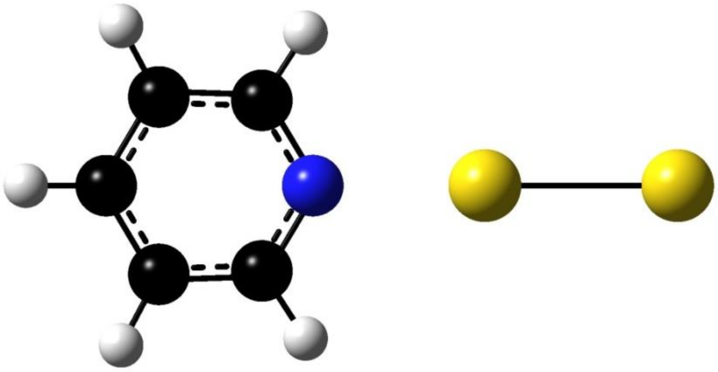


**Figure 1.4.1:** N···Ag Configuration

Knowing how the molecule is interacting with the Ag surface is important because the orientation needs to be the same for all compounds in order to directly compare characteristics. Also, the distance between the N and the Ag atoms can be determined, which will be discussed later, to understand how closely the molecules are interacting with one another.

# Chapter 2: Computational Chemistry Background

Simulation has become a key tool to study various systems, such as the weather, the human body, and engineering problems. A model is a mathematical representation of the system, while simulation is the calculations done on the model to understand the system.[22] Creating models saves time and resources, especially when studying compounds that may be challenging or dangerous to make in the lab, such as HEDMs.

Computational chemistry allows scientists to use computer programs to simulate molecules and to solve chemical problems. These programs can give information on the compound, such as its molecular geometry, its energy, and its spectra. Computational chemists have many methods they can use to solve these chemical problems. Molecular mechanics is based on classical physics. Although classical physics generally uses equations that can be solved more easily on a computer and are less computationally demanding, the results typically are less accurate. Computational quantum chemistry is based on quantum mechanics, which uses the Schrödinger equation to describe the behavior of the electrons as they interact with the electromagnetic force from nuclear charges and from each other. Solving the Schrödinger equation is more computationally demanding but can give more accurate results and describe molecular properties that depend on the electronic structure of the system. This branch of science was developed to correct for the limitations of classical physics, or the inability to describe matter as a wave and a particle. This forms the basis of quantum computational chemistry, which allows for the prediction of all properties of matter.[23]

## 2.1 Electronic Structure Theory

Quantum chemistry focuses on the electrons within atoms and molecules. Models of the molecule are built based on the electrons. By studying the electronic structure of the molecule, various properties can be described, such as the dipole moment, polarizability, electronic occupation, and electron density. The Schrödinger equation is used to describe these properties.[24]

### 2.1.1 Schrödinger Equation

In computational chemistry, the time-independent Schrödinger equation (equation 2.1.1) describes the total electronic energy of a system. A wavefunction ($\Psi$) represents all of the information about a molecule. When the molecular Hamiltonian operator ($\hat{H}$) acts on the wavefunction, the wavefunction is returned multiplied by the energy ($E$). This solution can be used to determine the total electronic energy of the system for that specific wavefunction.[5, 23]

$$\hat{H}\Psi = E\Psi \qquad \textbf{(2.1.1)}$$

The Schrödinger equation can be solved exactly only for systems containing one electron. As more electrons are added to a system, it becomes increasingly more complicated to describe each electron due to electron-electron repulsion.[25] The molecular Hamiltonian (equation 2.1.2) is used to describe the energy of the electrons ($e$) and the nuclei ($n$) in a molecule.[26] In this equation, $\hat{T}$ represents the kinetic energy. $\hat{T}_n$ indicates the kinetic energy for all of the nuclei, and $\hat{T}_e$ denotes the kinetic energy for all of the electrons. The potential energy ($\hat{V}$) is the attractive and repulsive forces occurring in the molecule. Equation 2.1.2 includes the sum of the potential energy of the repulsive forces between two nuclei ($\hat{V}_{n,n}$) and between two electrons ($\hat{V}_{e,e}$). The sum of the attractive forces between the nuclei and the electrons is represented by $\hat{V}_{n,e}$.[26]

$$\hat{H}_{elec} = \hat{T}_n + \hat{T}_e + \hat{V}_{n,n} + \hat{V}_{n,e} + \hat{V}_{e,e} \qquad \mathbf{(2.1.2)}$$

When solving the Schrödinger equation for molecules, the nuclei are assumed to be stationary, according to the Born-Oppenheimer approximation. This approximation allows for the separation of the nuclei and the electrons. Since nuclei are much larger than electrons, they move more slowly and can be considered frozen. As shown in equation 2.1.3, this removes the $\hat{T}_n$ and $\hat{V}_{n,n}$ terms from the molecular Hamiltonian. Because the nuclei are not moving, the kinetic energy ($\hat{T}_n$) becomes zero, and the potential energy of the repulsive forces between two nuclei ($\hat{V}_{n,n}$) remains constant. With this simplified molecular Hamiltonian, the total electronic energy of larger systems can be calculated.[26]

$$\hat{H}^{BO}_{elec} = 0 + \hat{T}_e + \text{constant} + \hat{V}_{n,e} + \hat{V}_{e,e} \qquad \mathbf{(2.1.3)}$$

### 2.1.1 Solving the Schrödinger Equation

Computational chemists use various approximate numerical procedures to find a solution to the Schrödinger equation. Some procedures are systematic and give extremely accurate results, but they are very demanding, which is not feasible for large systems, such as those containing more than 15-20 atoms.[23] These computations are demanding because they require a large amount of time, storage, and disk use. Density functional theory (DFT) methods are a compromise for this problem. Instead of using the wavefunction, DFT methods try to describe the molecule based on the electron density. DFT methods create a model of an idealized molecule with many electrons by making an electron cloud with uniform density.[5] The electron density has fewer variables than the wavefunction. Since electron density describes the volume of the electron cloud, only three variables are needed, x, y, and z. With fewer variables, DFT methods, in principle, are less computationally demanding than methods that use the wavefunction.[23]

## 2.2 Potential Energy Surface

The potential energy surface (PES) is a mathematical function that relates the energy of a molecule and its geometry. For a diatomic molecule, the potential energy of the molecule changes as the bond length, or distance between the two nuclei, changes.[23] This can be visualized in Figure 2.2.1. The repulsive forces cause the nuclei to move further apart from one another, and the attractive forces cause the nuclei in the two atoms to move closer together. At an equilibrium bond length, the energy of the molecule is the lowest. The first derivate of the potential energy curve at this point is zero, indicating that this geometry is a stationary state on this particular PES. By evaluating the second derivative, information about the nature of the stationary point is obtained. If all of the second derivatives are positive, the stationary point is considered a minimum on the PES.[23]

For compounds containing more than two atoms, the dimensionality is expanded to include additional geometric parameters, including more bond lengths, bond angles, and torsional angles, creating a more complex PES. Similar to the diatomic case, when the first derivatives of the energy with respect to each geometric parameter are zero and the second derivatives are positive, this indicates a minimum energy structure on the PES. There are local and global minimums on the PES for a particular system. The global minimum is also referred to as the lowest energy structure.[23] This stationary point is in an optimized geometric conformation, where the energy of the molecule has been minimized.[4] All of the compounds analyzed in this thesis were minimum energy structures on the PES for that particular system.

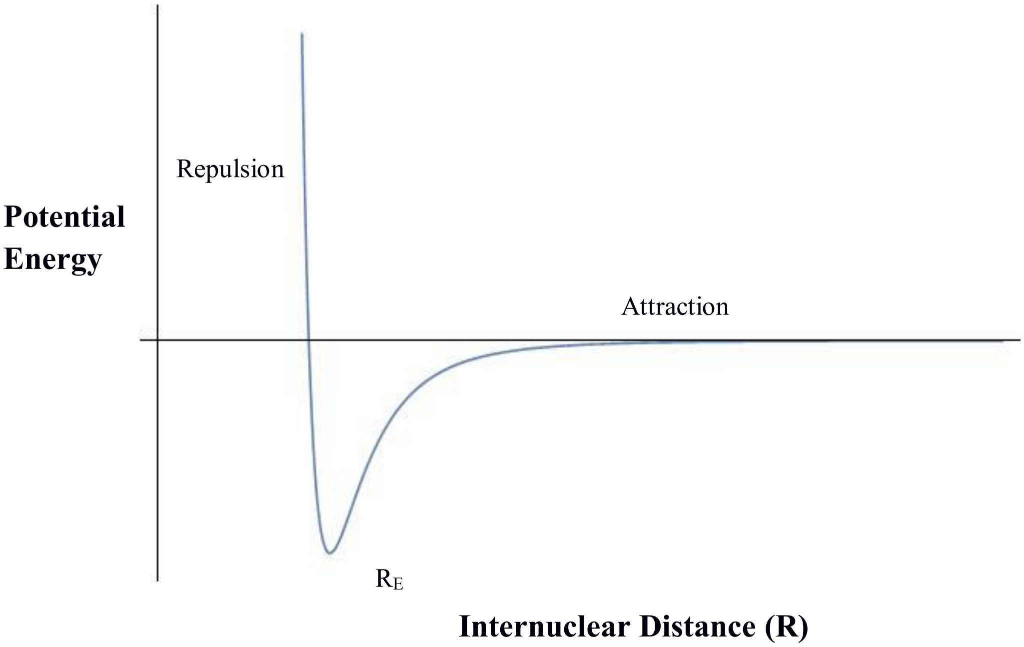


**Figure 2.2.1:** PES diagram for a diatomic molecule

# Chapter 3: Computational Details

## 3.1 Building the Structures

The initial structures were built by obtaining the geometry structure from the PubChem Database. This is a free online database maintained by the National Center for Biotechnology Information that gives compound information including chemical structure, chemical formula, molecular weight, and other physical and chemical properties.[27] The compound identification number was entered into the `PSI4` program[28], which searched for the structure's geometry in the database. This model gives a reasonable starting geometry of the molecule.[29] The coordinates from this output file were used to create initial structures in `Gaussian09`.[30]

## 3.2 Computational Method and Basis Sets

Once the initial structures were built using `PSI4`, they were fully optimized and harmonic vibrational computations were performed using B3LYP/6-31++G(*d,p*) in `Gaussian09`. The compounds in Group 3 (simpler byproducts) were also optimized and harmonic vibrational frequency computations were performed to obtain the IR and Raman spectra at the B3LYP/Def2-TZVPD level of theory. Because the byproducts are simpler systems, more computations can be performed to give a more in-depth understanding of these compounds.

A DFT method was chosen for this study due to the size of the systems, despite the fact that there is currently no systematic way to improve its accuracy.[4] In this thesis, the popular hybrid DFT method, B3LYP[31,32], was used. This method models the distribution of the electrons by combining parts of the Hartree-Fock theory, which observes how each electron behaves in relation to the mean field created by the remaining electrons, with computations that account for electron-electron interactions.[23,24]

Basis sets describe the electron space. A minimal basis set has the least number of functions required per atom to create the simplest representation of the molecule. Although calculations involving a minimal basis are relatively inexpensive, the electron space is not described completely. In order to create a more accurate representation of how the electrons act within an atom, larger basis sets are used. For example, in a split-valence basis set, the core atomic orbitals are described by one set of functions, and the valence atomic orbitals are represented by more than one set of functions. One of the simplest basis sets, double zeta, uses two sets of functions to describe each valence atomic orbital. A triple-zeta basis set uses three sets of functions per valence atomic orbital. This can be increased until an infinite number of basis functions are used to describe the atomic orbitals.[4] In this thesis, 6-31++G(*d,p*) denotes a double zeta basis set, and Def2-TZVPD indicates a triple zeta basis set.

Various basis functions can be added to create different representations of the molecule and obtain more accurate results. Diffuse functions describe how electrons behave far from the nucleus. The Def2-TZVPD basis set includes diffuse functions in the calculations, as indicated by the "D". The 6-31++G(*d,p*) basis set also includes diffuse functions, as indicated by "++". A single diffuse function, such as "+", indicates that diffuse *s* and *p* functions have been added for non-H atoms. A double diffuse function, such as "++", indicates that diffuse *s* functions have been added for H also.[4]

Polarization functions describe the electron clouds and how the charge in the molecule is redistributed when these clouds change shape. Including a polarization function in a basis set adds a function for additional atomic orbitals. These additional orbitals can mix with existing orbitals to give more flexibility and space in the atom for the electrons to move. For example, a *d*-polarization function can be added to a basis set with valence *p* orbitals. This new orbital can now polarize, or redistribute the electrons, when the molecule needs to change shape. Polarization functions are included in the Def2-TZVPD basis set, as indicated by the "P". For the 6-31++G(*d,p*) basis set, a set of *d*-polarization function was added to the basis set for all non-H atoms, and a *p*-polarization function was added for the H atoms. [24]

To model SERS, $Ag_2$ molecules were added to the optimized B3LYP/Def2-TZVPD byproduct structures. These byproduct/$Ag_2$ complexes were optimized and harmonic vibrational frequency computations were performed at the same level of theory. In the Def2-TZVPD basis set, the "Def2" refers to the 2nd generation default split valence basis sets developed by Reinhart Ahlrichs.[33] This basis set was chosen because it includes functions for Ag, which is needed to simulate SERS. Also, this basis set can use the effective core potential (ECP) function that is needed for the Ag atoms. The ECP function is added to reduce the number of basis functions for heavier atoms, such as Ag, by replacing the core electrons with a potential to model the center of the atom.[33] This basis set with the ECP function is not built into `Gaussian09`, so the basis set as well as the ECP parameters for Ag were obtained from the EMSL Basis Set Exchange database.[34]

In Figure 3.1.1, the optimized HEDM interacts with $Ag_2$ via the N atom. Only the N atoms with lone pairs were considered capable of having intermolecular interactions with $Ag_2$.[35] Some of the byproducts contained more than one unique N atom. In these systems, $Ag_2$ was added to each N atom, one at a time. For example, 1,2,4-triazine (Figure 3.1.1) has three N atoms with lone pairs in a different position within the compound. As shown in Box 1 in Figure 3.1.1, N1 (the N interacting with $Ag_2$) is located between a C atom and an N atom and is three atoms away from another N atom. In Box 2, N2 is also located between a C atom and an N atom, but it is only two atoms away from the other N. Finally, in Box 3, N4 is between two C atoms. Since each N will be affected differently by the addition of $Ag_2$ due to the various N-N and N-C connections, three possible interactions must be considered. Geometry optimizations and harmonic vibrational frequency computations were performed on each complex to understand how the IR and Raman spectra were affected by presence of $Ag_2$ at each location.

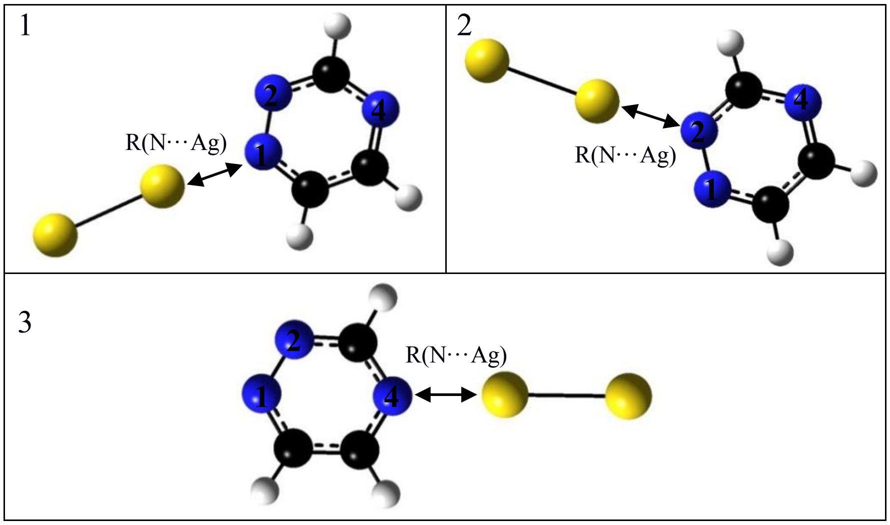


**Figure 3.1.1:** Optimized Structures of the 1,2,4-Triazine/$Ag_2$ complexes

Table 3.1.1 shows the distance between each of the N atoms and the Ag, which is denoted as R(N···Ag) in Figure 3.1.1, and the relative energies for each complex. The bold number in the names indicate with which N atom the $Ag_2$ interacted. For example, **1**,2,4-triazine indicates the first N atom interacted with $Ag_2$. 1,**2**,4-triazine is the lowest energy structure and has the shortest intermolecular N···Ag interaction. As discussed previously, the lowest energy structure is the global minimum on the PES. Knowing which complex is the lowest in energy can help determine which spectra to expect experimentally.

**Table 3.1.1**: Distance of N···Ag Interaction and Relative Energies in 1,2,4-Triazine/$Ag_2$ Complexes[a]

| Name | R(N···Ag) | Relative Energy |
|---|---|---|
| **1**,2,4-Triazine | 2.347 | 0.25 |
| 1,**2**,4-Triazine | 2.346 | 0.00 |
| 1,2,**4**-Triazine | 2.359 | 1.25 |

[a] R(N···Ag) distances in Å, $D_e$ in kcal $mol^{-1}$

# Chapter 4: Results and Discussion

## 4.1 Pyridine

Both the isolated pyridine molecule and the pyridine/$Ag_2$ complex (Figure 4.1.1) were optimized and their frequencies were calculated at the B3LYP/Def2-TZVPD level of theory in order to determine how the presence of the $Ag_2$ molecule affected the IR and Raman spectra of pyridine.

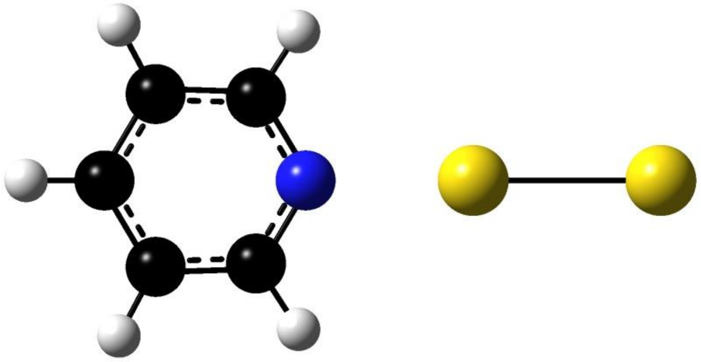


**Figure 4.1.1:** Optimized Structure of the Pyridine/$Ag_2$ complex

Table 4.1.1 shows select harmonic vibrational frequencies for both the pyridine molecule and the pyridine/$Ag_2$ complex. The full table of frequencies for pyridine can be found in the appendix (Table A-1).

The last section in the table shows the frequency shifts for each vibrational mode. This shift shows the changes from the isolated molecule to the complex, which demonstrates the effects that occur when $Ag_2$ interacts with the N in the pyridine. The frequencies listed only in the "Pyridine/$Ag_2$ complex" section (shown in Table A-1) correspond to the intermolecular vibrations between $Ag_2$ and the pyridine.

**Table 4.1.1:** Select Harmonic Vibrational Frequencies for Pyridine and Pyridine/$Ag_2$ Complex[a]

| Pyridine | | | Pyridine/$Ag_2$ complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | $\Delta\ \omega$ | Δ IR | Δ Raman |
| 719.0 | 63.8 | 0.1 | 718.3 | 49.2 | 0.5 | -0.6 | -14.6 | 0.5 |
| 1013.0 | 5.3 | 30.2 | 1027.8 | 22.0 | 55.8 | 14.8 | 16.7 | 25.6 |
| 1050.8 | 7.1 | 40.6 | 1055.6 | 9.0 | 48.4 | 4.7 | 1.9 | 7.8 |
| 1476.3 | 25.9 | 0.1 | 1482.2 | 29.4 | 0.0 | 5.9 | 3.5 | -0.1 |
| 3149.2 | 26.5 | 95.3 | 3179.1 | 3.0 | 30.4 | 29.9 | -23.5 | -64.9 |
| 3151.8 | 4.3 | 85.3 | 3177.4 | 4.1 | 32.9 | 25.7 | -0.2 | -52.5 |
| 3175.0 | 3.8 | 101.1 | 3186.2 | 0.1 | 62.5 | 11.1 | -3.7 | -38.6 |
| 3188.8 | 24.0 | 35.2 | 3200.8 | 9.9 | 91.7 | 12.0 | -14.1 | 56.5 |
| 3197.5 | 7.2 | 272.4 | 3206.4 | 12.4 | 443.5 | 8.9 | 5.2 | 171.1 |

[a] Frequencies ($\omega$) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

The IR and Raman spectra are shown in Figures 4.1.3 and 4.1.4, respectively. A Raman spectra showing 0-2000 $cm^{-1}$ is shown in Figure 4.1.5. These spectra were created using the *GaussView* 5 program.[30] This program plotted the calculated frequencies and intensities. It also added line broadening to simulate the types of peaks that would be seen in experimental data. The blue line in each corresponds to the isolated pyridine molecule, and the red line represents the pyridine/$Ag_2$ complex. In both spectra, the frequencies below 200 $cm^{-1}$ correspond to the intermolecular modes between $Ag_2$ and the pyridine.

Analyzing both the IR and the Raman spectra together may reveal interesting trends in the vibrational modes. For example, the C-H out-of-plane wagging (719.0 $cm^{-1}$ in pyridine; 718.3 $cm^{-1}$ in the complex) and the antisymmetric C-C stretching (1476.3 $cm^{-1}$ in pyridine; 1482.2 cm$^{-1}$ in the complex) modes are mainly IR active. In the isolated molecule, these modes show very little Raman activity, and adding $Ag_2$ did not make these modes become Raman active. For the vibrational mode of four symmetric C-H and one antisymmetric C-H stretching (3175.0 cm$^{-1}$ in pyridine; 3186.2 cm$^{-1}$ in the complex), the mode is mainly Raman active. However, adding $Ag_2$ dramatically decreases the IR intensity and reduces the Raman activity.

When $Ag_2$ was added to the pyridine, many of the frequencies shifted by less than 10 cm$^{-1}$, with a few exceptions. The magnitude of each of these shifts is shown in the $\Delta\omega$ column in Tables 4.1.1. Both IR and Raman modes corresponding to the four C-H antisymmetric stretches (3149.2 cm$^{-1}$ in pyridine; 3179.1 cm$^{-1}$ in the complex) and all the C-H antisymmetric stretches (3151.8 cm$^{-1}$ in pyridine; 3177.4 cm$^{-1}$ in the complex) have the two largest frequency shifts.

The two ring-breathing modes occur at 1027 cm$^{-1}$ (symmetric) and at 1055 cm$^{-1}$ (asymmetric). At this resolution, these two modes look like one peak on the complex's IR spectrum. However, these modes are more clearly seen in the complex's IR spectra, and the intensity of the peak makes it easier to detect this mode using IR.

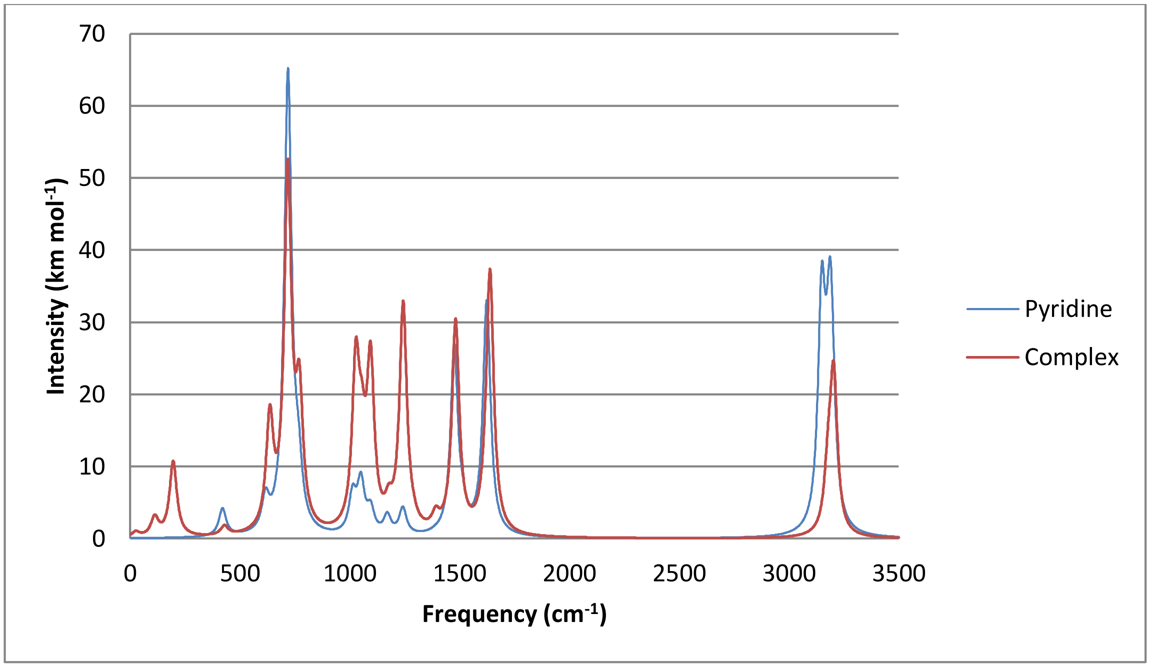


**Figure 4.1.3:** IR Spectrum of Pyridine and Pyridine/$Ag_2$ Complex

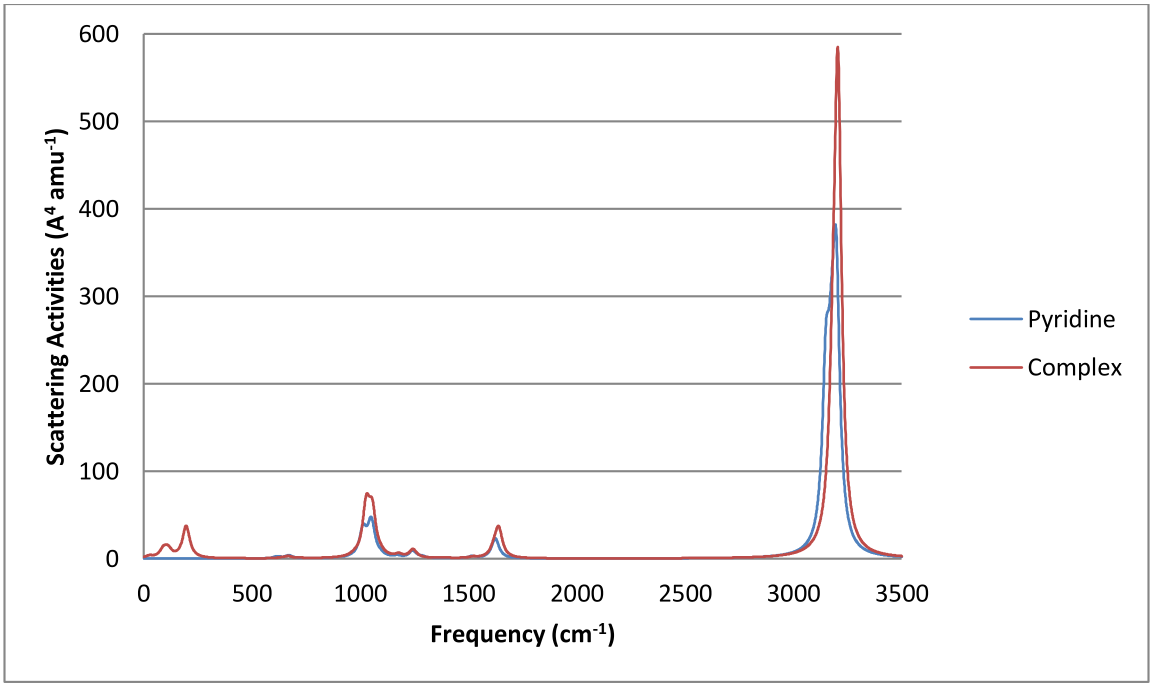


**Figure 4.1.4:** Raman Activity Spectrum of Pyridine and Pyridine/$Ag_2$ Complex

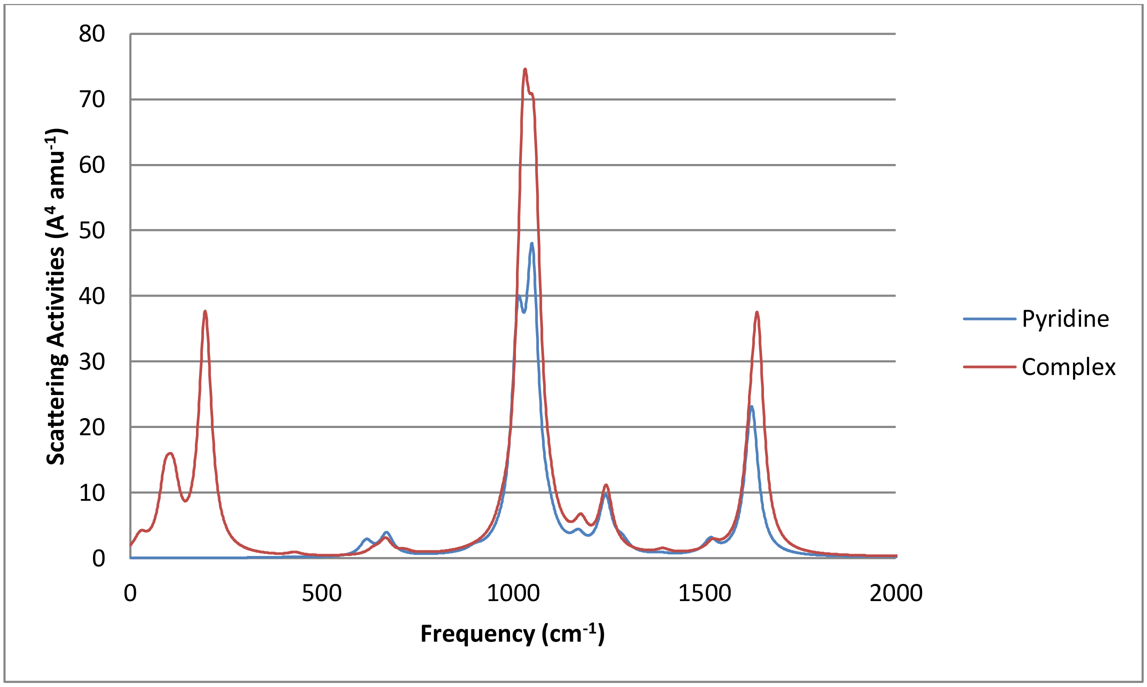


**Figure 4.1.5:** Raman Activity Spectrum (0-2000 cm$^{-1}$) of Pyridine and Pyridine/$Ag_2$ Complex

When the $Ag_2$ molecule was added, the Raman activity decreased significantly for the following modes of vibration: antisymmetric stretching of four C-H bonds (3149.2 cm$^{-1}$ in pyridine; 3179.1 cm$^{-1}$ in the complex), antisymmetric stretching of all C-H bonds (3151.8 cm$^{-1}$ in pyridine; 3177.4 cm$^{-1}$ in the complex), and four symmetric C-H and one antisymmetric C-H stretching (3175.0 cm$^{-1}$ in pyridine; 3186.2 cm$^{-1}$ in the complex). Adding the $Ag_2$ molecule to the pyridine caused an increase in Raman scattering activities for the following vibrational modes: symmetric C-H stretching (3188.8 cm$^{-1}$ in pyridine to 3200.8 cm$^{-1}$ in complex) and all C-H bonds stretching symmetrically (3197.5 cm$^{-1}$ in pyridine to 3206.4 cm$^{-1}$ in complex).

For the pyridine/$Ag_2$ complex, the mode with the greatest IR intensity is the symmetric C-H out-of-plane wag (718.3 cm$^{-1}$), and the mode with the greatest Raman activity is all C-H bonds stretching symmetrically (3206.4 $cm^{-1}$). These two peaks could be used in identifying the presence of pyridine when using SERS.

In general, for the case of pyridine, the frequency shifts were less than 10 $cm^{-1}$, the IR intensities changed by less than 10 km $mol^{-1}$, and the Raman scattering activities changed by less than 2 $A^4$ $amu^{-1}$, except for the ones listed in Table 4.1.1. The largest frequency shift was 29.9 $cm^{-1}$ (3149.2 $cm^{-1}$ in pyridine to 3179.1 $cm^{-1}$ in the complex). The greatest change in IR intensity was 27.8 km $mol^{-1}$ (1242.0 $cm^{-1}$ in pyridine to 1243.5 $cm^{-1}$ in the complex), and the greatest change in Raman activity was 171.1 $A^4$ $amu^{-1}$ (3197.5 $cm^{-1}$ in pyridine to 3206.4 $cm^{-1}$ in the complex).

## 4.2 1H-1,2,3-Triazole

The 1H-1,2,3-Triazole molecule has three N atoms. However, the $Ag_2$ molecule was only added to the two N atoms with lone electron pairs, as discussed previously. In the compound name, the bold number indicates with which N atom $Ag_2$ interacted. For example, 1H-1,**2**,3-triazole indicates the second N atom interacted with $Ag_2$. Figures 4.2.1 and 4.2.2 show 1H-1,**2**,3-triazole and 1H-1,2,**3**-triazole complexes, respectively. The 1H-1,2,**3**-triazole/$Ag_2$ complex is the lower energy structure by 1.70 kcal $mol^{-1}$. The isolated 1H-1,2,3-triazole molecule and the two complexes were optimized and their frequencies were calculated at the B3LYP/Def2-TZVPD level of theory.

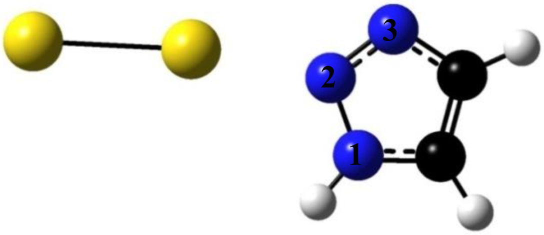


**Figure 4.2.1:** Optimized Structure of 1H-1,**2**,3-Trizaole/$Ag_2$ Complex

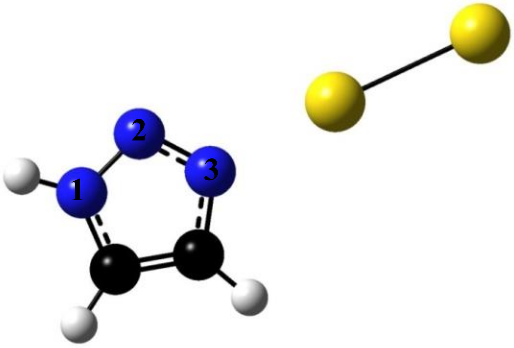


**Figure 4.2.2:** Optimized Structure of 1H-1,2,**3**-Trizaole/$Ag_2$ complex

Tables 4.2.1 and 4.2.2 show select harmonic vibrational frequencies of the 1H-1,2,3-triazole molecule and the 1H-1,**2**,3-triazole/$Ag_2$ and 1H-1,2,**3**-triazole/$Ag_2$ complexes. The full tables of frequencies for 1H-1,**2**,3-triazole/$Ag_2$ and 1H-1,2,**3**-triazole/$Ag_2$ can be found in the appendix (Tables A-10.1 and A-10.2, respectively).

The last section in the table shows the frequency shifts for each vibrational mode. This shift indicates the changes from the isolated molecule to the complex, which shows the effects that occur when $Ag_2$ interacts with each N in 1H-1,2,3-triazole. The frequencies listed only in the "1H-1,2,3-Triazole/$Ag_2$ complex" section (shown in Tables A-10.1 and A-10.2) correspond to the intermolecular vibrations between $Ag_2$ and the 1H-1,2,3-triazole.

The IR and Raman spectra for the 1H-1,**2**,3-triazole/$Ag_2$ complex (shown in red) are shown in Figures 4.2.4 and 4.2.5, respectively. A Raman spectra showing 0-2000 $cm^{-1}$ is shown in Figure 4.2.6. The IR and Raman spectra for the 1H-1,2,**3**-triazole/$Ag_2$ complex (shown in green) are shown in Figures 4.2.7 and 4.2.8, respectively. A Raman spectra showing 0-2000 $cm^{-1}$ is shown in Figure 4.2.9. The blue lines correspond to the isolated 1H-1,2,3-triazole molecule. In all of the spectra, the frequencies below 120 $cm^{-1}$ correspond to the intermolecular modes between $Ag_2$ and 1H-1,2,3-triazole.

**Table 4.2.1:** Select Harmonic Vibrational Frequencies for 1H-1,2,3-Triazole and 1H-1,**2**,3-Triazole/$Ag_2$ Complex[a]

| 1H-1,2,3-Triazole | | | 1H-1,**2**,3-Triazole/$Ag_2$ complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | $\Delta\ \omega$ | Δ IR | Δ Raman |
| 1036.1 | 26.2 | 4.3 | 1069.9 | 31.9 | 1.6 | 33.8 | 5.8 | -2.7 |
| 1104.3 | 32.1 | 0.4 | 1113.5 | 72.6 | 0.6 | 9.2 | 40.5 | 0.3 |
| 1178.7 | 11.8 | 23.3 | 1191.0 | 12.7 | 23.7 | 12.3 | 0.9 | 0.4 |
| 3287.1 | 0.1 | 102.5 | 3290.4 | 0.7 | 241.7 | 3.3 | 0.7 | 139.2 |
| 3635.4 | 80.0 | 110.6 | 3612.0 | 91.6 | 143.5 | -23.4 | 11.6 | 32.9 |

[a] Frequencies ($\omega$) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table 4.2.2:** Select Harmonic Vibrational Frequencies for 1H-1,2,3-Triazole and 1H-1,2,**3**-Triazole/$Ag_2$ Complex[a]

| 1H-1,2,3-Triazole | | | 1H-1,2,**3**-Triazole/$Ag_2$ complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | $\Delta\ \omega$ | Δ IR | Δ Raman |
| 591.9 | 56.8 | 0.3 | 623.0 | 38.0 | 0.6 | 31.0 | -18.8 | 0.3 |
| 1036.1 | 26.2 | 4.3 | 1074.9 | 32.4 | 7.2 | 38.7 | 6.2 | 2.9 |
| 1104.3 | 32.1 | 0.4 | 1109.2 | 61.0 | 0.2 | 4.9 | 28.9 | -0.2 |
| 1178.7 | 11.8 | 23.3 | 1195.6 | 3.8 | 44.8 | 16.9 | -8.0 | 21.5 |
| 3287.1 | 0.1 | 102.5 | 3293.8 | 1.6 | 181.4 | 6.7 | 1.5 | 78.9 |
| 3635.4 | 80.0 | 110.6 | 3625.4 | 113.2 | 390.5 | -10.0 | 33.2 | 279.9 |

[a] Frequencies ($\omega$) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

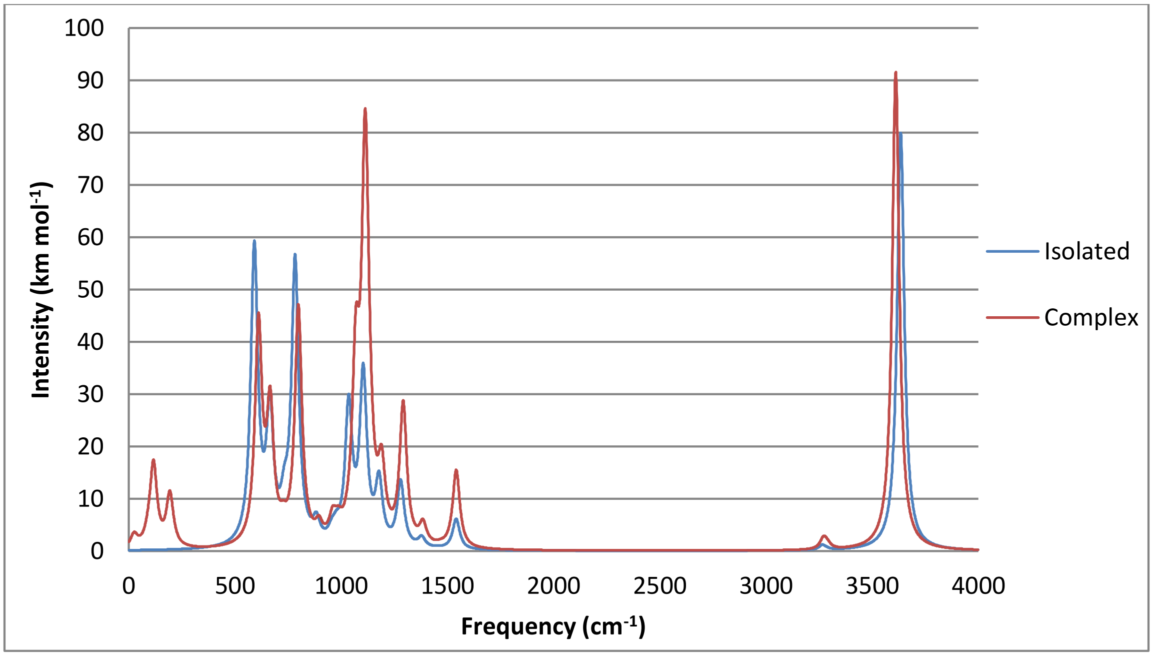


**Figure 4.2.4:** IR Spectrum of 1H-1,**2**,3-Triazole

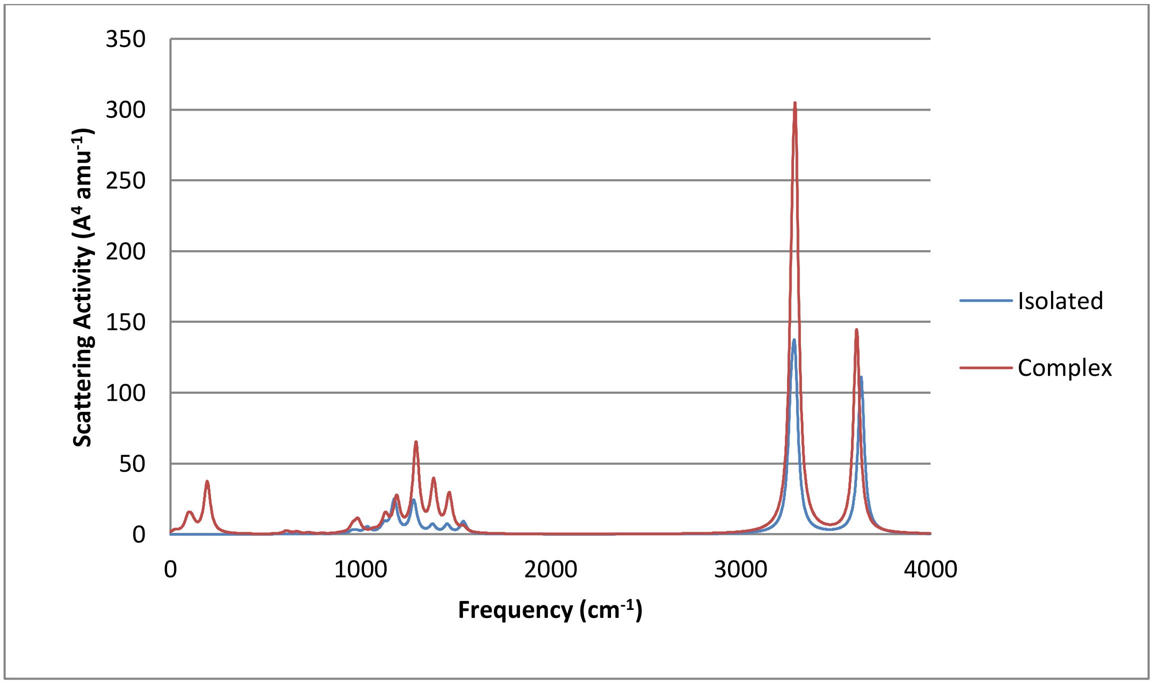


**Figure 4.2.5:** Raman Activity Spectrum of 1H-1,**2**,3-Triazole

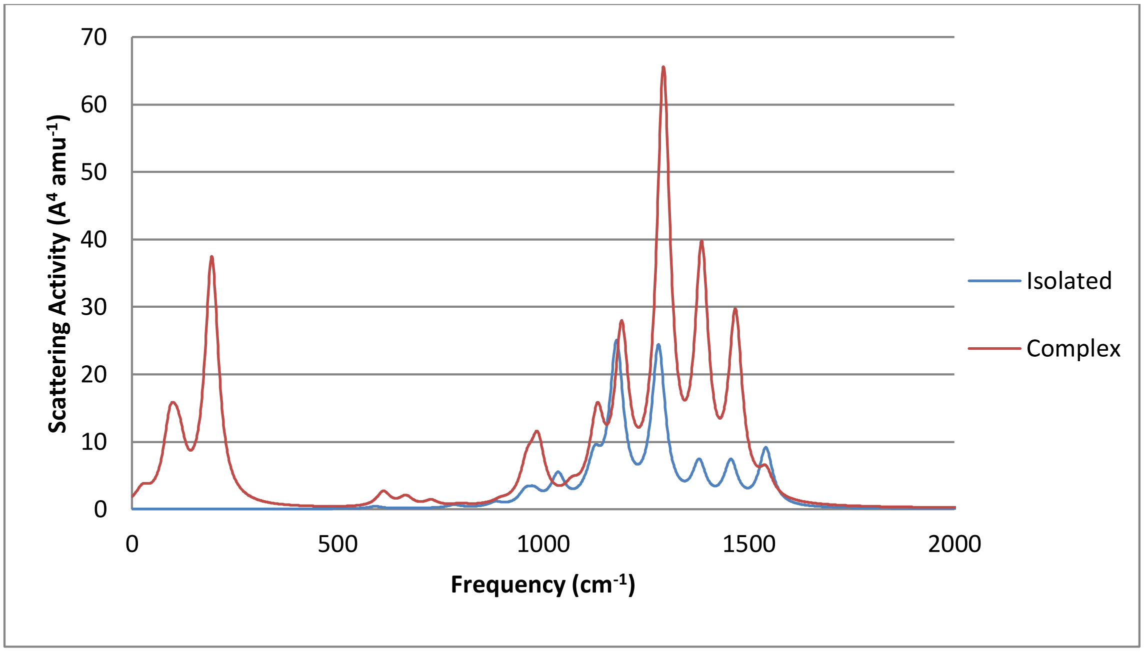


**Figure 4.2.6:** Raman Activity Spectrum (0-2000 cm$^{-1}$) of 1H-1,**2**,3-Triazole

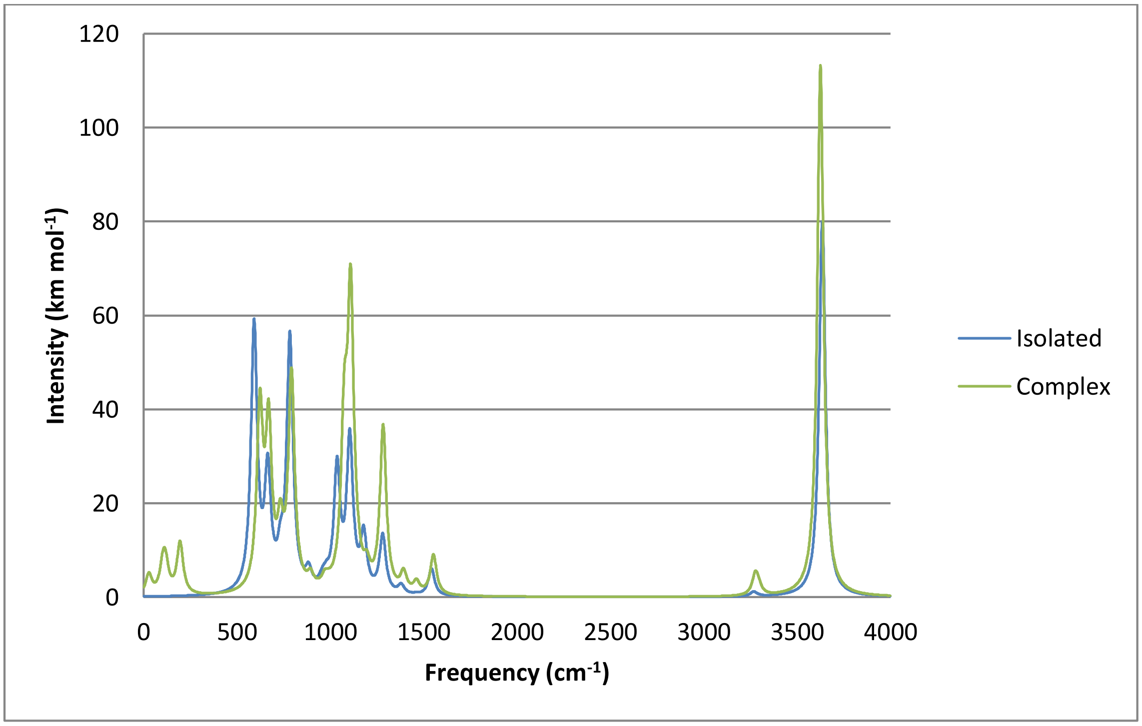


**Figure 4.2.7:** IR Spectrum of 1H-1,2,**3**-Triazole

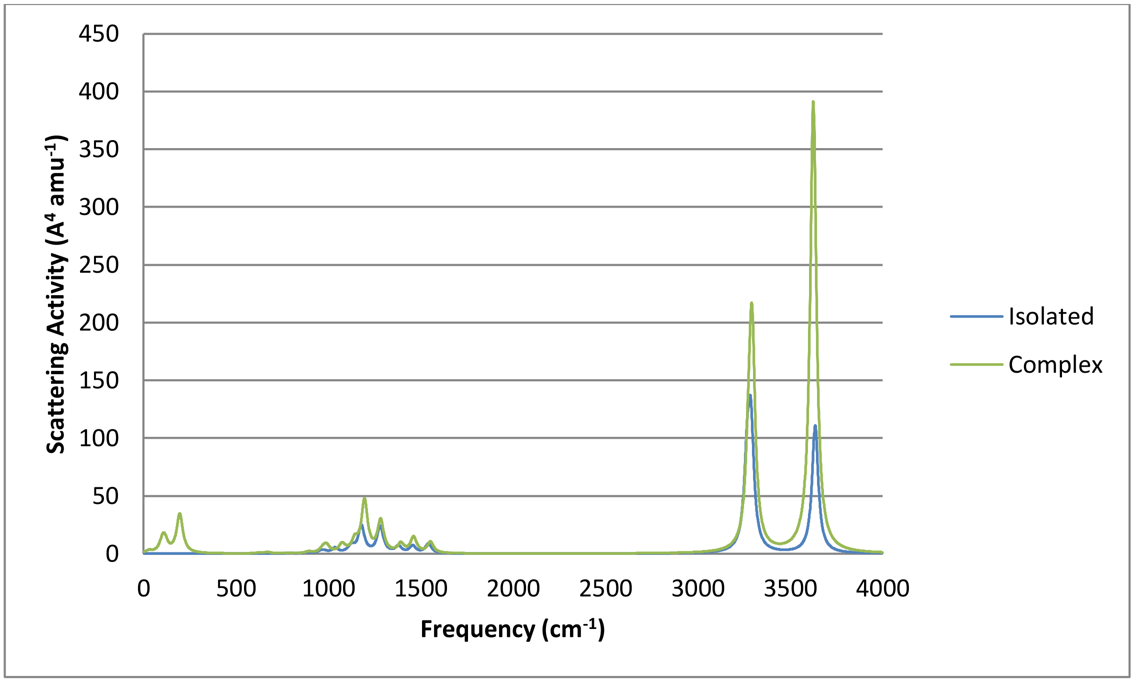


**Figure 4.2.8:** Raman Activity Spectrum of 1H-1,2,**3**-Triazole

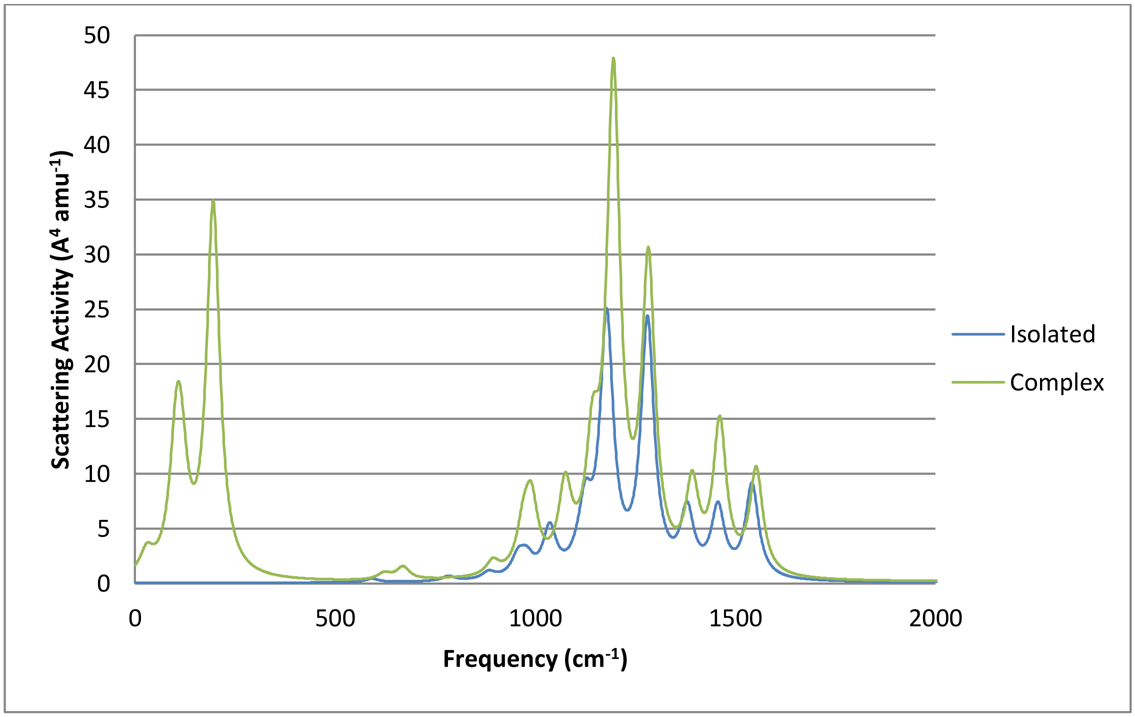


**Figure 4.2.9:** Raman Activity Spectrum (0-2000 cm$^{-1}$) of 1H-1,2,**3**-Triazole

When comparing the two Raman spectra together, the difference in the peak intensities and positions for certain modes can help differentiate between which N atom $Ag_2$ was interacting. In particular, three modes displayed the greatest Raman scattering in both complexes: antisymmetric C-H stretching (3267.0 $cm^{-1}$ in 1H-1,2,3-triazole; 3272.2 $cm^{-1}$ 1H-1,**2**,3-triazole/$Ag_2$ complex; 3276.4 $cm^{-1}$ in 1H-1,2,**3**-triazole/$Ag_2$ complex), symmetric C-H stretching (3287.1 $cm^{-1}$ in 1H-1,2,3-triazole; 3290.4 $cm^{-1}$ in 1H-1,**2**,3-triazole/$Ag_2$ complex; 3293.8 $cm^{-1}$ in 1H-1,2,**3**-triazole/$Ag_2$ complex), and the N-H stretch (3635.4 $cm^{-1}$ in 1H-1,2,3-triazole; 3612.0 $cm^{-1}$ in 1H-1,**2**,3-triazole/$Ag_2$ complex; 3625.4 $cm^{-1}$ in 1H-1,2,**3**-triazole/$Ag_2$ complex). Since the frequencies corresponding to the antisymmetric and symmetric C-H stretching are very close, the two peaks at these frequencies show up as one in the Raman spectra. In the 1H-1,**2**,3-triazole/$Ag_2$ complex, the symmetric C-H stretching mode at 3290.4 $cm^{-1}$ exhibited significantly more scattering activity than the N-H stretching mode at 3612.0 $cm^{-1}$. However, in the 1H-1,**2**,3-triazole/$Ag_2$ complex, the N-H stretching mode at 3625.4 $cm^{-1}$ displayed almost twice as much scattering activity than the symmetric C-H mode at 3293.8 $cm^{-1}$. Also, for the $Ag_2$ interacting with N2 complex, the modes between 1300 and 1500 $cm^{-1}$ exhibited slightly more Raman scattering activity than the other complex.

When $Ag_2$ was added to the 1H-1,2,3-triazole, two significant frequency shifts of greater than 20 $cm^{-1}$ occurred in each complex. The magnitude of these shifts is shown in the $\Delta\omega$ columns in Tables 4.2.1 and 4.2.2. In the 1H-1,**2**,3-triazole/$Ag_2$ complex, the frequencies shifted from 1036.1 $cm^{-1}$ to 1069.9 $cm^{-1}$ (N1-N2 stretch) and from 3635.4 $cm^{-1}$ to 3612.0 $cm^{-1}$ (N1-H stretch). In the 1H-1,2,**3**-triazole/$Ag_2$ complex, the frequencies shifted from 591.9 cm$^{-1}$ to 623.0 cm$^{-1}$ (C-H + N1-H out-of-plane wagging) and 1036.1 cm$^{-1}$ to 1074.9 cm$^{-1}$ (N1-N2 stretch).

The ring-breathing mode occurred at 1191.0 cm$^{-1}$ in the 1H-1,**2**,3-triazole/$Ag_2$ complex and 1195.6 cm$^{-1}$ in the 1H-1,2,**3**-triazole/$Ag_2$ complex. This mode is more clearly seen in the complexes, and the intensities of the peaks make it easier to detect this mode using IR.

## 4.3 1,2,4,5-Tetrazine and 1,2,3,5-Tetrazine

1,2,4,5-tetrazine and 1,2,3,5-tetrazine displayed very large increases in Raman activity for certain vibrational modes when $Ag_2$ interacted with N. The isolated 1,2,4,5-tetrazine and 1,2,3,5-tetrazine molecules and their respective $Ag_2$ complexes were each optimized and their frequencies were calculated at the B3LYP/Def2-TZVPD level of theory. Since 1,2,4,5-tetrazine only has one unique N atom, only one model of the complex was constructed (Figure 4.3.1). 1,2,3,5-tetrazine has three unique N atoms with lone electron pairs, so three complexes were modeled. However, only the complex with $Ag_2$ interacting with the second N atom showed significant enhancement of the Raman scattering activities on the order of $10^2$-$10^4$. Only this complex will be discussed. In the compound name (1,**2**,3,5-tetrazine, Figure 4.3.2), the bold number indicates with that $Ag_2$ interacted with the second N. Table 4.3.1 shows the relative energies for these complexes. The lowest energy structure is the 1,**2**,3,5-tetrazine/$Ag_2$ complex. It is also isoenergetic to the **1**,2,3,5-tetrazine/$Ag_2$ complex at this level of theory, so both structures may be seen when 1,2,3,5-tetrazine interacts with $Ag_2$.

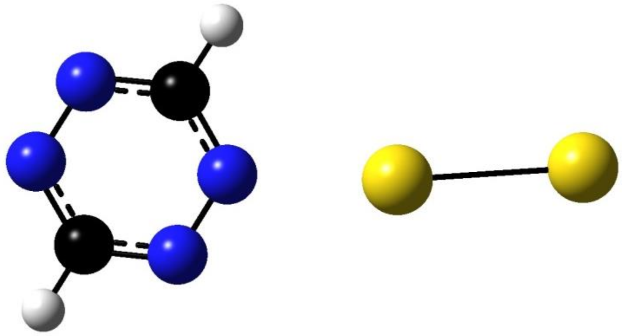


**Figure 4.3.1:** Optimized Structure of the 1,2,4,5-Tetrazine/Ag$_2$ complex

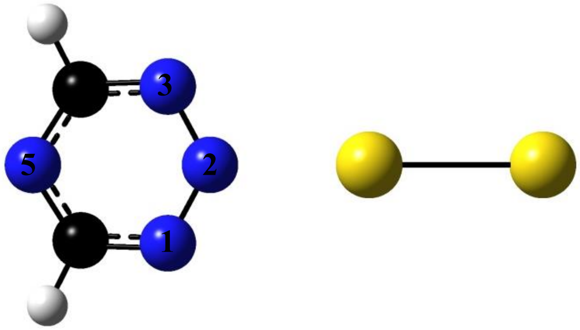


**Figure 4.3.3:** Optimized Structure of the 1,**2**,3,5-Tetrazine/Ag$_2$ complex

**Table 4.3.1:** Relative Energies of 1,2,3,5-Tetrazine/Ag2 Complexes[a]

| Name | Relative Energy |
|---|---|
| **1**,2,3,5-Tetrazine/Ag$_2$ complex | 0.07 |
| 1,**2**,3,5-Tetrazine/Ag$_2$ complex | 0.00 |
| 1,2,3,**5**-Tetrazine/Ag$_2$ complex | 0.91 |

[a] Relative Energies in kcal mol$^{-1}$

Table 4.3.2 shows select harmonic vibrational frequencies for both the 1,2,4,5-tetrazine molecule and the 1,2,4,5-tetrazine/Ag$_2$ complex. The Raman scattering activities for these modes were on the order of $10^2$-$10^4$ $A^4$ $amu^{-1}$. The full table of frequencies for 1,2,4,5-tetrazine can be found in the appendix (Table A-6).

**Table 4.3.2**: Select Harmonic Vibrational Frequencies for 1,2,4,5-Tetrazine and 1,2,4,5-Tetrazine/$Ag_2$ Complex[a]

| 1,2,4,5-Tetrazine | | | 1,2,4,5-Tetrazine/$Ag_2$ complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ *ω* | Δ IR | Δ Raman |
| 655.8 | 0.0 | 2.2 | 662.3 | 0.7 | 134.3 | 6.5 | 0.7 | 132.0 |
| 755.1 | 0.0 | 5.0 | 754.7 | 5.8 | 630.5 | -0.4 | 5.8 | 625.5 |
| 837.2 | 0.0 | 0.6 | 827.8 | 4.5 | 94.9 | -9.4 | 4.5 | 94.2 |
| 935.7 | 1.2 | 0.0 | 939.1 | 12.1 | 224.7 | 3.5 | 11.0 | 224.7 |
| 1052.6 | 0.0 | 42.3 | 1046.1 | 35.6 | 8358.2 | -6.5 | 35.6 | 8315.9 |
| 1150.3 | 8.6 | 0.0 | 1147.0 | 5.3 | 732.8 | -3.3 | -3.3 | 732.8 |
| 1328.4 | 0.0 | 5.6 | 1326.3 | 2.8 | 441.6 | -2.1 | 2.8 | 436.0 |
| 1477.7 | 0.0 | 3.0 | 1456.2 | 313.9 | 35477.5 | -21.5 | 313.9 | 35474.5 |
| 1558.7 | 0.0 | 7.1 | 1553.6 | 21.8 | 1192.1 | -5.1 | 21.8 | 1185.0 |
| 3199.5 | 5.9 | 0.0 | 3206.8 | 2.8 | 342.3 | 7.3 | -3.1 | 342.3 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

Adding $Ag_2$ to 1,2,4,5-tetrazine caused several modes to display large Raman scattering activities, and some even became Raman active. Many of these modes were also IR inactive before the addition of $Ag_2$ to the system. In this particular case, this shows that allowing $Ag_2$ to interact with N can significantly affect the molecule's IR intensities and Raman activities, which can lead to better spectroscopic detection. Table 4.3.3 shows the type of vibrational modes that were affected by the addition of $Ag_2$.

**Table 4.3.3**: Vibrational Modes for Select Frequencies in 1,2,4,5-Tetrazine and 1,2,4,5-Tetrazine/$Ag_2$ Complex[a]

| 1,2,4,5-Tetrazine | 1,2,4,5-Tetrazine/$Ag_2$ complex | Vibrational Mode |
|---|---|---|
| $\omega$ | $\omega$ | |
| 655.8 | 662.3 | ring stretch |
| 755.1 | 754.7 | ring stretch |
| 837.2 | 827.8 | ring bend |
| 935.7 | 939.1 | symmetric C-H out-of-plane wag |
| 1052.6 | 1046.1 | symmetric ring breathing |
| 1150.3 | 1147.0 | symmetric C-H in-plane wag |
| 1328.4 | 1326.3 | antisymmetric C-H in-plane wag |
| 1477.7 | 1456.2 | symmetric N-N stretch |
| 1558.7 | 1553.6 | antisymmetric N-C stretch |
| 3199.5 | 3206.8 | antisymmetric C-H stretch |

[a] Frequencies ($\omega$) in $cm^{-1}$

Select harmonic vibrational frequencies for both the 1,2,4,5-tetrazine molecule and the 1,**2**,3,5-tetrazine/$Ag_2$ complex are shown in Table 4.3.4. The Raman scattering activities for these modes were on the order of $10^2$-$10^4$ $A^4$ $amu^{-1}$ as well. The full table of frequencies for 1,**2**,3,5-tetrazine can be found in the appendix (Table A-13.2).

**Table 4.3.4**: Select Vibrational Frequencies for 1,2,3,5-Tetrazine and 1,**2**,3,5-Tetrazine/$Ag_2$ Complex[a]

| 1,2,3,5-Tetrazine | | | 1,**2**,3,5-Tetrazine/$Ag_2$ complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | $\Delta\ \omega$ | Δ IR | Δ Raman |
| 679.2 | 5.6 | 3.1 | 685.0 | 23.9 | 206.3 | 5.8 | 18.3 | 203.2 |
| 813.5 | 9.8 | 0.2 | 810.9 | 23.4 | 217.3 | -2.7 | 13.6 | 217.1 |
| 1018.8 | 0.4 | 27.7 | 1008.6 | 50.8 | 5076.4 | -10.1 | 50.4 | 5048.7 |
| 1143.5 | 4.7 | 9.0 | 1154.7 | 12.9 | 1054.7 | 11.2 | 8.2 | 1045.7 |
| 1397.7 | 37.8 | 1.6 | 1386.4 | 508.2 | 11235.9 | -11.2 | 470.4 | 11234.4 |
| 1580.1 | 30.4 | 6.1 | 1568.3 | 420.8 | 11980.4 | -11.8 | 390.4 | 11974.2 |

[a] Frequencies ($\omega$) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

For 1,2,3,5-tetrazine, $Ag_2$ had the greatest effect on the Raman activities when it interacted with N2. Most of these selected modes (from Table 4.3.2) showed little Raman activity in the isolated molecule, and the addition of $Ag_2$ enhanced these activities dramatically. This likely happened because N2 was between two N atoms. The $Ag_2$ molecule's interaction with N2 may have caused the molecule to have a larger change in polarizability. Table 4.3.5 shows the type of vibrational modes that were affected by the addition of $Ag_2$.

**Table 4.3.5**: Vibrational Modes for Select Frequencies in 1,2,3,5-Tetrazine and 1,**2**,3,5-Tetrazine/$Ag_2$ Complex[a]

| 1,2,3,5-Tetrazine | 1,**2**,3,5-Tetrazine/ $Ag_2$ complex | Vibrational Mode |
|---|---|---|
| $\omega$ | $\omega$ | |
| 679.2 | 685.0 | ring bend |
| 813.5 | 810.9 | ring out-of-plane wag |
| 1018.8 | 1008.6 | symmetric ring breathing |
| 1143.5 | 1154.7 | antisymmetric ring breathing |
| 1397.7 | 1386.4 | symmetric C-H in-plane wag + N-N stretch |
| 1580.1 | 1568.3 | symmetric C-H in-plane wag + N=C stretch |

[a] Frequencies ($\omega$) in $cm^{-1}$

## 4.4 N···Ag Distances and Dissociation Energies

Table 4.4.1 shows the distance between the N atom and the Ag atom in each of the Group 3 byproduct/$Ag_2$ complexes. The dissociation energy ($D_e$), which is the amount of energy required to break the N···Ag intermolecular bond, for each complex have also been determined. These calculations were done by comparing the energies of the isolated molecule and the isolated $Ag_2$ to the energy of the molecule/$Ag_2$ complex.

As discussed previously, the 1,2,4,5-tetrazine/$Ag_2$ and 1,**2**,3,5-tetrazine/$Ag_2$ complexes showed significant enhancement of the Raman scattering activities on the order of $10^2$-$10^4$ $A^4$ $amu^{-1}$. When comparing the distance between N and Ag and the $D_e$ of each byproduct/complex, these two had some of the largest intermolecular distances and smallest $D_e$'s. This shows that when these byproducts interacted with the $Ag_2$ molecule, a weaker intermolecular interaction occurred. This weaker interaction allows the byproduct to have a larger change in polarizability, leading to an increase in the Raman scattering activities. This can be seen in the data provided in Tables 4.3.2, 4.3.4, and 4.4.1.

**Table 4.4.1**: Distance of N···Ag Interactions and Dissociation Energies ($D_e$) for Each Complex$^a$

| Name | R | $D_e$ | | Name | R | $D_e$ |
|---|---|---|---|---|---|---|
| Pyridine | 2.32 | 12.42 | | 2-Methylpyrazine (**N1**) | 2.34 | 10.73 |
| Pyridazine | 2.33 | 11.57 | | 2-Methylpyrazine (**N4**) | 2.33 | 10.85 |
| Pyrimidine | 2.33 | 10.69 | | Phenanthridine | 2.33 | 12.27 |
| Pyrazine | 2.34 | 10.30 | | Benzotriazole | 2.32 | 9.60 |
| 1H-Pyrazole | 2.30 | 12.02 | | Indazole | 2.30 | 11.35 |
| 1,3,5-Triazine | 2.35 | 8.89 | | Benzimidazole | 2.28 | 13.62 |
| **1**,2,3-Triazine | 2.35 | 9.39 | | Quinoline | 2.32 | 12.33 |
| 1,**2**,3-Triazine | 2.35 | 9.52 | | Phenazine | 2.35 | 10.74 |
| **1**,2,4-Triazine | 2.35 | 9.40 | | Quinoxaline | 2.34 | 10.62 |
| 1,**2**,4-Triazine | 2.35 | 9.65 | | Acridine | 2.34 | 12.11 |
| 1,2,**4**-Triazine | 2.36 | 8.40 | | Isoquinoline | 2.31 | 12.73 |
| 1H-1,**2**,3-Triazole | 2.33 | 9.63 | | 3-Methylquinoline | 2.32 | 12.60 |
| 1H-1,2,**3**-Triazole | 2.32 | 11.32 | | Phthalazine | 2.31 | 12.47 |
| 1H-1,**2**,4-Triazole | 2.32 | 10.03 | | Purine (**N3**) | 2.32 | 11.37 |
| 1H-1,2,**4**-Triazole | 2.30 | 11.68 | | Purine (**N5**) | 2.33 | 11.13 |
| 1,2,4,5-Tetrazine | 2.35 | 7.36 | | Purine (**N7**) | 2.33 | 11.38 |
| **1**,2,3,5-Tetrazine | 2.38 | 7.43 | | Cinnoline (**N1**) | 2.32 | 12.02 |
| 1,**2**,3,5-Tetrazine | 2.34 | 7.49 | | Cinnoline (**N2**) | 2.33 | 11.65 |
| 1,2,3,**5**-Tetrazine | 2.39 | 6.58 | | Quinazoline (**N1**) | 2.32 | 11.29 |
| | | | | Quinazoline (**N3**) | 2.33 | 11.17 |

$^a$ R(N···Ag) in Å, $D_e$ in kcal $mol^{-1}$

# Chapter 5: Conclusions

In order to simulate the SERS detection of HEDM byproducts, an $Ag_2$ molecule was added to the N atoms in the small byproducts (Group 3). The IR and Raman spectra of the isolated byproduct and the byproduct/$Ag_2$ complex were compared to determine how the presence of $Ag_2$ affected the harmonic vibrational modes of the compounds.

In general, there was no clear trend in the change of IR intensities when $Ag_2$ was added. Most of the frequency shifts were less than 10 $cm^{-1}$. Two molecules (1,2,4,5-tetrazine and 1,2,3,5-tetrazine) displayed significant increases in some Raman scattering activities. Adding the $Ag_2$ molecule caused multiple modes to dramatically increase the Raman scattering activity on the order of $10^2$-$10^4$ $A^4$ $amu^{-1}$.

The N···Ag intermolecular bond distances and $D_e$'s for the Group 3 byproducts were determined. When comparing the 1,2,4,5-tetrazine/$Ag_2$ and 1,**2**,3,5-tetrazine/$Ag_2$ complexes to the remaining byproduct/$Ag_2$ complexes, these two had some of the largest intermolecular distances and smallest $D_e$'s. This weaker interaction between the Ag and the N in these complexes likely allowed the byproducts to have a larger change in polarizability, which caused the significant enhancements in the Raman scattering activities (on the order of $10^2$-$10^4$ $A^4$ $amu^{-1}$) for certain vibrational modes.

Modeling these byproduct/$Ag_2$ complexes aids in the understanding of the effectiveness of the SERS detection technique. Adding $Ag_2$ to the systems caused increases in the Raman scattering activities for some modes. On this scale, this suggests that adding only two Ag atoms can have an effect on the enhancement of the Raman activities. Larger Ag clusters may be required to adequately model the surface enhancement of Raman scattering activities for these compounds.

To further explore if SERS is a viable detection technique for these types of compounds in the real world, other molecules commonly found in the environment can be added to the systems. For example, $H_2O$ can interact with the HEDMs to see how the vibrational spectra are affected.

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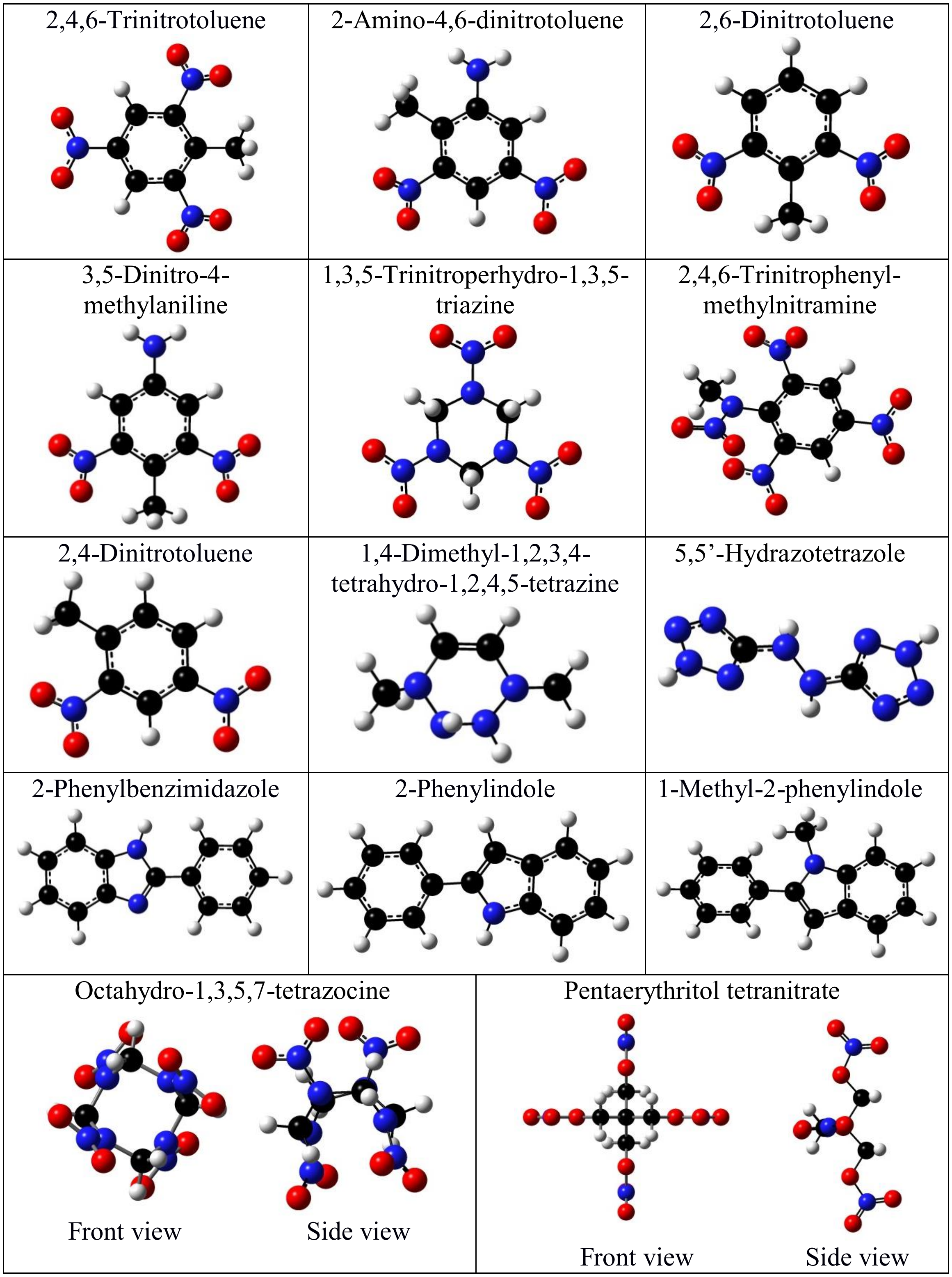
# APPENDIX



2,4,6-Trinitrotoluene

2-Amino-4,6-dinitrotoluene

2,6-Dinitrotoluene

3,5-Dinitro-4-methylaniline

1,3,5-Trinitroperhydro-1,3,5-triazine

2,4,6-Trinitrophenyl-methylnitramine

2,4-Dinitrotoluene

1,4-Dimethyl-1,2,3,4-tetrahydro-1,2,4,5-tetrazine

5,5'-Hydrazotetrazole

2-Phenylbenzimidazole

2-Phenylindole

1-Methyl-2-phenylindole

Octahydro-1,3,5,7-tetrazocine

Front view

Side view

Pentaerythritol tetranitrate

Front view

Side view

**Figure A-1:** Group 1 Molecules

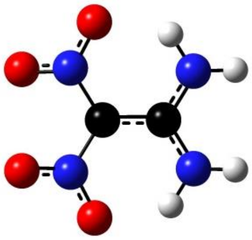
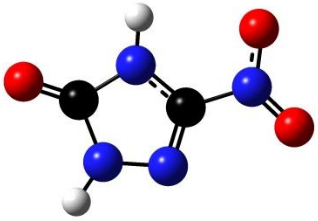
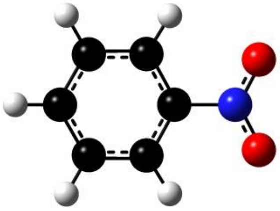
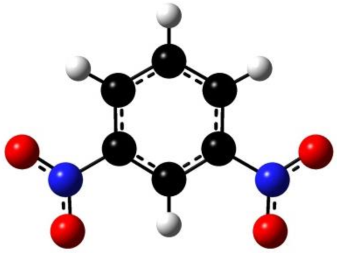
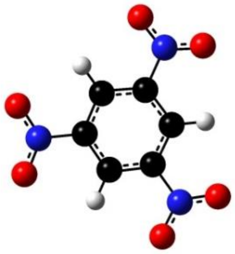
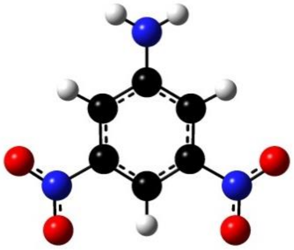
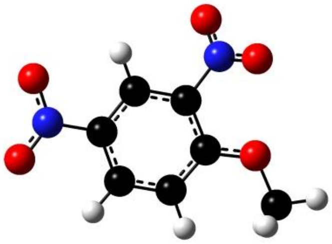
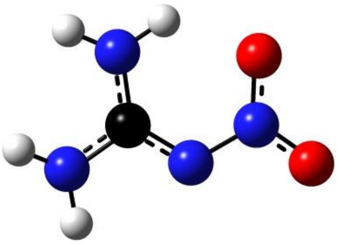
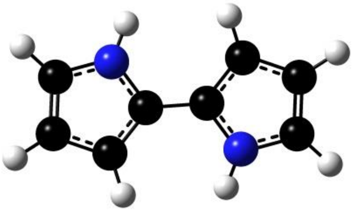
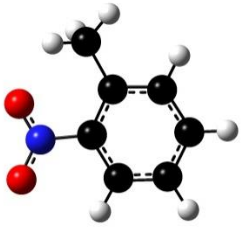
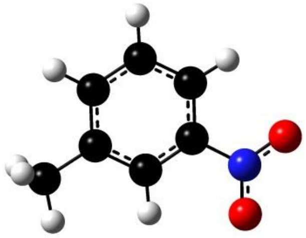
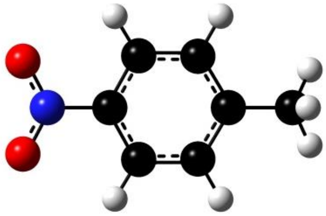
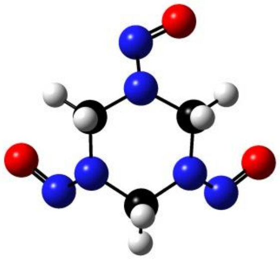
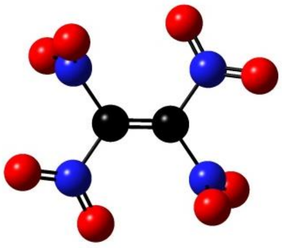
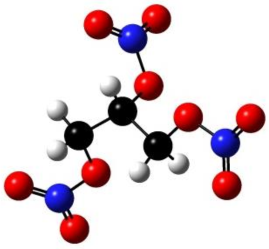
| | | |
|---|---|---|
| 2,2-Dintroethene-1,1-diamine (FOX-7)<br> | Nitrotriazolone<br> | Nitrobenzene<br> |
| 1,3-Dinitrobenzene<br> | 1,3,5-Trinitrobenzene<br> | 3,5-Dinitroaniline<br> |
| 2,4-Dinitroanisole<br> | Nitroguanidine<br> | 2,2'-Bipyrrol<br> |
| 2-Nitrotoluene<br> | 3-Nitrotoluene<br> | 4-Nitrotoluene<br> |
| Hexahydro-1,3,5-trinitroso-1,3,5-triazine<br> | 1,1,2,2-Tetranitroethene<br> | Trinitroglycerin<br> |

**Figure A-2:** Group 2 Molecules

**Table A-1:** Harmonic Vibrational Frequencies for Pyridine and Pyridine/$Ag_2$ Complex[a]

| Pyridine | | | Pyridine/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 25.6 | 0.5 | 0.0 | | | |
| | | | 26.7 | 0.2 | 2.3 | | | |
| | | | 91.1 | 0.0 | 9.0 | | | |
| | | | 111.7 | 2.5 | 8.4 | | | |
| | | | 122.1 | 0.1 | 0.9 | | | |
| | | | 196.1 | 10.4 | 36.7 | | | |
| 383.9 | 0.0 | 0.0 | 391.2 | 0.0 | 0.0 | 7.3 | 0.0 | 0.0 |
| 420.8 | 3.8 | 0.1 | 429.7 | 1.3 | 0.5 | 8.9 | -2.6 | 0.3 |
| 616.7 | 4.5 | 2.3 | 636.2 | 15.2 | 0.7 | 19.5 | 10.8 | -1.6 |
| 670.1 | 0.2 | 3.4 | 667.3 | 0.0 | 2.4 | -2.8 | -0.1 | -1.0 |
| 719.0 | 63.8 | 0.1 | 718.3 | 49.2 | 0.5 | -0.6 | -14.6 | 0.5 |
| 766.6 | 7.1 | 0.0 | 770.5 | 17.6 | 0.1 | 3.9 | 10.5 | 0.1 |
| 899.8 | 0.0 | 0.6 | 900.4 | 0.0 | 0.0 | 0.6 | 0.0 | -0.5 |
| 962.5 | 0.0 | 0.3 | 971.6 | 0.0 | 1.5 | 9.1 | 0.0 | 1.2 |
| 1011.0 | 0.0 | 0.0 | 1014.5 | 0.0 | 0.1 | 3.6 | 0.0 | 0.1 |
| 1013.0 | 5.3 | 30.2 | 1027.8 | 22.0 | 55.8 | 14.8 | 16.7 | 25.6 |
| 1024.2 | 0.0 | 0.0 | 1032.5 | 0.1 | 0.1 | 8.3 | 0.1 | 0.1 |
| 1050.8 | 7.1 | 40.6 | 1055.6 | 9.0 | 48.4 | 4.7 | 1.9 | 7.8 |
| 1079.5 | 0.1 | 0.3 | 1089.2 | 0.9 | 0.2 | 9.8 | 0.8 | -0.1 |
| 1095.4 | 3.2 | 1.8 | 1095.2 | 21.8 | 1.9 | -0.2 | 18.6 | 0.1 |
| 1171.1 | 2.6 | 2.0 | 1177.6 | 2.7 | 3.4 | 6.5 | 0.1 | 1.4 |
| 1242.0 | 3.7 | 8.5 | 1243.5 | 31.5 | 9.6 | 1.5 | 27.8 | 1.2 |
| 1285.3 | 0.0 | 1.5 | 1288.4 | 0.6 | 0.1 | 3.1 | 0.6 | -1.4 |
| 1387.1 | 0.1 | 0.2 | 1391.6 | 2.0 | 0.6 | 4.4 | 1.9 | 0.4 |
| 1476.3 | 25.9 | 0.1 | 1482.2 | 29.4 | 0.0 | 5.9 | 3.5 | -0.1 |
| 1516.1 | 2.1 | 2.1 | 1521.1 | 0.0 | 1.4 | 5.0 | -2.1 | -0.8 |
| 1619.6 | 9.9 | 9.0 | 1619.2 | 2.1 | 9.1 | -0.3 | -7.8 | 0.1 |
| 1626.1 | 23.3 | 14.5 | 1639.2 | 35.7 | 32.6 | 13.2 | 12.4 | 18.1 |
| 3149.2 | 26.5 | 95.3 | 3177.4 | 4.1 | 32.9 | 29.9 | -23.5 | -64.9 |
| 3151.8 | 4.3 | 85.3 | 3179.1 | 3.0 | 30.4 | 25.7 | -0.2 | -52.5 |
| 3175.0 | 3.8 | 101.1 | 3186.2 | 0.1 | 62.5 | 11.1 | -3.7 | -38.6 |
| 3188.8 | 24.0 | 35.2 | 3200.8 | 9.9 | 91.7 | 12.0 | -14.1 | 56.5 |
| 3197.5 | 7.2 | 272.4 | 3206.4 | 12.4 | 443.5 | 8.9 | 5.2 | 171.1 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-2:** Harmonic Vibrational Frequencies for Pyridazine and Pyridazine/$Ag_2$ Complex[a]

| Pyridazine | | | Pyridazine/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 23.0 | 1.0 | 0.1 | | | |
| | | | 27.0 | 1.2 | 2.3 | | | |
| | | | 89.1 | 1.1 | 10.7 | | | |
| | | | 107.4 | 3.0 | 4.7 | | | |
| | | | 113.5 | 1.9 | 1.0 | | | |
| | | | 194.0 | 9.7 | 42.0 | | | |
| 376.1 | 8.9 | 0.2 | 384.1 | 4.6 | 1.0 | 8.0 | -4.3 | 0.8 |
| 378.8 | 0.0 | 0.1 | 392.3 | 0.4 | 0.7 | 13.4 | 0.4 | 0.6 |
| 636.0 | 0.1 | 2.9 | 646.3 | 0.9 | 2.2 | 10.3 | 0.8 | -0.6 |
| 682.2 | 3.2 | 2.8 | 685.5 | 6.5 | 2.2 | 3.3 | 3.3 | -0.6 |
| 764.8 | 41.2 | 0.0 | 768.5 | 28.0 | 0.2 | 3.7 | -13.3 | 0.2 |
| 780.5 | 0.0 | 0.1 | 780.1 | 14.8 | 0.4 | -0.4 | 14.8 | 0.3 |
| 947.4 | 0.0 | 0.1 | 952.6 | 0.0 | 0.3 | 5.2 | 0.0 | 0.2 |
| 990.0 | 0.0 | 0.0 | 997.6 | 0.0 | 0.3 | 7.7 | 0.0 | 0.3 |
| 1014.2 | 6.6 | 40.9 | 1016.2 | 19.2 | 57.1 | 2.0 | 12.6 | 16.2 |
| 1031.0 | 0.0 | 0.0 | 1037.4 | 0.1 | 0.1 | 6.4 | 0.1 | 0.1 |
| 1061.8 | 0.8 | 0.5 | 1075.5 | 2.2 | 3.0 | 13.7 | 1.4 | 2.5 |
| 1087.9 | 1.5 | 1.3 | 1093.4 | 2.3 | 2.0 | 5.5 | 0.8 | 0.7 |
| 1093.0 | 11.6 | 16.2 | 1096.7 | 15.4 | 25.0 | 3.7 | 3.8 | 8.8 |
| 1175.3 | 0.0 | 5.7 | 1180.9 | 0.3 | 5.6 | 5.6 | 0.3 | -0.1 |
| 1181.8 | 0.0 | 6.9 | 1204.2 | 0.4 | 29.2 | 22.4 | 0.4 | 22.3 |
| 1314.1 | 2.8 | 3.7 | 1319.9 | 4.8 | 2.6 | 5.8 | 2.0 | -1.2 |
| 1443.2 | 16.7 | 0.2 | 1448.9 | 14.3 | 1.7 | 5.6 | -2.4 | 1.4 |
| 1481.7 | 1.0 | 2.4 | 1486.4 | 4.2 | 4.2 | 4.7 | 3.2 | 1.8 |
| 1604.7 | 3.7 | 8.7 | 1610.2 | 7.8 | 21.9 | 5.5 | 4.1 | 13.1 |
| 1611.0 | 4.4 | 4.1 | 1615.7 | 0.7 | 36.2 | 4.8 | -3.6 | 32.1 |
| 3168.6 | 6.7 | 35.5 | 3181.0 | 2.0 | 62.4 | 12.4 | -4.7 | 26.9 |
| 3173.1 | 0.1 | 164.4 | 3188.7 | 2.9 | 112.7 | 15.7 | 2.7 | -51.7 |
| 3186.1 | 17.0 | 43.9 | 3197.3 | 3.4 | 59.3 | 11.2 | -13.5 | 15.4 |
| 3199.0 | 7.5 | 229.1 | 3208.0 | 7.9 | 373.7 | 8.9 | 0.5 | 144.6 |

[a] Frequencies ($\omega$) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-3:** Harmonic Vibrational Frequencies for Pyrimidine and Pyrimidine/$Ag_2$ Complex[a]

| Pyrimidine | | | Pyrimidine/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 25.0 | 0.1 | 0.1 | | | |
| | | | 26.6 | 0.3 | 2.2 | | | |
| | | | 90.6 | 0.1 | 9.3 | | | |
| | | | 106.8 | 3.2 | 6.6 | | | |
| | | | 119.2 | 1.2 | 1.5 | | | |
| | | | 194.8 | 9.1 | 38.2 | | | |
| 352.5 | 3.5 | 0.1 | 357.1 | 1.8 | 0.2 | 4.6 | -1.7 | 0.1 |
| 410.9 | 0.0 | 0.4 | 418.9 | 0.8 | 0.3 | 8.0 | 0.8 | -0.1 |
| 635.8 | 11.6 | 2.2 | 645.8 | 23.7 | 1.2 | 9.9 | 12.0 | -1.1 |
| 696.4 | 2.8 | 4.1 | 698.6 | 5.4 | 2.5 | 2.2 | 2.5 | -1.6 |
| 740.0 | 41.0 | 0.1 | 734.7 | 33.4 | 0.8 | -5.3 | -7.6 | 0.7 |
| 826.7 | 4.6 | 0.0 | 831.0 | 8.1 | 0.1 | 4.2 | 3.5 | 0.1 |
| 989.2 | 0.1 | 0.2 | 991.8 | 0.0 | 0.3 | 2.7 | 0.0 | 0.1 |
| 1006.6 | 0.0 | 0.0 | 1012.0 | 0.0 | 0.6 | 5.3 | 0.0 | 0.6 |
| 1011.8 | 3.9 | 20.3 | 1024.4 | 14.5 | 24.3 | 12.6 | 10.6 | 4.0 |
| 1033.1 | 0.0 | 0.1 | 1035.1 | 0.0 | 0.3 | 1.9 | 0.0 | 0.1 |
| 1083.3 | 1.1 | 33.4 | 1085.1 | 3.8 | 63.7 | 1.8 | 2.7 | 30.3 |
| 1096.2 | 2.8 | 1.8 | 1101.2 | 15.7 | 1.6 | 5.0 | 13.0 | -0.2 |
| 1164.1 | 1.6 | 9.8 | 1163.8 | 5.1 | 13.3 | -0.4 | 3.5 | 3.5 |
| 1214.5 | 5.1 | 0.6 | 1218.0 | 20.5 | 4.9 | 3.5 | 15.4 | 4.3 |
| 1254.0 | 8.2 | 5.7 | 1258.1 | 24.4 | 5.3 | 4.2 | 16.2 | -0.4 |
| 1396.3 | 0.3 | 0.5 | 1399.1 | 2.6 | 1.9 | 2.8 | 2.3 | 1.4 |
| 1439.6 | 58.8 | 0.6 | 1445.6 | 61.0 | 0.7 | 6.0 | 2.2 | 0.1 |
| 1497.8 | 5.6 | 1.4 | 1501.4 | 3.4 | 2.6 | 3.6 | -2.2 | 1.3 |
| 1609.4 | 83.8 | 7.7 | 1605.8 | 36.2 | 9.1 | -3.7 | -47.6 | 1.4 |
| 1610.1 | 45.0 | 10.1 | 1624.6 | 119.0 | 29.0 | 14.5 | 74.1 | 18.8 |
| 3152.3 | 14.1 | 119.8 | 3164.4 | 12.3 | 137.8 | 12.1 | -1.8 | 18.0 |
| 3155.5 | 18.1 | 63.7 | 3179.6 | 3.6 | 21.4 | 24.2 | -14.5 | -42.4 |
| 3166.4 | 13.1 | 112.6 | 3185.2 | 1.3 | 55.8 | 18.8 | -11.8 | -56.7 |
| 3200.0 | 8.9 | 169.2 | 3209.7 | 7.4 | 266.8 | 9.6 | -1.5 | 97.6 |

[a] Frequencies ($\omega$) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-4:** Harmonic Vibrational Frequencies for Pyrazine and Pyrazine/$Ag_2$ Complex[a]

| Pyrazine | | | Pyrazine/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 24.0 | 0.0 | 0.1 | | | |
| | | | 25.9 | 0.0 | 2.9 | | | |
| | | | 89.1 | 1.6 | 7.5 | | | |
| | | | 105.2 | 2.9 | 5.5 | | | |
| | | | 118.9 | 1.7 | 0.5 | | | |
| | | | 194.3 | 8.4 | 40.2 | | | |
| 352.0 | 0.0 | 0.0 | 356.5 | 0.0 | 0.0 | 4.5 | 0.0 | 0.0 |
| 435.8 | 24.3 | 0.0 | 446.5 | 15.4 | 2.0 | 10.7 | -8.9 | 2.0 |
| 612.7 | 0.0 | 1.9 | 629.1 | 2.0 | 1.6 | 16.5 | 2.0 | -0.3 |
| 720.6 | 0.0 | 5.0 | 717.2 | 0.5 | 3.4 | -3.4 | 0.5 | -1.6 |
| 782.7 | 0.0 | 0.4 | 776.5 | 0.0 | 0.1 | -6.2 | 0.0 | -0.3 |
| 806.7 | 28.6 | 0.0 | 812.2 | 28.9 | 0.1 | 5.5 | 0.3 | 0.1 |
| 947.7 | 0.0 | 0.5 | 942.5 | 0.0 | 0.0 | -5.2 | 0.0 | -0.5 |
| 998.3 | 0.0 | 0.2 | 1000.8 | 0.0 | 1.1 | 2.5 | 0.0 | 0.9 |
| 1009.5 | 0.0 | 0.0 | 1010.7 | 0.0 | 0.0 | 1.2 | 0.0 | 0.0 |
| 1037.0 | 35.0 | 0.0 | 1040.9 | 7.9 | 64.8 | 4.0 | -27.0 | 64.8 |
| 1043.7 | 0.0 | 54.8 | 1054.0 | 59.6 | 24.3 | 10.3 | 59.6 | -30.5 |
| 1091.8 | 12.8 | 0.0 | 1099.6 | 5.4 | 1.6 | 7.8 | -7.4 | 1.6 |
| 1166.1 | 5.4 | 0.0 | 1162.5 | 26.4 | 0.3 | -3.6 | 21.0 | 0.3 |
| 1219.9 | 4.8 | 0.0 | 1219.7 | 10.9 | 2.4 | -0.3 | 6.2 | 2.4 |
| 1253.3 | 0.0 | 14.9 | 1254.8 | 5.1 | 14.0 | 1.5 | 5.1 | -1.0 |
| 1375.6 | 0.0 | 0.8 | 1377.8 | 0.6 | 0.1 | 2.2 | 0.6 | -0.8 |
| 1445.1 | 31.4 | 0.0 | 1450.0 | 41.5 | 0.0 | 4.9 | 10.1 | 0.0 |
| 1516.9 | 0.5 | 0.0 | 1518.6 | 0.8 | 1.3 | 1.7 | 0.3 | 1.3 |
| 1581.7 | 0.0 | 6.9 | 1580.0 | 1.6 | 7.1 | -1.7 | 1.6 | 0.2 |
| 1615.1 | 0.0 | 26.9 | 1624.7 | 0.2 | 30.7 | 9.6 | 0.2 | 3.7 |
| 3150.6 | 0.0 | 135.6 | 3168.9 | 9.3 | 123.9 | 18.3 | 9.3 | -11.8 |
| 3151.8 | 2.8 | 0.0 | 3170.8 | 0.0 | 89.9 | 19.0 | -2.8 | 89.9 |
| 3165.7 | 64.1 | 0.0 | 3188.9 | 15.0 | 5.4 | 23.2 | -49.2 | 5.4 |
| 3171.8 | 0.0 | 386.9 | 3192.4 | 13.1 | 291.5 | 20.6 | 13.1 | -95.4 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-5:** Harmonic Vibrational Frequencies for 1,3,5-Triazine and 1,3,5-Triazine/$Ag_2$ Complex[a]

| 1,3,5-Triazine | | | 1,3,5-Triazine/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 23.6 | 0.0 | 0.1 | | | |
| | | | 25.6 | 0.0 | 2.1 | | | |
| | | | 87.8 | 1.0 | 9.0 | | | |
| | | | 100.4 | 3.4 | 4.9 | | | |
| | | | 114.7 | 1.7 | 1.3 | | | |
| | | | 193.3 | 7.8 | 40.0 | | | |
| 352.6 | 0.0 | 0.6 | 357.6 | 0.0 | 0.6 | 4.9 | 0.0 | 0.0 |
| 352.6 | 0.0 | 0.6 | 357.9 | 1.4 | 0.2 | 5.2 | 1.4 | -0.4 |
| 693.5 | 15.6 | 3.4 | 686.9 | 12.0 | 2.2 | -6.6 | -3.5 | -1.2 |
| 693.5 | 15.6 | 3.4 | 707.7 | 34.9 | 2.3 | 14.2 | 19.4 | -1.1 |
| 759.4 | 31.5 | 0.0 | 751.9 | 26.4 | 1.2 | -7.5 | -5.2 | 1.2 |
| 955.9 | 0.0 | 0.0 | 961.1 | 0.0 | 0.0 | 5.2 | 0.0 | 0.0 |
| 1012.5 | 0.0 | 16.7 | 1023.1 | 4.6 | 20.2 | 10.6 | 4.6 | 3.5 |
| 1047.1 | 0.0 | 0.1 | 1043.5 | 0.0 | 0.2 | -3.5 | 0.0 | 0.1 |
| 1047.1 | 0.0 | 0.1 | 1051.5 | 0.0 | 0.1 | 4.4 | 0.0 | 0.0 |
| 1159.8 | 0.0 | 36.3 | 1153.9 | 18.7 | 68.8 | -5.9 | 18.7 | 32.5 |
| 1169.1 | 0.0 | 0.0 | 1168.4 | 1.6 | 1.0 | -0.7 | 1.6 | 1.0 |
| 1197.0 | 1.2 | 1.6 | 1192.3 | 21.3 | 8.2 | -4.7 | 20.1 | 6.6 |
| 1197.0 | 1.2 | 1.6 | 1209.2 | 5.9 | 0.3 | 12.1 | 4.7 | -1.3 |
| 1401.9 | 0.0 | 0.0 | 1403.1 | 0.7 | 2.7 | 1.2 | 0.7 | 2.7 |
| 1444.2 | 67.6 | 2.1 | 1447.8 | 76.3 | 2.8 | 3.6 | 8.6 | 0.7 |
| 1444.2 | 67.6 | 2.1 | 1448.7 | 65.1 | 3.1 | 4.5 | -2.6 | 1.1 |
| 1594.8 | 142.1 | 4.8 | 1586.5 | 96.2 | 2.3 | -8.3 | -45.9 | -2.5 |
| 1594.9 | 142.1 | 4.8 | 1610.0 | 256.2 | 30.1 | 15.2 | 114.1 | 25.3 |
| 3165.3 | 20.4 | 61.0 | 3177.1 | 8.8 | 110.4 | 11.7 | -11.6 | 49.4 |
| 3165.4 | 20.4 | 61.0 | 3182.0 | 2.7 | 8.2 | 16.6 | -17.7 | -52.8 |
| 3170.5 | 0.0 | 200.6 | 3184.5 | 1.6 | 149.0 | 14.1 | 1.6 | -51.6 |

[a] Frequencies ($\omega$) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

**Table A-6:** Harmonic Vibrational Frequencies for 1,2,4,5-Tetrazine and 1,2,4,5-Tetrazine/$Ag_2$ Complex[a]

| 1,2,4,5-Tetrazine | | | 1,2,4,5-Tetrazine/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | $\Delta\omega$ | Δ IR | Δ Raman |
| | | | 17.7 | 2.0 | 28.0 | | | |
| | | | 26.8 | 0.0 | 6.2 | | | |
| | | | 79.0 | 3.9 | 85.6 | | | |
| | | | 99.8 | 1.9 | 33.8 | | | |
| | | | 109.6 | 0.9 | 14.7 | | | |
| | | | 187.8 | 0.1 | 898.3 | | | |
| 258.4 | 54.2 | 0.0 | 272.1 | 93.9 | 449.2 | 13.7 | 39.7 | 449.2 |
| 356.8 | 0.0 | 0.0 | 368.4 | 3.1 | 3.8 | 11.6 | 3.1 | 3.8 |
| 655.8 | 0.0 | 2.2 | 662.3 | 0.7 | 134.3 | 6.5 | 0.7 | 132.0 |
| 755.1 | 0.0 | 5.0 | 754.7 | 5.8 | 630.5 | -0.4 | 5.8 | 625.5 |
| 837.2 | 0.0 | 0.6 | 827.8 | 4.5 | 94.9 | -9.4 | 4.5 | 94.2 |
| 935.7 | 1.2 | 0.0 | 939.1 | 12.1 | 224.7 | 3.5 | 11.0 | 224.7 |
| 971.5 | 34.8 | 0.0 | 983.5 | 74.5 | 13.5 | 12.0 | 39.7 | 13.5 |
| 1006.5 | 0.0 | 0.0 | 1005.0 | 2.5 | 1.6 | -1.5 | 2.5 | 1.6 |
| 1052.6 | 0.0 | 42.3 | 1046.1 | 35.6 | 8358.2 | -6.5 | 35.6 | 8315.9 |
| 1102.0 | 0.7 | 0.0 | 1108.5 | 1.1 | 32.1 | 6.5 | 0.5 | 32.1 |
| 1150.3 | 8.6 | 0.0 | 1147.0 | 5.3 | 732.8 | -3.3 | -3.3 | 732.8 |
| 1237.9 | 62.9 | 0.0 | 1243.1 | 56.7 | 2.3 | 5.2 | -6.2 | 2.3 |
| 1328.4 | 0.0 | 5.6 | 1326.3 | 2.8 | 441.6 | -2.1 | 2.8 | 436.0 |
| 1477.7 | 0.0 | 3.0 | 1456.2 | 313.9 | 35477.5 | -21.5 | 313.9 | 35474.5 |
| 1478.7 | 1.9 | 0.0 | 1476.9 | 4.1 | 57.9 | -1.8 | 2.2 | 57.9 |
| 1558.7 | 0.0 | 7.1 | 1553.6 | 21.8 | 1192.1 | -5.1 | 21.8 | 1185.0 |
| 3199.5 | 5.9 | 0.0 | 3206.8 | 2.8 | 342.3 | 7.3 | -3.1 | 342.3 |
| 3200.7 | 0.0 | 221.7 | 3208.4 | 2.1 | 277.4 | 7.7 | 2.1 | 55.8 |

[a] Frequencies ($\omega$) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-7:** Harmonic Vibrational Frequencies for 1H-Pyrazole and 1H-Pyrazole/$Ag_2$ Complex[a]

| 1H-Pyrazole | | | 1H-Pyrazole/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 27.4 | 0.5 | 1.6 | | | |
| | | | 28.1 | 0.3 | 0.1 | | | |
| | | | 94.6 | 0.1 | 8.2 | | | |
| | | | 117.9 | 1.1 | 7.9 | | | |
| | | | 125.9 | 4.8 | 4.8 | | | |
| | | | 198.4 | 11.6 | 31.3 | | | |
| 542.2 | 56.4 | 0.2 | 548.3 | 49.0 | 2.7 | 6.1 | -7.4 | 2.5 |
| 639.7 | 0.1 | 0.0 | 636.8 | 0.1 | 0.1 | -2.8 | 0.0 | 0.1 |
| 693.0 | 18.5 | 0.0 | 684.8 | 11.7 | 1.5 | -8.3 | -6.7 | 1.4 |
| 760.3 | 93.6 | 0.4 | 771.9 | 80.0 | 0.1 | 11.6 | -13.6 | -0.3 |
| 854.7 | 7.6 | 0.9 | 870.4 | 4.0 | 0.5 | 15.7 | -3.6 | -0.4 |
| 905.2 | 4.1 | 0.1 | 918.1 | 2.8 | 0.2 | 12.9 | -1.3 | 0.0 |
| 925.2 | 9.1 | 1.6 | 928.1 | 7.3 | 1.7 | 2.9 | -1.8 | 0.0 |
| 943.6 | 5.2 | 0.7 | 957.5 | 10.1 | 7.7 | 13.9 | 4.9 | 7.0 |
| 1047.1 | 36.5 | 1.9 | 1058.8 | 69.3 | 1.4 | 11.8 | 32.9 | -0.5 |
| 1055.9 | 6.2 | 2.2 | 1070.7 | 21.9 | 1.2 | 14.7 | 15.7 | -1.0 |
| 1141.6 | 20.3 | 6.0 | 1146.7 | 57.0 | 2.7 | 5.1 | 36.7 | -3.3 |
| 1179.0 | 0.3 | 30.8 | 1183.4 | 17.9 | 42.9 | 4.4 | 17.6 | 12.2 |
| 1281.1 | 2.4 | 16.8 | 1292.3 | 5.3 | 36.1 | 11.2 | 2.9 | 19.3 |
| 1384.0 | 5.0 | 13.2 | 1390.1 | 22.7 | 27.0 | 6.1 | 17.7 | 13.8 |
| 1421.8 | 12.2 | 17.4 | 1430.2 | 15.8 | 58.8 | 8.4 | 3.6 | 41.5 |
| 1478.3 | 6.4 | 3.1 | 1495.4 | 14.4 | 4.0 | 17.0 | 8.0 | 0.9 |
| 1565.1 | 6.4 | 2.7 | 1568.5 | 9.9 | 2.8 | 3.4 | 3.5 | 0.1 |
| 3240.2 | 2.8 | 93.9 | 3253.1 | 0.1 | 65.5 | 12.8 | -2.7 | -28.4 |
| 3254.6 | 1.2 | 41.7 | 3262.0 | 0.5 | 75.1 | 7.4 | -0.7 | 33.4 |
| 3271.8 | 0.4 | 143.3 | 3278.8 | 0.2 | 307.8 | 7.0 | -0.2 | 164.5 |
| 3653.0 | 83.0 | 96.2 | 3639.0 | 104.3 | 132.9 | -14.1 | 21.3 | 36.7 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-8.1:** Harmonic Vibrational Frequencies for 1,2,3-Triazine and **1**,2,3-Triazine/Ag$_2$ Complex[a]

| 1,2,3-Triazine | | | **1**,2,3-Triazine/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 21.4 | 0.1 | 0.0 | | | |
| | | | 26.1 | 1.8 | 2.3 | | | |
| | | | 85.5 | 0.5 | 11.5 | | | |
| | | | 100.0 | 4.3 | 2.9 | | | |
| | | | 109.1 | 5.4 | 1.1 | | | |
| | | | 192.1 | 8.0 | 44.3 | | | |
| 310.2 | 1.3 | 0.1 | 317.7 | 1.2 | 0.4 | 7.5 | -0.1 | 0.3 |
| 367.3 | 0.0 | 0.5 | 380.9 | 1.0 | 1.7 | 13.6 | 1.0 | 1.2 |
| 668.7 | 6.2 | 2.2 | 673.7 | 7.7 | 1.9 | 5.0 | 1.6 | -0.3 |
| 682.3 | 0.1 | 3.9 | 688.3 | 5.3 | 3.4 | 6.0 | 5.3 | -0.5 |
| 787.2 | 19.2 | 0.0 | 783.4 | 15.6 | 0.3 | -3.7 | -3.6 | 0.3 |
| 830.1 | 3.9 | 0.0 | 833.4 | 7.9 | 0.6 | 3.2 | 4.0 | 0.6 |
| 976.2 | 11.7 | 1.1 | 980.9 | 35.5 | 12.9 | 4.8 | 23.8 | 11.7 |
| 999.8 | 0.0 | 0.0 | 1006.1 | 0.0 | 0.6 | 6.3 | 0.0 | 0.6 |
| 1013.0 | 3.7 | 35.5 | 1031.3 | 4.7 | 55.8 | 18.3 | 1.1 | 20.3 |
| 1029.0 | 0.0 | 0.2 | 1034.1 | 0.0 | 0.6 | 5.1 | 0.0 | 0.4 |
| 1098.6 | 0.5 | 16.1 | 1100.7 | 0.9 | 34.1 | 2.1 | 0.4 | 18.0 |
| 1105.8 | 0.2 | 3.8 | 1113.3 | 0.2 | 4.3 | 7.4 | 0.0 | 0.5 |
| 1139.8 | 0.4 | 1.8 | 1144.1 | 3.2 | 0.2 | 4.3 | 2.8 | -1.6 |
| 1225.2 | 0.1 | 3.0 | 1227.3 | 3.3 | 4.4 | 2.1 | 3.1 | 1.5 |
| 1390.1 | 15.8 | 1.6 | 1393.8 | 27.1 | 1.5 | 3.7 | 11.4 | -0.1 |
| 1442.4 | 3.3 | 0.6 | 1445.5 | 2.1 | 6.7 | 3.1 | -1.2 | 6.1 |
| 1591.1 | 45.4 | 3.4 | 1591.6 | 8.7 | 4.8 | 0.4 | -36.7 | 1.5 |
| 1591.8 | 0.1 | 6.6 | 1598.1 | 33.8 | 38.6 | 6.3 | 33.7 | 32.1 |
| 3172.2 | 1.9 | 122.9 | 3183.8 | 3.9 | 125.2 | 11.6 | 2.0 | 2.4 |
| 3177.7 | 8.8 | 51.4 | 3189.8 | 0.3 | 22.6 | 12.1 | -8.5 | -28.8 |
| 3200.5 | 7.1 | 183.3 | 3209.6 | 5.4 | 303.5 | 9.2 | -1.6 | 120.2 |

[a] Frequencies ($\omega$) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

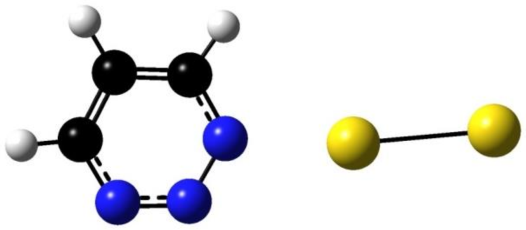


**Figure A-8.1:** **1**,2,3-Triazine/Ag$_2$ Complex

**Table A-8.2:** Harmonic Vibrational Frequencies for 1,2,3-Triazine and 1,**2**,3-Triazine/$Ag_2$ Complex[a]

| 1,2,3-Triazine | | | 1,**2**,3-Triazine/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 16.1 | 2.9 | 0.4 | | | |
| | | | 27.9 | 1.6 | 2.2 | | | |
| | | | 83.4 | 3.1 | 15.2 | | | |
| | | | 98.5 | 2.5 | 0.7 | | | |
| | | | 101.8 | 2.4 | 0.5 | | | |
| | | | 191.1 | 8.3 | 50.7 | | | |
| 310.2 | 1.3 | 0.1 | 331.6 | 0.2 | 4.9 | 21.4 | -1.1 | 4.8 |
| 367.3 | 0.0 | 0.5 | 374.2 | 0.0 | 0.7 | 6.9 | 0.0 | 0.2 |
| 668.7 | 6.2 | 2.2 | 669.0 | 8.1 | 2.6 | 0.3 | 2.0 | 0.4 |
| 682.3 | 0.1 | 3.9 | 691.5 | 0.0 | 4.1 | 9.2 | -0.1 | 0.3 |
| 787.2 | 19.2 | 0.0 | 794.2 | 22.6 | 3.3 | 7.0 | 3.4 | 3.3 |
| 830.1 | 3.9 | 0.0 | 829.0 | 6.0 | 0.0 | -1.2 | 2.1 | 0.0 |
| 976.2 | 11.7 | 1.1 | 1005.2 | 0.0 | 0.0 | 29.0 | -11.7 | -1.1 |
| 999.8 | 0.0 | 0.0 | 1014.3 | 8.3 | 0.1 | 14.5 | 8.3 | 0.1 |
| 1013.0 | 3.7 | 35.5 | 1014.4 | 5.7 | 99.3 | 1.4 | 2.0 | 63.7 |
| 1029.0 | 0.0 | 0.2 | 1035.6 | 0.1 | 0.1 | 6.7 | 0.1 | -0.1 |
| 1098.6 | 0.5 | 16.1 | 1101.6 | 0.0 | 24.0 | 2.9 | -0.5 | 7.9 |
| 1105.8 | 0.2 | 3.8 | 1117.4 | 0.4 | 2.4 | 11.5 | 0.2 | -1.4 |
| 1139.8 | 0.4 | 1.8 | 1154.8 | 0.5 | 11.8 | 15.0 | 0.1 | 10.0 |
| 1225.2 | 0.1 | 3.0 | 1232.9 | 0.0 | 4.5 | 7.6 | -0.1 | 1.5 |
| 1390.1 | 15.8 | 1.6 | 1396.6 | 33.3 | 17.4 | 6.5 | 17.5 | 15.8 |
| 1442.4 | 3.3 | 0.6 | 1444.9 | 4.6 | 0.1 | 2.5 | 1.4 | -0.5 |
| 1591.1 | 45.4 | 3.4 | 1591.1 | 45.4 | 3.9 | 0.0 | 0.0 | 0.5 |
| 1591.8 | 0.1 | 6.6 | 1594.0 | 4.9 | 87.7 | 2.2 | 4.7 | 81.1 |
| 3172.2 | 1.9 | 122.9 | 3183.0 | 4.4 | 116.3 | 10.8 | 2.5 | -6.6 |
| 3177.7 | 8.8 | 51.4 | 3188.4 | 2.8 | 108.2 | 10.7 | -6.0 | 56.8 |
| 3200.5 | 7.1 | 183.3 | 3208.8 | 3.9 | 293.7 | 8.3 | -3.1 | 110.3 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

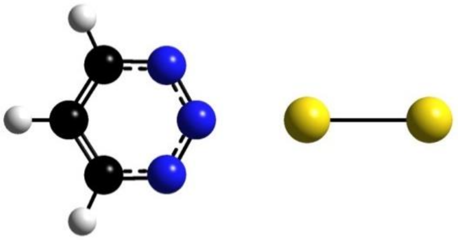


**Figure A-8.2:** 1,**2**,3-Triazine/$Ag_2$ Complex

**Table A-9.1:** Harmonic Vibrational Frequencies for 1,2,4-Triazine and **1**,2,4-Triazine/Ag$_2$ Complex[a]

| 1,2,4-Triazine | | | **1**,2,4-Triazine/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 19.3 | 0.0 | 0.1 | | | |
| | | | 26.1 | 0.6 | 2.8 | | | |
| | | | 86.4 | 0.2 | 10.1 | | | |
| | | | 100.3 | 2.7 | 2.2 | | | |
| | | | 111.2 | 2.5 | 0.6 | | | |
| | | | 192.4 | 7.5 | 45.9 | | | |
| 322.2 | 13.1 | 0.2 | 328.0 | 7.4 | 2.9 | 5.8 | -5.7 | 2.7 |
| 388.1 | 12.9 | 0.1 | 404.2 | 8.2 | 3.7 | 16.1 | -4.7 | 3.6 |
| 637.3 | 2.1 | 2.2 | 649.5 | 0.8 | 4.4 | 12.2 | -1.3 | 2.2 |
| 731.0 | 3.0 | 4.5 | 730.0 | 5.6 | 4.5 | -1.0 | 2.6 | -0.1 |
| 797.6 | 8.0 | 0.3 | 797.3 | 10.0 | 0.7 | -0.2 | 2.0 | 0.4 |
| 865.8 | 6.5 | 0.0 | 866.5 | 8.0 | 0.2 | 0.7 | 1.5 | 0.2 |
| 996.9 | 0.1 | 0.0 | 999.5 | 0.0 | 0.5 | 2.6 | 0.0 | 0.5 |
| 1019.2 | 8.1 | 25.1 | 1015.9 | 12.1 | 44.6 | -3.4 | 4.1 | 19.4 |
| 1021.3 | 0.0 | 0.0 | 1025.0 | 0.0 | 0.2 | 3.7 | 0.0 | 0.2 |
| 1069.0 | 18.5 | 0.1 | 1083.2 | 31.9 | 0.8 | 14.2 | 13.4 | 0.7 |
| 1101.7 | 2.2 | 12.9 | 1108.0 | 1.8 | 18.2 | 6.3 | -0.4 | 5.3 |
| 1139.4 | 10.3 | 13.6 | 1154.3 | 11.5 | 45.0 | 14.8 | 1.2 | 31.5 |
| 1183.2 | 9.6 | 4.1 | 1182.8 | 9.6 | 3.3 | -0.4 | 0.0 | -0.8 |
| 1316.4 | 13.2 | 5.7 | 1322.0 | 12.0 | 4.1 | 5.6 | -1.2 | -1.6 |
| 1405.7 | 28.8 | 0.6 | 1408.7 | 29.0 | 2.7 | 3.0 | 0.1 | 2.1 |
| 1472.8 | 1.0 | 1.2 | 1473.6 | 3.7 | 3.3 | 0.8 | 2.7 | 2.1 |
| 1566.6 | 25.0 | 2.9 | 1571.4 | 26.4 | 4.4 | 4.9 | 1.4 | 1.6 |
| 1596.4 | 10.0 | 11.5 | 1599.6 | 39.5 | 48.3 | 3.2 | 29.4 | 36.7 |
| 3155.3 | 9.0 | 97.4 | 3167.4 | 6.5 | 153.1 | 12.1 | -2.6 | 55.7 |
| 3183.5 | 19.5 | 1.3 | 3194.0 | 4.8 | 119.8 | 10.5 | -14.7 | 118.4 |
| 3186.1 | 0.9 | 268.1 | 3199.1 | 6.4 | 157.6 | 13.0 | 5.5 | -110.4 |

[a] Frequencies ($\omega$) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

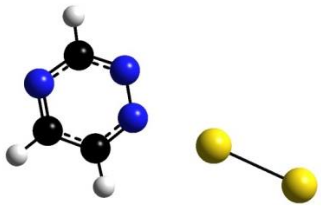


**Figure A-9.1:** **1**,2,4-Triazine/Ag$_2$ Complex

**Table A-9.2:** Harmonic Vibrational Frequencies for 1,2,4-Triazine and 1,**2**,4-Triazine/Ag$_2$ Complex[a]

| 1,2,4-Triazine | | | 1,**2**,4-Triazine/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 21.7 | 0.7 | 0.1 | | | |
| | | | 27.3 | 0.4 | 2.0 | | | |
| | | | 88.3 | 0.2 | 13.1 | | | |
| | | | 102.1 | 2.5 | 2.8 | | | |
| | | | 111.3 | 0.5 | 2.0 | | | |
| | | | 193.0 | 8.3 | 44.4 | | | |
| 322.2 | 13.1 | 0.2 | 326.6 | 7.3 | 4.8 | 4.4 | -5.8 | 4.6 |
| 388.1 | 12.9 | 0.1 | 399.2 | 13.4 | 0.4 | 11.1 | 0.5 | 0.3 |
| 637.3 | 2.1 | 2.2 | 642.1 | 3.6 | 2.4 | 4.9 | 1.5 | 0.1 |
| 731.0 | 3.0 | 4.5 | 736.2 | 5.3 | 5.1 | 5.2 | 2.3 | 0.6 |
| 797.6 | 8.0 | 0.3 | 790.3 | 5.7 | 0.8 | -7.3 | -2.3 | 0.5 |
| 865.8 | 6.5 | 0.0 | 873.3 | 9.1 | 0.9 | 7.5 | 2.6 | 0.9 |
| 996.9 | 0.1 | 0.0 | 999.7 | 0.1 | 0.1 | 2.9 | 0.1 | 0.1 |
| 1019.2 | 8.1 | 25.1 | 1024.6 | 30.6 | 37.0 | 5.4 | 22.5 | 11.9 |
| 1021.3 | 0.0 | 0.0 | 1026.8 | 0.0 | 0.0 | 5.5 | 0.0 | 0.0 |
| 1069.0 | 18.5 | 0.1 | 1072.0 | 22.2 | 1.2 | 3.0 | 3.7 | 1.1 |
| 1101.7 | 2.2 | 12.9 | 1110.1 | 2.1 | 12.3 | 8.4 | 0.0 | -0.6 |
| 1139.4 | 10.3 | 13.6 | 1149.6 | 5.9 | 74.4 | 10.1 | -4.4 | 60.8 |
| 1183.2 | 9.6 | 4.1 | 1192.5 | 8.2 | 0.7 | 9.2 | -1.4 | -3.4 |
| 1316.4 | 13.2 | 5.7 | 1321.1 | 15.1 | 4.4 | 4.7 | 1.9 | -1.3 |
| 1405.7 | 28.8 | 0.6 | 1409.2 | 26.0 | 3.3 | 3.4 | -2.9 | 2.7 |
| 1472.8 | 1.0 | 1.2 | 1477.4 | 3.6 | 7.3 | 4.6 | 2.7 | 6.1 |
| 1566.6 | 25.0 | 2.9 | 1576.4 | 18.6 | 28.5 | 9.8 | -6.4 | 25.6 |
| 1596.4 | 10.0 | 11.5 | 1595.6 | 21.3 | 37.8 | -0.8 | 11.3 | 26.2 |
| 3155.3 | 9.0 | 97.4 | 3165.4 | 5.6 | 127.6 | 10.1 | -3.4 | 30.2 |
| 3183.5 | 19.5 | 1.3 | 3192.8 | 9.0 | 122.8 | 9.3 | -10.5 | 121.4 |
| 3186.1 | 0.9 | 268.1 | 3196.0 | 0.7 | 181.4 | 9.9 | -0.3 | -86.6 |

[a] Frequencies (*ω*) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

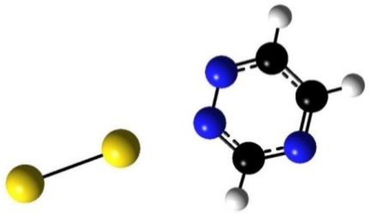


**Figure A-9.2:** 1,**2**,4-Triazine/Ag$_2$ Complex

**Table A-9.3:** Harmonic Vibrational Frequencies for 1,2,4-Triazine and 1,2,**4**-Triazine/$Ag_2$ Complex[a]

| 1,2,4-Triazine | | | 1,2,**4**-Triazine/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 22.2 | 0.4 | 0.1 | | | |
| | | | 24.9 | 0.5 | 2.6 | | | |
| | | | 86.3 | 4.2 | 7.6 | | | |
| | | | 97.9 | 3.5 | 3.4 | | | |
| | | | 114.6 | 4.2 | 0.9 | | | |
| | | | 192.7 | 6.7 | 43.4 | | | |
| 322.2 | 13.1 | 0.2 | 326.0 | 10.9 | 0.9 | 3.8 | -2.3 | -12.3 |
| 388.1 | 12.9 | 0.1 | 397.6 | 5.5 | 2.0 | 9.5 | -7.4 | -10.9 |
| 637.3 | 2.1 | 2.2 | 651.4 | 10.8 | 3.9 | 14.1 | 8.7 | 1.8 |
| 731.0 | 3.0 | 4.5 | 727.3 | 1.5 | 3.2 | -3.7 | -1.5 | 0.2 |
| 797.6 | 8.0 | 0.3 | 790.6 | 5.2 | 0.3 | -6.9 | -2.8 | -7.7 |
| 865.8 | 6.5 | 0.0 | 870.3 | 8.4 | 0.1 | 4.6 | 1.9 | -6.4 |
| 996.9 | 0.1 | 0.0 | 995.7 | 0.0 | 0.2 | -1.2 | 0.0 | 0.1 |
| 1019.2 | 8.1 | 25.1 | 1019.4 | 9.0 | 39.0 | 0.2 | 0.9 | 30.9 |
| 1021.3 | 0.0 | 0.0 | 1022.0 | 0.0 | 0.2 | 0.7 | 0.0 | 0.2 |
| 1069.0 | 18.5 | 0.1 | 1076.9 | 30.4 | 1.7 | 7.9 | 11.9 | -16.7 |
| 1101.7 | 2.2 | 12.9 | 1103.8 | 12.8 | 27.2 | 2.1 | 10.7 | 25.0 |
| 1139.4 | 10.3 | 13.6 | 1147.3 | 7.2 | 19.9 | 7.9 | -3.1 | 9.6 |
| 1183.2 | 9.6 | 4.1 | 1174.8 | 30.6 | 9.8 | -8.4 | 21.0 | 0.2 |
| 1316.4 | 13.2 | 5.7 | 1320.0 | 20.7 | 4.8 | 3.6 | 7.5 | -8.4 |
| 1405.7 | 28.8 | 0.6 | 1409.4 | 37.0 | 0.2 | 3.7 | 8.2 | -28.6 |
| 1472.8 | 1.0 | 1.2 | 1470.6 | 1.3 | 2.4 | -2.2 | 0.4 | 1.4 |
| 1566.6 | 25.0 | 2.9 | 1562.7 | 13.5 | 2.1 | -3.8 | -11.5 | -22.9 |
| 1596.4 | 10.0 | 11.5 | 1606.8 | 15.2 | 36.6 | 10.5 | 5.1 | 26.6 |
| 3155.3 | 9.0 | 97.4 | 3176.5 | 4.0 | 27.0 | 21.2 | -5.0 | 18.0 |
| 3183.5 | 19.5 | 1.3 | 3194.7 | 7.8 | 185.8 | 11.2 | -11.7 | 166.3 |
| 3186.1 | 0.9 | 268.1 | 3199.8 | 2.0 | 104.3 | 13.8 | 1.1 | 103.4 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

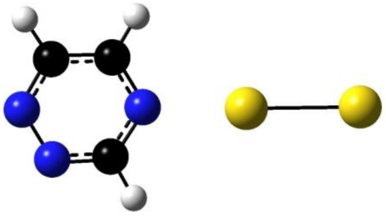


**Figure A-9.3:** 1,2,**4**-Triazine/$Ag_2$ Complex

**Table A-10.1:** Harmonic Vibrational Frequencies for 1H-1,2,3-Triazole and 1H-1,**2**,3-Triazole/Ag$_2$ Complex[a]

| 1H-1,2,3-Triazole | | | 1H-1,**2**,3-Triazole/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 25.7 | 2.5 | 1.8 | | | |
| | | | 26.5 | 0.0 | 0.2 | | | |
| | | | 92.0 | 1.5 | 9.4 | | | |
| | | | 107.9 | 0.2 | 4.4 | | | |
| | | | 117.1 | 15.8 | 3.8 | | | |
| | | | 194.1 | 10.2 | 36.6 | | | |
| 591.9 | 56.8 | 0.3 | 611.5 | 41.7 | 2.2 | 19.5 | -15.1 | 1.9 |
| 665.1 | 24.6 | 0.0 | 666.3 | 25.0 | 1.4 | 1.2 | 0.4 | 1.4 |
| 733.1 | 5.8 | 0.0 | 727.9 | 2.3 | 0.8 | -5.2 | -3.5 | 0.8 |
| 783.6 | 54.1 | 0.4 | 799.2 | 45.1 | 0.3 | 15.6 | -9.0 | -0.2 |
| 883.9 | 3.8 | 0.7 | 895.8 | 2.8 | 0.5 | 11.9 | -1.0 | -0.2 |
| 957.3 | 1.9 | 1.8 | 960.7 | 3.9 | 4.9 | 3.5 | 2.1 | 3.1 |
| 978.8 | 2.2 | 1.6 | 987.0 | 2.4 | 8.7 | 8.2 | 0.2 | 7.1 |
| 1036.1 | 26.2 | 4.3 | 1069.9 | 31.9 | 1.6 | 33.8 | 5.8 | -2.7 |
| 1104.3 | 32.1 | 0.4 | 1113.5 | 72.6 | 0.6 | 9.2 | 40.5 | 0.3 |
| 1125.2 | 0.6 | 5.7 | 1131.8 | 9.0 | 11.3 | 6.6 | 8.3 | 5.6 |
| 1178.7 | 11.8 | 23.3 | 1191.0 | 12.7 | 23.7 | 12.3 | 0.9 | 0.4 |
| 1280.8 | 12.3 | 23.1 | 1292.7 | 26.6 | 62.5 | 12.0 | 14.3 | 39.5 |
| 1379.7 | 1.9 | 5.8 | 1385.7 | 3.8 | 35.0 | 6.0 | 2.0 | 29.3 |
| 1456.8 | 0.1 | 6.2 | 1467.8 | 0.2 | 26.5 | 11.0 | 0.1 | 20.3 |
| 1541.9 | 5.8 | 8.5 | 1542.3 | 14.9 | 3.6 | 0.4 | 9.1 | -5.0 |
| 3267.0 | 0.9 | 63.5 | 3272.2 | 2.2 | 107.4 | 5.2 | 1.2 | 43.9 |
| 3287.1 | 0.1 | 102.5 | 3290.4 | 0.7 | 241.7 | 3.3 | 0.7 | 139.2 |
| 3635.4 | 80.0 | 110.6 | 3612.0 | 91.6 | 143.5 | -23.4 | 11.6 | 32.9 |

[a] Frequencies (*ω*) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

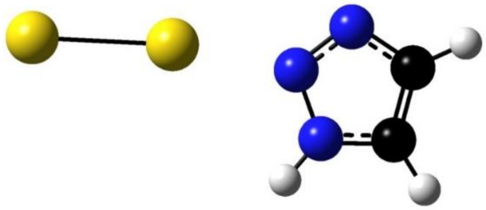


**Figure A-10.1:** 1H-1,**2**,3-Triazole/Ag$_2$ Complex

**Table A-10.2:** Harmonic Vibrational Frequencies for 1H-1,2,3-Triazole and 1H-1,2,**3**-Triazole/$Ag_2$ Complex[a]

| 1H-1,2,3-Triazole | | | 1H-1,2,**3**-Triazole/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 27.2 | 2.6 | 0.1 | | | |
| | | | 29.2 | 1.8 | 1.9 | | | |
| | | | 102.7 | 4.9 | 9.8 | | | |
| | | | 113.7 | 2.4 | 6.7 | | | |
| | | | 119.4 | 3.6 | 1.7 | | | |
| | | | 195.3 | 11.1 | 33.9 | | | |
| 591.9 | 56.8 | 0.3 | 623.0 | 38.0 | 0.6 | 31.0 | -18.8 | 0.3 |
| 665.1 | 24.6 | 0.0 | 669.8 | 33.7 | 1.2 | 4.7 | 9.1 | 1.2 |
| 733.1 | 5.8 | 0.0 | 732.4 | 11.7 | 0.0 | -0.7 | 5.9 | 0.0 |
| 783.6 | 54.1 | 0.4 | 792.2 | 45.6 | 0.1 | 8.7 | -8.5 | -0.4 |
| 883.9 | 3.8 | 0.7 | 893.7 | 2.6 | 1.3 | 9.8 | -1.2 | 0.6 |
| 957.3 | 1.9 | 1.8 | 970.5 | 1.9 | 3.7 | 13.3 | 0.1 | 1.9 |
| 978.8 | 2.2 | 1.6 | 990.1 | 0.6 | 6.1 | 11.3 | -1.5 | 4.5 |
| 1036.1 | 26.2 | 4.3 | 1074.9 | 32.4 | 7.2 | 38.7 | 6.2 | 2.9 |
| 1104.3 | 32.1 | 0.4 | 1109.2 | 61.0 | 0.2 | 4.9 | 28.9 | -0.2 |
| 1125.2 | 0.6 | 5.7 | 1143.6 | 2.0 | 9.7 | 18.3 | 1.4 | 4.0 |
| 1178.7 | 11.8 | 23.3 | 1195.6 | 3.8 | 44.8 | 16.9 | -8.0 | 21.5 |
| 1280.8 | 12.3 | 23.1 | 1283.1 | 35.2 | 27.6 | 2.3 | 22.8 | 4.6 |
| 1379.7 | 1.9 | 5.8 | 1392.5 | 4.1 | 7.6 | 12.8 | 2.2 | 1.8 |
| 1456.8 | 0.1 | 6.2 | 1461.5 | 2.4 | 13.5 | 4.6 | 2.2 | 7.3 |
| 1541.9 | 5.8 | 8.5 | 1552.6 | 8.5 | 9.5 | 10.7 | 2.7 | 1.0 |
| 3267.0 | 0.9 | 63.5 | 3276.4 | 4.3 | 57.9 | 9.4 | 3.3 | -5.7 |
| 3287.1 | 0.1 | 102.5 | 3293.8 | 1.6 | 181.4 | 6.7 | 1.5 | 78.9 |
| 3635.4 | 80.0 | 110.6 | 3625.4 | 113.2 | 390.5 | -10.0 | 33.2 | 279.9 |

[a] Frequencies ($\omega$) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

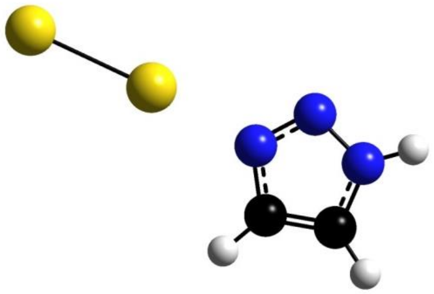


**Figure A-10.2:** 1H-1,2,**3**-Triazole/$Ag_2$ Complex

**Table A-11.1:** Harmonic Vibrational Frequencies for 1H-1,2,4-Triazole and 1H-1,**2**,4-Triazole/Ag$_2$ Complex[a]

| 1H-1,2,4-Triazole | | | 1H-1,**2**,4-Triazole/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 25.8 | 1.1 | 1.8 | | | |
| | | | 26.8 | 0.2 | 0.2 | | | |
| | | | 93.4 | 0.8 | 8.0 | | | |
| | | | 111.6 | 1.8 | 6.8 | | | |
| | | | 119.6 | 10.3 | 3.7 | | | |
| | | | 195.9 | 9.9 | 32.9 | | | |
| 570.9 | 71.1 | 0.2 | 577.0 | 60.9 | 2.7 | 6.1 | -10.3 | 2.5 |
| 683.2 | 1.4 | 0.0 | 679.0 | 1.5 | 0.6 | -4.2 | 0.1 | 0.5 |
| 701.5 | 45.0 | 0.1 | 692.7 | 31.5 | 1.3 | -8.8 | -13.6 | 1.2 |
| 865.6 | 18.1 | 0.3 | 881.5 | 15.0 | 0.2 | 15.9 | -3.1 | -0.1 |
| 912.1 | 8.6 | 0.1 | 921.9 | 6.0 | 0.0 | 9.8 | -2.6 | -0.1 |
| 961.1 | 5.2 | 0.3 | 962.9 | 7.5 | 1.9 | 1.8 | 2.3 | 1.7 |
| 992.3 | 18.2 | 0.6 | 1007.7 | 20.9 | 5.1 | 15.4 | 2.7 | 4.5 |
| 1077.1 | 36.9 | 4.1 | 1090.7 | 98.6 | 5.1 | 13.6 | 61.7 | 1.1 |
| 1139.1 | 15.3 | 4.9 | 1144.0 | 47.3 | 5.9 | 4.8 | 32.0 | 1.0 |
| 1179.4 | 12.5 | 9.1 | 1193.4 | 4.7 | 8.9 | 14.1 | -7.9 | -0.2 |
| 1277.9 | 0.6 | 21.3 | 1279.3 | 2.2 | 48.1 | 1.4 | 1.5 | 26.8 |
| 1318.1 | 23.0 | 2.9 | 1332.8 | 22.4 | 10.7 | 14.7 | -0.6 | 7.8 |
| 1387.6 | 10.2 | 29.7 | 1387.9 | 41.5 | 70.5 | 0.3 | 31.4 | 40.8 |
| 1462.5 | 19.9 | 6.3 | 1474.5 | 36.7 | 10.9 | 12.0 | 16.8 | 4.7 |
| 1551.2 | 25.8 | 0.2 | 1550.6 | 35.3 | 3.9 | -0.6 | 9.5 | 3.7 |
| 3253.2 | 1.4 | 37.3 | 3259.5 | 1.1 | 120.9 | 6.3 | -0.4 | 83.5 |
| 3258.8 | 1.5 | 133.9 | 3267.0 | 0.9 | 84.1 | 8.2 | -0.5 | -49.8 |
| 3640.6 | 77.6 | 110.3 | 3622.9 | 92.3 | 144.9 | -17.7 | 14.7 | 34.6 |

[a] Frequencies ($\omega$) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

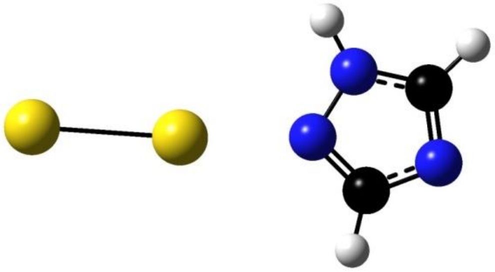


**Figure A-11.1:** 1H-1,**2**,4-Triazole/Ag$_2$ Complex

**Table A-11.2:** Harmonic Vibrational Frequencies for 1H-1,2,4-Triazole and 1H-1,2,**4**-Triazole/Ag$_2$ Complex[a]

| 1H-1,2,4-Triazole | | | 1H-1,2,**4**-Triazole/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 28.1 | 0.2 | 0.3 | | | |
| | | | 28.3 | 0.7 | 2.1 | | | |
| | | | 105.3 | 0.0 | 7.7 | | | |
| | | | 116.6 | 3.9 | 9.1 | | | |
| | | | 121.9 | 1.7 | 1.8 | | | |
| | | | 197.5 | 11.1 | 29.5 | | | |
| 570.9 | 71.1 | 0.2 | 600.4 | 60.7 | 1.0 | 29.5 | -10.4 | 0.8 |
| 683.2 | 1.4 | 0.0 | 682.8 | 1.7 | 0.2 | -0.4 | 0.4 | 0.1 |
| 701.5 | 45.0 | 0.1 | 699.2 | 43.7 | 0.6 | -2.4 | -1.3 | 0.5 |
| 865.6 | 18.1 | 0.3 | 875.6 | 12.4 | 0.3 | 9.9 | -5.8 | 0.0 |
| 912.1 | 8.6 | 0.1 | 912.7 | 9.4 | 0.3 | 0.6 | 0.8 | 0.2 |
| 961.1 | 5.2 | 0.3 | 978.2 | 5.1 | 1.7 | 17.0 | -0.1 | 1.4 |
| 992.3 | 18.2 | 0.6 | 995.1 | 20.6 | 4.1 | 2.8 | 2.4 | 3.5 |
| 1077.1 | 36.9 | 4.1 | 1075.9 | 62.1 | 7.2 | -1.2 | 25.2 | 3.1 |
| 1139.1 | 15.3 | 4.9 | 1158.2 | 17.6 | 4.6 | 19.0 | 2.3 | -0.3 |
| 1179.4 | 12.5 | 9.1 | 1174.4 | 53.2 | 19.0 | -5.0 | 40.7 | 9.9 |
| 1277.9 | 0.6 | 21.3 | 1284.4 | 2.1 | 28.1 | 6.5 | 1.4 | 6.8 |
| 1318.1 | 23.0 | 2.9 | 1318.6 | 15.7 | 1.8 | 0.5 | -7.3 | -1.1 |
| 1387.6 | 10.2 | 29.7 | 1400.2 | 3.6 | 25.3 | 12.5 | -6.6 | -4.4 |
| 1462.5 | 19.9 | 6.3 | 1482.1 | 38.5 | 8.7 | 19.6 | 18.7 | 2.5 |
| 1551.2 | 25.8 | 0.2 | 1561.3 | 74.9 | 1.7 | 10.1 | 49.1 | 1.5 |
| 3253.2 | 1.4 | 37.3 | 3268.1 | 4.4 | 17.4 | 14.8 | 3.0 | -20.0 |
| 3258.8 | 1.5 | 133.9 | 3273.3 | 5.0 | 86.3 | 14.5 | 3.6 | -47.6 |
| 3640.6 | 77.6 | 110.3 | 3634.7 | 118.6 | 335.6 | -5.9 | 41.0 | 225.3 |

[a] Frequencies (*ω*) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

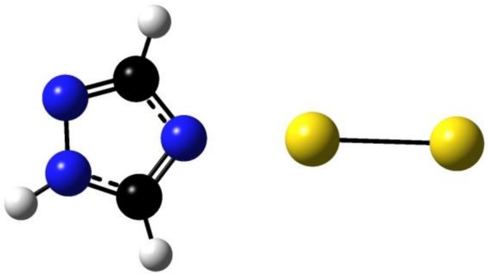


**Figure A-11.2:** 1H-1,2,**4**-Triazole/Ag$_2$ Complex

**Table A-12.1:** Harmonic Vibrational Frequencies for 2-Methylpyrazine and 2-Methylpyrazin/Ag$_2$ Complex (**N1**)[a]

| 2-Methylpyrazine | | | 2-Methylpyrazine/Ag$_2$ complex (**N1**) | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 23.1 | 0.1 | 0.1 | | | |
| | | | 27.0 | 0.0 | 3.4 | | | |
| 75.3 | 0.2 | 0.2 | 74.5 | 1.9 | 4.8 | -0.8 | 1.7 | 4.6 |
| | | | 90.9 | 0.3 | 3.3 | | | |
| | | | 97.8 | 2.1 | 3.9 | | | |
| | | | 110.1 | 1.4 | 3.4 | | | |
| | | | 193.9 | 8.7 | 35.9 | | | |
| 194.8 | 1.5 | 1.8 | 203.4 | 0.3 | 2.0 | 8.5 | -1.2 | 0.2 |
| 351.8 | 1.4 | 0.7 | 366.9 | 5.5 | 1.2 | 15.1 | 4.2 | 0.5 |
| 420.3 | 17.3 | 0.1 | 428.4 | 9.4 | 3.1 | 8.2 | -7.9 | 3.0 |
| 481.6 | 2.2 | 0.2 | 487.2 | 2.0 | 0.4 | 5.6 | -0.2 | 0.2 |
| 567.0 | 0.4 | 6.7 | 573.7 | 0.2 | 6.7 | 6.8 | -0.2 | 0.0 |
| 648.2 | 0.6 | 3.7 | 656.4 | 0.3 | 2.4 | 8.2 | -0.2 | -1.3 |
| 777.7 | 2.4 | 0.4 | 775.2 | 3.3 | 0.0 | -2.5 | 0.9 | -0.3 |
| 842.5 | 0.3 | 14.2 | 839.6 | 1.1 | 19.7 | -2.9 | 0.7 | 5.5 |
| 849.0 | 15.7 | 0.2 | 850.6 | 16.9 | 0.1 | 1.6 | 1.1 | -0.1 |
| 958.9 | 0.0 | 0.5 | 959.0 | 0.0 | 0.3 | 0.2 | 0.0 | -0.2 |
| 997.4 | 0.0 | 0.2 | 1000.4 | 0.2 | 0.9 | 3.0 | 0.1 | 0.6 |
| 1001.3 | 1.5 | 2.7 | 1007.9 | 4.1 | 2.5 | 6.6 | 2.6 | -0.2 |
| 1041.5 | 21.7 | 12.4 | 1053.3 | 48.3 | 9.6 | 11.8 | 26.6 | -2.9 |
| 1065.3 | 4.5 | 0.5 | 1066.2 | 3.8 | 0.3 | 1.0 | -0.7 | -0.2 |
| 1084.0 | 10.0 | 18.8 | 1090.6 | 6.0 | 33.3 | 6.6 | -3.9 | 14.4 |
| 1203.6 | 11.8 | 6.9 | 1206.7 | 14.0 | 6.1 | 3.0 | 2.1 | -0.8 |
| 1220.1 | 8.4 | 0.7 | 1216.7 | 16.5 | 5.7 | -3.4 | 8.2 | 5.0 |
| 1271.9 | 12.3 | 8.0 | 1274.1 | 3.2 | 20.8 | 2.2 | -9.1 | 12.7 |
| 1330.5 | 10.8 | 4.9 | 1334.6 | 22.9 | 7.9 | 4.1 | 12.2 | 3.0 |
| 1415.3 | 4.8 | 11.4 | 1420.0 | 5.6 | 9.9 | 4.6 | 0.9 | -1.4 |
| 1430.8 | 29.6 | 3.1 | 1432.7 | 21.6 | 4.3 | 1.9 | -8.0 | 1.2 |
| 1476.7 | 6.7 | 5.1 | 1475.8 | 13.8 | 3.5 | -0.9 | 7.0 | -1.6 |
| 1488.2 | 23.8 | 6.3 | 1485.9 | 58.0 | 1.8 | -2.3 | 34.1 | -4.5 |
| 1510.7 | 10.7 | 0.5 | 1513.1 | 9.4 | 3.6 | 2.3 | -1.3 | 3.2 |
| 1580.2 | 6.4 | 11.0 | 1576.9 | 2.6 | 8.8 | -3.3 | -3.8 | -2.2 |
| 1614.7 | 7.3 | 30.6 | 1622.0 | 2.1 | 21.4 | 7.4 | -5.2 | -9.2 |
| 3040.3 | 12.4 | 242.3 | 3040.9 | 2.7 | 208.2 | 0.6 | -9.7 | -34.1 |
| 3094.0 | 7.9 | 83.3 | 3094.2 | 2.7 | 36.4 | 0.2 | -5.3 | -47.0 |
| 3118.2 | 10.6 | 47.1 | 3123.7 | 18.0 | 77.5 | 5.5 | 7.5 | 30.4 |
| 3150.6 | 4.7 | 69.2 | 3163.9 | 17.5 | 157.6 | 13.4 | 12.9 | 88.4 |
| 3152.2 | 27.0 | 95.6 | 3171.3 | 0.9 | 83.3 | 19.1 | -26.1 | -12.3 |
| 3170.1 | 27.6 | 244.3 | 3188.4 | 15.4 | 194.6 | 18.3 | -12.2 | -49.7 |

[a] Frequencies (*ω*) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

**Table A-12.2:** Harmonic Vibrational Frequencies for 2-Methylpyrazine and 2-Methylpyrazine/$Ag_2$ Complex (**N4**)[a]

| 2-Methylpyrazine | | | 2-Methylpyrazine/$Ag_2$ complex (**N4**) | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 23.4 | 0.0 | 0.3 | | | |
| | | | 24.4 | 0.0 | 3.5 | | | |
| 75.3 | 0.2 | 0.2 | 71.8 | 0.0 | 1.4 | -3.5 | -0.2 | 1.2 |
| | | | 91.5 | 1.4 | 6.1 | | | |
| | | | 95.5 | 1.3 | 3.3 | | | |
| | | | 111.2 | 2.5 | 2.6 | | | |
| | | | 194.4 | 9.0 | 41.1 | | | |
| 194.8 | 1.5 | 1.8 | 196.4 | 2.0 | 1.4 | 1.6 | 0.5 | -0.4 |
| 351.8 | 1.4 | 0.7 | 358.7 | 3.6 | 0.6 | 7.0 | 2.3 | 0.0 |
| 420.3 | 17.3 | 0.1 | 424.9 | 11.2 | 0.8 | 4.6 | -6.1 | 0.7 |
| 481.6 | 2.2 | 0.2 | 493.3 | 0.9 | 1.1 | 11.7 | -1.3 | 0.9 |
| 567.0 | 0.4 | 6.7 | 567.5 | 0.7 | 5.2 | 0.6 | 0.3 | -1.5 |
| 648.2 | 0.6 | 3.7 | 662.7 | 5.1 | 4.0 | 14.5 | 4.5 | 0.4 |
| 777.7 | 2.4 | 0.4 | 771.8 | 1.1 | 0.1 | -5.9 | -1.3 | -0.2 |
| 842.5 | 0.3 | 14.2 | 849.1 | 3.1 | 15.3 | 6.6 | 2.7 | 1.1 |
| 849.0 | 15.7 | 0.2 | 852.9 | 15.6 | 0.5 | 3.9 | -0.2 | 0.2 |
| 958.9 | 0.0 | 0.5 | 953.5 | 0.0 | 0.1 | -5.3 | 0.0 | -0.4 |
| 997.4 | 0.0 | 0.2 | 999.9 | 0.0 | 0.8 | 2.5 | 0.0 | 0.6 |
| 1001.3 | 1.5 | 2.7 | 1004.7 | 1.7 | 6.7 | 3.4 | 0.2 | 3.9 |
| 1041.5 | 21.7 | 12.4 | 1045.5 | 16.3 | 38.4 | 4.0 | -5.4 | 26.0 |
| 1065.3 | 4.5 | 0.5 | 1066.5 | 4.4 | 1.2 | 1.2 | -0.1 | 0.7 |
| 1084.0 | 10.0 | 18.8 | 1091.7 | 32.3 | 21.0 | 7.7 | 22.3 | 2.1 |
| 1203.6 | 11.8 | 6.9 | 1200.4 | 47.9 | 9.3 | -3.2 | 36.1 | 2.4 |
| 1220.1 | 8.4 | 0.7 | 1221.6 | 15.7 | 1.5 | 1.5 | 7.3 | 0.8 |
| 1271.9 | 12.3 | 8.0 | 1275.7 | 16.4 | 9.8 | 3.8 | 4.1 | 1.8 |
| 1330.5 | 10.8 | 4.9 | 1332.5 | 6.9 | 6.5 | 2.0 | -3.9 | 1.6 |
| 1415.3 | 4.8 | 11.4 | 1417.7 | 7.0 | 15.6 | 2.4 | 2.2 | 4.2 |
| 1430.8 | 29.6 | 3.1 | 1435.2 | 37.6 | 3.8 | 4.4 | 8.0 | 0.7 |
| 1476.7 | 6.7 | 5.1 | 1476.2 | 7.0 | 5.1 | -0.5 | 0.3 | 0.0 |
| 1488.2 | 23.8 | 6.3 | 1488.9 | 29.8 | 6.6 | 0.7 | 5.9 | 0.3 |
| 1510.7 | 10.7 | 0.5 | 1511.6 | 8.9 | 0.5 | 0.9 | -1.7 | 0.0 |
| 1580.2 | 6.4 | 11.0 | 1580.1 | 16.9 | 17.5 | -0.1 | 10.4 | 6.4 |
| 1614.7 | 7.3 | 30.6 | 1625.0 | 10.2 | 24.8 | 10.3 | 2.9 | -5.8 |
| 3040.3 | 12.4 | 242.3 | 3044.0 | 7.6 | 305.0 | 3.8 | -4.8 | 62.7 |
| 3094.0 | 7.9 | 83.3 | 3099.3 | 4.7 | 100.6 | 5.3 | -3.2 | 17.3 |
| 3118.2 | 10.6 | 47.1 | 3124.2 | 8.6 | 54.1 | 6.0 | -2.0 | 7.0 |
| 3150.6 | 4.7 | 69.2 | 3165.7 | 8.4 | 132.2 | 15.2 | 3.7 | 63.0 |
| 3152.2 | 27.0 | 95.6 | 3180.4 | 10.5 | 43.9 | 28.2 | -16.5 | -51.7 |
| 3170.1 | 27.6 | 244.3 | 3192.7 | 13.9 | 146.8 | 22.6 | -13.7 | -97.5 |

[a] Frequencies (*ω*) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

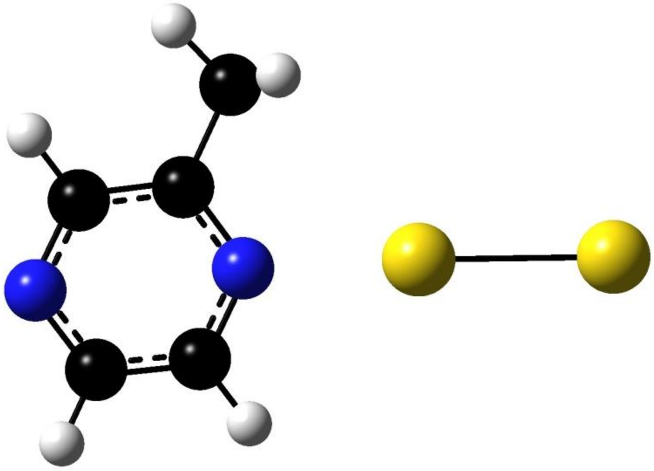


**Figure A-12.1:** 2-Methylpyrazine/$Ag_2$ Complex (**N1**)

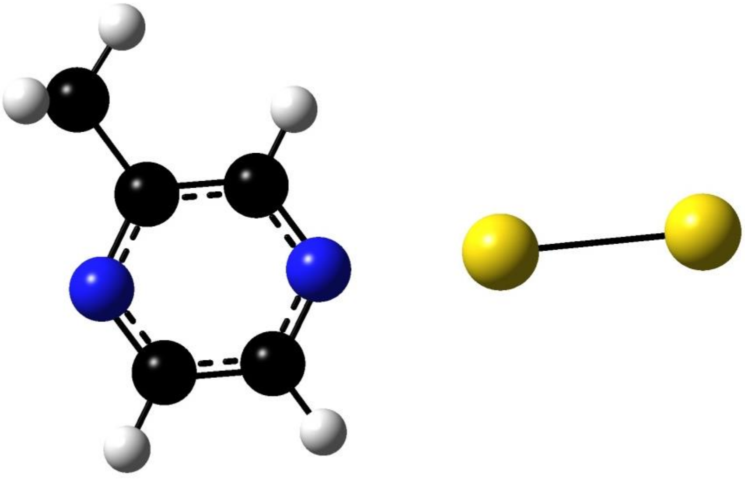


**Figure A-12.2:** 2-Methylpyrazine/$Ag_2$ Complex (**N4**)

**Table A-13.1:** Harmonic Vibrational Frequencies for 1,2,3,5-Tetrazine and **1**,2,3,5-Tetrazine/Ag$_2$ Complex[a]

| 1,2,3,5-Tetrazine | | | **1**,2,3,5-Tetrazine/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | $\Delta\ \omega$ | $\Delta$ IR | $\Delta$ Raman |
| | | | 15.0 | 0.0 | 0.5 | | | |
| | | | 25.4 | 0.6 | 2.1 | | | |
| | | | 78.3 | 0.0 | 17.2 | | | |
| | | | 91.0 | 3.4 | 1.2 | | | |
| | | | 105.2 | 3.1 | 1.6 | | | |
| | | | 190.4 | 6.5 | 47.0 | | | |
| 292.6 | 0.0 | 0.7 | 293.9 | 0.1 | 16.9 | 1.3 | 0.1 | 16.1 |
| 306.3 | 15.6 | 0.0 | 313.5 | 16.0 | 1.2 | 7.3 | 0.4 | 1.2 |
| 679.2 | 5.6 | 3.1 | 678.9 | 5.8 | 3.1 | -0.4 | 0.2 | 0.0 |
| 732.4 | 8.7 | 4.0 | 739.2 | 13.5 | 5.1 | 6.7 | 4.9 | 1.1 |
| 813.5 | 9.8 | 0.2 | 805.7 | 8.2 | 0.6 | -7.8 | -1.6 | 0.4 |
| 929.7 | 27.8 | 0.7 | 937.1 | 57.0 | 2.2 | 7.4 | 29.2 | 1.5 |
| 964.4 | 0.0 | 0.0 | 968.5 | 0.1 | 1.4 | 4.1 | 0.1 | 1.4 |
| 1018.8 | 0.4 | 27.7 | 1031.1 | 1.5 | 65.8 | 12.3 | 1.1 | 38.1 |
| 1040.4 | 0.0 | 0.0 | 1043.3 | 0.0 | 0.1 | 2.9 | 0.0 | 0.1 |
| 1143.5 | 4.7 | 9.0 | 1140.4 | 11.0 | 27.8 | -3.1 | 6.3 | 18.7 |
| 1184.6 | 7.6 | 0.4 | 1183.6 | 2.9 | 0.4 | -1.0 | -4.7 | 0.0 |
| 1201.0 | 1.6 | 9.3 | 1204.0 | 5.5 | 14.8 | 3.0 | 3.9 | 5.4 |
| 1397.7 | 37.8 | 1.6 | 1399.3 | 54.9 | 2.2 | 1.7 | 17.1 | 0.6 |
| 1415.5 | 24.8 | 1.4 | 1415.9 | 23.5 | 6.1 | 0.3 | -1.3 | 4.7 |
| 1526.1 | 98.7 | 1.3 | 1534.6 | 104.8 | 35.5 | 8.5 | 6.1 | 34.2 |
| 1580.1 | 30.4 | 6.1 | 1578.0 | 35.0 | 19.9 | -2.2 | 4.6 | 13.8 |
| 3178.3 | 12.4 | 53.9 | 3187.1 | 1.3 | 28.5 | 8.8 | -11.1 | -25.4 |
| 3181.5 | 1.6 | 171.6 | 3190.7 | 2.6 | 202.3 | 9.2 | 0.9 | 30.7 |

[a] Frequencies ($\omega$) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

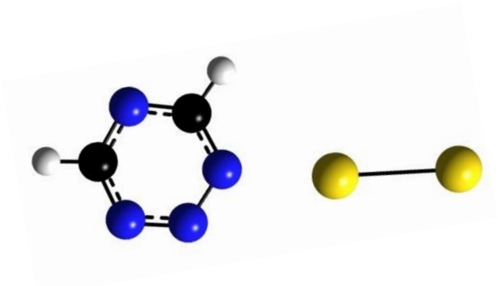


**Figure A-13.1:** **1**,2,3,5-Tetrazine/Ag$_2$ Complex

**Table A-13.2:** Harmonic Vibrational Frequencies for 1,2,3,5-Tetrazine and 1,**2**,3,5-Tetrazine/$Ag_2$ Complex[a]

| 1,2,3,5-Tetrazine | | | 1,**2**,3,5-Tetrazine/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 18.5 | 2.9 | 5.3 | | | |
| | | | 29.7 | 0.3 | 3.2 | | | |
| | | | 79.4 | 3.6 | 16.3 | | | |
| | | | 102.8 | 1.7 | 33.8 | | | |
| | | | 103.0 | 0.5 | 1.6 | | | |
| | | | 186.6 | 0.1 | 622.5 | | | |
| 292.6 | 0.0 | 0.7 | 303.2 | 0.0 | 2.6 | 10.6 | 0.0 | 1.9 |
| 306.3 | 15.6 | 0.0 | 338.3 | 47.1 | 22.6 | 32.1 | 31.4 | 22.5 |
| 679.2 | 5.6 | 3.1 | 685.0 | 23.9 | 206.3 | 5.8 | 18.3 | 203.2 |
| 732.4 | 8.7 | 4.0 | 732.1 | 12.6 | 5.0 | -0.4 | 3.9 | 1.0 |
| 813.5 | 9.8 | 0.2 | 810.9 | 23.4 | 217.3 | -2.7 | 13.6 | 217.1 |
| 929.7 | 27.8 | 0.7 | 964.5 | 8.5 | 74.2 | 34.8 | -19.3 | 73.5 |
| 964.4 | 0.0 | 0.0 | 965.2 | 19.5 | 19.2 | 0.8 | 19.5 | 19.2 |
| 1018.8 | 0.4 | 27.7 | 1008.6 | 50.8 | 5076.4 | -10.1 | 50.4 | 5048.7 |
| 1040.4 | 0.0 | 0.0 | 1040.5 | 0.0 | 0.2 | 0.1 | 0.0 | 0.2 |
| 1143.5 | 4.7 | 9.0 | 1154.7 | 12.9 | 1054.7 | 11.2 | 8.2 | 1045.7 |
| 1184.6 | 7.6 | 0.4 | 1194.4 | 2.9 | 11.3 | 9.8 | -4.7 | 10.8 |
| 1201.0 | 1.6 | 9.3 | 1194.5 | 9.5 | 6.3 | -6.5 | 7.9 | -3.1 |
| 1397.7 | 37.8 | 1.6 | 1386.4 | 508.2 | 11235.9 | -11.2 | 470.4 | 11234.4 |
| 1415.5 | 24.8 | 1.4 | 1414.6 | 26.9 | 0.6 | -1.0 | 2.2 | -0.8 |
| 1526.1 | 98.7 | 1.3 | 1511.0 | 85.8 | 4.0 | -15.2 | -13.0 | 2.7 |
| 1580.1 | 30.4 | 6.1 | 1568.3 | 420.8 | 11980.4 | -11.8 | 390.4 | 11974.2 |
| 3178.3 | 12.4 | 53.9 | 3186.7 | 6.2 | 181.8 | 8.4 | -6.2 | 127.9 |
| 3181.5 | 1.6 | 171.6 | 3189.8 | 5.3 | 340.8 | 8.3 | 3.6 | 169.1 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

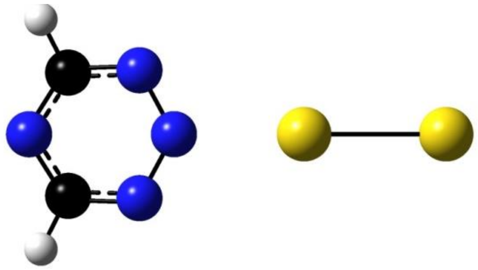


**Figure A-13.2:** 1,**2**,3,5-Tetrazine/$Ag_2$ Complex

**Table A-13.3:** Harmonic Vibrational Frequencies for 1,2,3,5-Tetrazine and 1,2,3,**5**-Tetrazine/Ag$_2$ Complex[a]

| 1,2,3,5-Tetrazine | | | 1,2,3,**5**-Tetrazine/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 18.9 | 1.3 | 0.1 | | | |
| | | | 23.7 | 0.5 | 2.5 | | | |
| | | | 81.1 | 8.4 | 8.0 | | | |
| | | | 89.8 | 3.4 | 1.8 | | | |
| | | | 109.0 | 5.9 | 0.8 | | | |
| | | | 191.3 | 5.3 | 46.6 | | | |
| 292.6 | 0.0 | 0.7 | 296.1 | 0.0 | 0.9 | 3.6 | 0.0 | 0.1 |
| 306.3 | 15.6 | 0.0 | 312.3 | 5.8 | 4.3 | 6.0 | -9.8 | 4.3 |
| 679.2 | 5.6 | 3.1 | 692.6 | 17.0 | 6.7 | 13.4 | 11.4 | 3.6 |
| 732.4 | 8.7 | 4.0 | 726.1 | 5.4 | 2.6 | -6.3 | -3.3 | -1.4 |
| 813.5 | 9.8 | 0.2 | 806.5 | 7.3 | 0.4 | -7.0 | -2.6 | 0.2 |
| 929.7 | 27.8 | 0.7 | 927.3 | 34.0 | 2.8 | -2.4 | 6.2 | 2.1 |
| 964.4 | 0.0 | 0.0 | 968.1 | 0.1 | 0.1 | 3.7 | 0.1 | 0.1 |
| 1018.8 | 0.4 | 27.7 | 1022.8 | 0.7 | 47.2 | 4.0 | 0.3 | 19.5 |
| 1040.4 | 0.0 | 0.0 | 1036.6 | 0.0 | 0.2 | -3.8 | 0.0 | 0.1 |
| 1143.5 | 4.7 | 9.0 | 1144.7 | 3.0 | 25.1 | 1.1 | -1.8 | 16.1 |
| 1184.6 | 7.6 | 0.4 | 1190.1 | 39.1 | 17.1 | 5.5 | 31.5 | 16.7 |
| 1201.0 | 1.6 | 9.3 | 1192.6 | 2.2 | 2.4 | -8.4 | 0.6 | -6.9 |
| 1397.7 | 37.8 | 1.6 | 1398.2 | 38.8 | 0.2 | 0.5 | 0.9 | -1.3 |
| 1415.5 | 24.8 | 1.4 | 1418.1 | 33.4 | 0.1 | 2.5 | 8.7 | -1.3 |
| 1526.1 | 98.7 | 1.3 | 1515.2 | 62.6 | 0.2 | -10.9 | -36.1 | -1.1 |
| 1580.1 | 30.4 | 6.1 | 1587.4 | 50.9 | 55.6 | 7.2 | 20.4 | 49.4 |
| 3178.3 | 12.4 | 53.9 | 3191.7 | 0.9 | 4.0 | 13.4 | -11.5 | -49.9 |
| 3181.5 | 1.6 | 171.6 | 3193.4 | 2.7 | 111.0 | 11.9 | 1.1 | -60.6 |

[a] Frequencies (*ω*) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

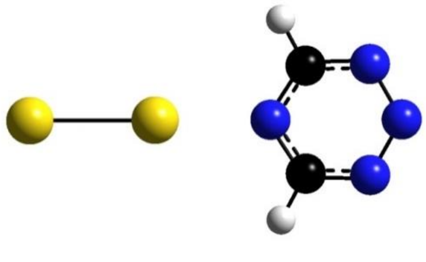


**Figure A-13.3:** 1,2,3,**5**-Tetrazine/Ag$_2$ Complex

**Table A-14:** Harmonic Vibrational Frequencies for Benzotriazole and Benzotriazole/$Ag_2$ Complex[a]

| Benzotriazole | | | Benzotriazole/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 20.0 | 0.1 | 3.2 | | | |
| | | | 21.1 | 0.0 | 0.2 | | | |
| | | | 70.3 | 0.4 | 11.3 | | | |
| | | | 75.2 | 1.0 | 2.8 | | | |
| | | | 104.8 | 3.6 | 3.4 | | | |
| | | | 194.1 | 9.7 | 41.4 | | | |
| 223.6 | 3.9 | 0.1 | 223.4 | 3.8 | 0.2 | -0.2 | -0.1 | 0.0 |
| 270.7 | 0.0 | 0.0 | 277.6 | 0.6 | 0.8 | 6.9 | 0.6 | 0.8 |
| 427.3 | 7.3 | 0.3 | 438.6 | 22.9 | 2.0 | 11.3 | 15.6 | 1.7 |
| 444.7 | 9.8 | 0.7 | 445.0 | 7.9 | 0.6 | 0.3 | -1.9 | -0.1 |
| 550.7 | 0.0 | 6.0 | 551.9 | 1.3 | 7.2 | 1.2 | 1.3 | 1.2 |
| 591.1 | 0.0 | 0.2 | 586.4 | 0.1 | 0.0 | -4.7 | 0.1 | -0.2 |
| 635.6 | 1.7 | 6.6 | 636.6 | 22.0 | 0.6 | 1.0 | 20.4 | -6.0 |
| 644.1 | 21.3 | 0.0 | 639.4 | 5.5 | 7.1 | -4.8 | -15.7 | 7.1 |
| 717.6 | 27.7 | 0.1 | 709.3 | 20.4 | 1.9 | -8.3 | -7.3 | 1.7 |
| 769.4 | 92.1 | 0.2 | 771.3 | 75.5 | 0.1 | 1.9 | -16.6 | 0.0 |
| 794.4 | 5.2 | 31.3 | 795.3 | 10.3 | 36.5 | 0.9 | 5.2 | 5.2 |
| 797.9 | 0.0 | 0.0 | 798.8 | 0.3 | 0.0 | 0.9 | 0.3 | 0.0 |
| 875.5 | 0.0 | 0.2 | 877.5 | 0.2 | 0.6 | 2.0 | 0.2 | 0.4 |
| 917.7 | 3.7 | 0.4 | 920.4 | 12.0 | 1.3 | 2.7 | 8.3 | 1.0 |
| 976.8 | 1.1 | 0.9 | 981.7 | 0.5 | 1.5 | 4.9 | -0.6 | 0.5 |
| 986.6 | 10.0 | 1.1 | 995.8 | 11.4 | 0.5 | 9.1 | 1.4 | -0.6 |
| 1008.3 | 0.0 | 0.7 | 1014.2 | 0.0 | 1.0 | 5.9 | 0.0 | 0.2 |
| 1019.7 | 0.0 | 34.9 | 1025.4 | 0.1 | 46.9 | 5.6 | 0.1 | 12.0 |
| 1152.0 | 7.3 | 7.8 | 1154.7 | 11.9 | 14.5 | 2.6 | 4.5 | 6.7 |
| 1165.3 | 4.7 | 4.5 | 1170.6 | 7.5 | 9.5 | 5.2 | 2.8 | 5.0 |
| 1187.5 | 7.7 | 16.0 | 1193.2 | 55.5 | 22.6 | 5.7 | 47.8 | 6.6 |
| 1218.4 | 70.8 | 2.5 | 1229.3 | 135.3 | 9.9 | 11.0 | 64.5 | 7.3 |
| 1271.2 | 7.6 | 1.0 | 1275.9 | 23.7 | 1.8 | 4.7 | 16.1 | 0.8 |
| 1328.9 | 2.2 | 10.3 | 1330.3 | 8.9 | 17.4 | 1.3 | 6.6 | 7.2 |
| 1357.1 | 8.2 | 0.7 | 1362.7 | 9.7 | 6.2 | 5.7 | 1.6 | 5.5 |
| 1417.5 | 5.0 | 60.6 | 1420.6 | 1.3 | 119.3 | 3.1 | -3.7 | 58.7 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-14 Continued**[a]

| Benzotriazole | | | Benzotriazole/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| 1476.0 | 0.2 | 49.2 | 1475.9 | 4.7 | 77.5 | 0.0 | 4.5 | 28.3 |
| 1489.7 | 1.7 | 3.0 | 1495.1 | 3.5 | 4.1 | 5.5 | 1.8 | 1.1 |
| 1541.3 | 0.3 | 9.1 | 1544.2 | 3.6 | 29.3 | 2.9 | 3.3 | 20.2 |
| 1592.6 | 7.3 | 47.3 | 1596.0 | 17.5 | 58.5 | 3.5 | 10.2 | 11.2 |
| 1662.8 | 0.0 | 1.0 | 1663.6 | 4.7 | 14.8 | 0.8 | 4.7 | 13.8 |
| 3172.8 | 2.8 | 52.5 | 3179.0 | 2.4 | 57.4 | 6.1 | -0.4 | 4.9 |
| 3185.5 | 6.9 | 113.2 | 3191.1 | 6.0 | 134.1 | 5.5 | -0.9 | 20.9 |
| 3200.6 | 9.1 | 15.6 | 3205.1 | 3.6 | 21.0 | 4.5 | -5.5 | 5.5 |
| 3203.8 | 6.1 | 297.9 | 3208.5 | 4.7 | 331.8 | 4.8 | -1.5 | 33.9 |
| 3620.3 | 162.1 | 142.3 | 3605.6 | 187.5 | 101.3 | -14.7 | 25.5 | -41.0 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-15:** Harmonic Vibrational Frequencies for Indazole and Indazole/$Ag_2$ Complex[a]

| Indazole | | | Indazole/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 18.8 | 0.0 | 0.1 | | | |
| | | | 21.2 | 0.1 | 1.3 | | | |
| | | | 67.7 | 0.1 | 10.2 | | | |
| | | | 93.1 | 0.6 | 4.0 | | | |
| | | | 98.6 | 3.8 | 4.7 | | | |
| | | | 194.3 | 10.6 | 46.5 | | | |
| 211.9 | 1.6 | 0.4 | 224.8 | 3.5 | 0.0 | 12.9 | 1.9 | -0.3 |
| 253.6 | 0.1 | 0.1 | 252.7 | 0.2 | 0.0 | -0.9 | 0.0 | -0.1 |
| 403.3 | 1.1 | 0.4 | 414.2 | 4.2 | 0.5 | 10.9 | 3.1 | 0.2 |
| 426.5 | 55.0 | 0.3 | 422.9 | 47.4 | 1.7 | -3.6 | -7.6 | 1.4 |
| 438.9 | 2.3 | 0.1 | 439.1 | 0.0 | 1.3 | 0.2 | -2.2 | 1.2 |
| 545.7 | 0.4 | 7.3 | 554.1 | 1.7 | 8.0 | 8.5 | 1.3 | 0.7 |
| 585.9 | 3.0 | 0.0 | 580.8 | 2.1 | 0.1 | -5.1 | -0.9 | 0.1 |
| 629.9 | 1.7 | 6.7 | 629.0 | 2.2 | 6.3 | -0.9 | 0.5 | -0.5 |
| 671.5 | 47.4 | 0.1 | 665.3 | 29.5 | 1.9 | -6.2 | -17.9 | 1.8 |
| 758.0 | 45.9 | 0.5 | 761.0 | 46.2 | 0.6 | 3.0 | 0.4 | 0.1 |
| 777.9 | 5.5 | 0.0 | 775.4 | 7.1 | 0.0 | -2.5 | 1.6 | 0.0 |
| 782.5 | 5.6 | 29.1 | 789.6 | 13.9 | 36.6 | 7.1 | 8.3 | 7.5 |
| 855.7 | 11.0 | 0.1 | 860.1 | 7.7 | 0.2 | 4.4 | -3.3 | 0.1 |
| 877.9 | 15.3 | 0.5 | 884.8 | 15.1 | 0.1 | 6.9 | -0.2 | -0.3 |
| 908.2 | 2.8 | 1.3 | 910.8 | 2.7 | 2.5 | 2.6 | -0.1 | 1.2 |
| 952.4 | 35.1 | 6.0 | 965.6 | 54.4 | 19.9 | 13.2 | 19.3 | 13.9 |
| 962.4 | 1.6 | 0.5 | 969.7 | 1.3 | 0.8 | 7.2 | -0.3 | 0.3 |
| 998.3 | 0.0 | 0.3 | 1005.6 | 0.0 | 0.3 | 7.3 | 0.0 | 0.0 |
| 1029.7 | 9.3 | 23.3 | 1030.3 | 13.1 | 36.6 | 0.6 | 3.8 | 13.3 |
| 1103.1 | 16.6 | 19.5 | 1109.8 | 77.4 | 50.2 | 6.8 | 60.8 | 30.7 |
| 1146.4 | 3.8 | 6.7 | 1150.0 | 7.6 | 9.3 | 3.6 | 3.8 | 2.6 |
| 1172.6 | 5.9 | 1.0 | 1175.5 | 7.5 | 3.6 | 2.9 | 1.6 | 2.6 |
| 1228.7 | 5.5 | 6.9 | 1236.9 | 3.0 | 25.7 | 8.2 | -2.5 | 18.7 |
| 1269.7 | 6.4 | 3.5 | 1272.6 | 13.0 | 3.5 | 3.0 | 6.6 | 0.0 |
| 1289.6 | 2.1 | 13.6 | 1291.0 | 5.0 | 20.1 | 1.4 | 2.9 | 6.6 |
| 1338.4 | 3.7 | 12.9 | 1348.7 | 10.0 | 32.0 | 10.3 | 6.4 | 19.2 |
| 1379.6 | 22.6 | 17.2 | 1384.8 | 34.3 | 34.5 | 5.2 | 11.7 | 17.3 |
| 1421.6 | 6.9 | 16.8 | 1425.0 | 19.5 | 32.5 | 3.5 | 12.7 | 15.7 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-15 Continued**[a]

| Indazole | | | Indazole/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | Δ ω | Δ IR | Δ Raman |
| 1452.7 | 5.6 | 36.2 | 1456.8 | 1.7 | 125.8 | 4.1 | -3.9 | 89.6 |
| 1521.2 | 3.4 | 38.5 | 1523.9 | 9.3 | 137.7 | 2.7 | 5.9 | 99.2 |
| 1535.8 | 12.2 | 15.2 | 1544.1 | 29.4 | 48.3 | 8.4 | 17.3 | 33.1 |
| 1619.8 | 1.0 | 13.1 | 1621.2 | 2.7 | 11.0 | 1.4 | 1.7 | -2.2 |
| 1659.5 | 14.8 | 7.0 | 1664.4 | 30.5 | 24.0 | 4.9 | 15.7 | 17.0 |
| 3169.8 | 0.1 | 36.0 | 3176.0 | 0.2 | 38.5 | 6.2 | 0.1 | 2.6 |
| 3177.4 | 3.0 | 122.6 | 3184.3 | 1.8 | 125.3 | 6.9 | -1.2 | 2.7 |
| 3187.0 | 20.7 | 38.6 | 3193.7 | 11.9 | 56.8 | 6.7 | -8.8 | 18.1 |
| 3196.0 | 11.8 | 289.5 | 3201.0 | 11.4 | 355.4 | 5.0 | -0.4 | 65.9 |
| 3237.0 | 3.5 | 119.6 | 3249.6 | 0.1 | 64.2 | 12.6 | -3.4 | -55.4 |
| 3660.1 | 89.3 | 119.8 | 3648.7 | 119.9 | 145.0 | -11.4 | 30.5 | 25.3 |

[a] Frequencies ($\omega$) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-16:** Harmonic Vibrational Frequencies for Benzimidazole and Benzimidazole/$Ag_2$ Complex[a]

| Benzimidazole | | | Benzimidazole/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 22.0 | 0.1 | 3.8 | | | |
| | | | 24.4 | 0.9 | 0.2 | | | |
| | | | 77.5 | 0.0 | 10.8 | | | |
| | | | 78.3 | 0.6 | 1.8 | | | |
| | | | 116.8 | 1.7 | 8.3 | | | |
| | | | 196.9 | 12.7 | 31.6 | | | |
| 221.6 | 7.8 | 0.0 | 222.9 | 8.5 | 0.1 | 1.2 | 0.7 | 0.1 |
| 256.8 | 3.8 | 0.1 | 269.1 | 1.1 | 0.4 | 12.3 | -2.7 | 0.3 |
| 420.1 | 8.1 | 0.2 | 431.4 | 14.1 | 0.4 | 11.3 | 6.0 | 0.3 |
| 432.2 | 17.6 | 0.4 | 433.2 | 9.9 | 0.3 | 1.0 | -7.7 | -0.1 |
| 460.4 | 72.4 | 0.4 | 502.2 | 69.4 | 1.3 | 41.8 | -3.1 | 0.9 |
| 553.2 | 0.3 | 5.3 | 554.4 | 1.3 | 5.1 | 1.2 | 1.1 | -0.1 |
| 594.3 | 3.4 | 0.1 | 592.0 | 3.2 | 0.0 | -2.3 | -0.2 | -0.1 |
| 630.8 | 0.1 | 5.4 | 637.7 | 0.6 | 4.1 | 7.0 | 0.5 | -1.3 |
| 652.1 | 2.0 | 0.3 | 651.9 | 5.0 | 0.4 | -0.2 | 3.0 | 0.1 |
| 757.7 | 71.8 | 0.7 | 762.0 | 66.5 | 0.2 | 4.2 | -5.3 | -0.5 |
| 787.8 | 3.7 | 0.3 | 790.5 | 2.9 | 0.2 | 2.7 | -0.8 | -0.1 |
| 791.8 | 4.5 | 33.2 | 791.8 | 5.8 | 41.2 | 0.0 | 1.3 | 8.0 |
| 862.5 | 2.2 | 1.1 | 869.9 | 1.4 | 0.3 | 7.4 | -0.9 | -0.9 |
| 877.3 | 8.5 | 0.4 | 880.6 | 6.1 | 0.9 | 3.3 | -2.4 | 0.5 |
| 893.4 | 2.8 | 0.4 | 898.3 | 6.7 | 1.1 | 4.9 | 3.9 | 0.7 |
| 947.6 | 1.3 | 3.4 | 962.0 | 1.2 | 0.7 | 14.5 | -0.2 | -2.7 |
| 955.2 | 2.7 | 0.3 | 967.7 | 5.3 | 0.8 | 12.5 | 2.6 | 0.5 |
| 995.4 | 0.0 | 0.1 | 1003.5 | 0.0 | 0.2 | 8.0 | 0.0 | 0.1 |
| 1029.6 | 5.6 | 24.3 | 1031.4 | 7.1 | 30.5 | 1.8 | 1.5 | 6.2 |
| 1096.7 | 18.3 | 12.7 | 1124.0 | 30.5 | 12.8 | 27.3 | 12.2 | 0.2 |
| 1133.4 | 1.8 | 2.7 | 1139.7 | 0.1 | 9.9 | 6.3 | -1.7 | 7.2 |
| 1171.9 | 1.9 | 4.4 | 1175.3 | 0.8 | 2.5 | 3.4 | -1.1 | -1.8 |
| 1206.3 | 1.0 | 3.1 | 1208.6 | 6.4 | 3.8 | 2.4 | 5.4 | 0.7 |
| 1273.3 | 22.0 | 48.4 | 1276.0 | 14.9 | 64.9 | 2.7 | -7.1 | 16.5 |
| 1288.2 | 30.7 | 15.8 | 1291.1 | 53.5 | 10.8 | 2.8 | 22.8 | -5.1 |
| 1336.6 | 7.7 | 16.8 | 1339.8 | 10.7 | 12.8 | 3.2 | 3.0 | -4.0 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-16 Continued[a]**

| Benzimidazole | | | Benzimidazole/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| 1380.0 | 24.9 | 34.2 | 1385.9 | 8.6 | 39.9 | 5.9 | -16.3 | 5.7 |
| 1420.0 | 28.4 | 25.0 | 1428.1 | 56.7 | 39.4 | 8.0 | 28.2 | 14.4 |
| 1480.2 | 23.8 | 8.3 | 1487.0 | 25.3 | 13.1 | 6.9 | 1.5 | 4.7 |
| 1522.6 | 5.9 | 6.7 | 1529.8 | 8.6 | 1.3 | 7.1 | 2.7 | -5.4 |
| 1534.6 | 24.0 | 50.6 | 1536.2 | 95.3 | 56.9 | 1.6 | 71.3 | 6.3 |
| 1622.9 | 3.5 | 17.9 | 1628.8 | 9.0 | 20.7 | 6.0 | 5.6 | 2.8 |
| 1661.1 | 7.3 | 5.2 | 1662.5 | 15.3 | 7.7 | 1.4 | 8.0 | 2.4 |
| 3170.2 | 0.0 | 46.6 | 3177.1 | 0.0 | 48.0 | 6.9 | 0.0 | 1.3 |
| 3179.4 | 9.4 | 105.0 | 3186.2 | 6.0 | 131.3 | 6.9 | -3.4 | 26.3 |
| 3190.9 | 16.2 | 91.5 | 3195.6 | 12.8 | 78.2 | 4.7 | -3.5 | -13.4 |
| 3199.5 | 9.0 | 245.9 | 3203.0 | 4.7 | 285.9 | 3.4 | -4.3 | 40.0 |
| 3234.4 | 1.3 | 127.5 | 3253.4 | 6.9 | 63.6 | 19.0 | 5.6 | -63.9 |
| 3648.3 | 64.0 | 136.7 | 3643.8 | 90.0 | 282.0 | -4.6 | 26.1 | 145.2 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-17.1:** Harmonic Vibrational Frequencies for Purine and Purine/$Ag_2$ Complex (**N3**)[a]

| Purine | | | Purine/$Ag_2$ Complex (**N3**) | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 22.4 | 1.1 | 3.7 | | | |
| | | | 22.4 | 1.2 | 0.1 | | | |
| | | | 69.4 | 2.6 | 1.5 | | | |
| | | | 75.2 | 0.1 | 10.7 | | | |
| | | | 109.3 | 0.4 | 5.1 | | | |
| | | | 193.3 | 10.5 | 37.7 | | | |
| 224.0 | 0.0 | 0.0 | 230.9 | 0.7 | 0.1 | 6.9 | 0.6 | 0.1 |
| 249.1 | 8.1 | 0.2 | 253.8 | 4.9 | 0.8 | 4.7 | -3.2 | 0.7 |
| 429.8 | 1.5 | 0.3 | 429.9 | 1.2 | 0.4 | 0.2 | -0.3 | 0.1 |
| 457.6 | 4.0 | 0.3 | 464.9 | 9.5 | 0.8 | 7.3 | 5.6 | 0.5 |
| 465.3 | 97.7 | 0.4 | 505.7 | 88.2 | 1.4 | 40.4 | -9.5 | 1.0 |
| 572.2 | 3.4 | 5.0 | 574.4 | 0.1 | 6.1 | 2.3 | -3.2 | 1.2 |
| 629.1 | 2.7 | 0.0 | 627.7 | 2.6 | 0.2 | -1.4 | -0.1 | 0.2 |
| 654.9 | 2.5 | 0.9 | 654.4 | 6.1 | 0.6 | -0.5 | 3.6 | -0.3 |
| 661.9 | 0.8 | 6.1 | 668.0 | 0.8 | 5.0 | 6.0 | 0.0 | -1.1 |
| 803.9 | 5.8 | 25.8 | 804.5 | 13.0 | 35.3 | 0.6 | 7.2 | 9.5 |
| 832.7 | 10.4 | 0.0 | 832.4 | 9.6 | 0.1 | -0.3 | -0.8 | 0.0 |
| 901.4 | 12.6 | 0.4 | 907.3 | 8.9 | 0.6 | 5.9 | -3.7 | 0.1 |
| 908.2 | 22.7 | 0.8 | 910.1 | 37.2 | 0.4 | 1.9 | 14.6 | -0.4 |
| 931.1 | 8.2 | 0.4 | 934.9 | 7.1 | 0.5 | 3.7 | -1.2 | 0.0 |
| 944.6 | 2.9 | 5.2 | 964.0 | 4.9 | 3.9 | 19.4 | 2.0 | -1.3 |
| 992.8 | 0.2 | 0.0 | 998.5 | 0.2 | 0.0 | 5.8 | 0.0 | 0.0 |
| 1097.4 | 18.8 | 12.8 | 1123.9 | 23.3 | 15.5 | 26.6 | 4.5 | 2.7 |
| 1134.8 | 6.0 | 16.6 | 1135.8 | 10.8 | 20.9 | 1.0 | 4.8 | 4.3 |
| 1200.5 | 4.2 | 2.8 | 1201.7 | 5.8 | 2.1 | 1.2 | 1.6 | -0.7 |
| 1257.3 | 13.8 | 3.8 | 1255.1 | 22.4 | 7.3 | -2.2 | 8.6 | 3.5 |
| 1290.4 | 39.5 | 25.3 | 1295.1 | 32.8 | 51.1 | 4.7 | -6.7 | 25.8 |
| 1318.7 | 1.6 | 8.6 | 1316.9 | 17.1 | 11.8 | -1.8 | 15.5 | 3.2 |
| 1369.1 | 12.3 | 30.9 | 1367.3 | 11.1 | 23.8 | -1.8 | -1.2 | -7.0 |
| 1402.8 | 152.0 | 44.2 | 1412.7 | 197.1 | 41.2 | 9.9 | 45.1 | -3.0 |
| 1423.3 | 52.5 | 4.3 | 1431.7 | 29.3 | 6.8 | 8.4 | -23.3 | 2.5 |
| 1493.5 | 13.1 | 1.8 | 1498.8 | 32.1 | 3.5 | 5.4 | 19.0 | 1.7 |
| 1524.5 | 39.2 | 28.2 | 1525.7 | 53.1 | 31.9 | 1.2 | 13.9 | 3.6 |
| 1591.9 | 57.2 | 6.8 | 1603.7 | 43.2 | 15.1 | 11.8 | -14.0 | 8.3 |
| 1646.0 | 48.5 | 4.6 | 1643.0 | 121.6 | 9.6 | -3.1 | 73.1 | 5.0 |
| 3145.7 | 18.2 | 120.4 | 3153.6 | 14.9 | 177.1 | 7.8 | -3.3 | 56.8 |
| 3173.1 | 15.1 | 142.6 | 3184.1 | 9.6 | 134.1 | 11.0 | -5.5 | -8.5 |
| 3236.7 | 0.7 | 119.1 | 3252.1 | 8.8 | 60.4 | 15.4 | 8.1 | -58.8 |
| 3639.4 | 72.8 | 150.6 | 3632.5 | 99.2 | 317.3 | -6.9 | 26.4 | 166.8 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-17.2:** Harmonic Vibrational Frequencies for Purine and Purine/$Ag_2$ Complex (**N5**)[a]

| Purine | | | Purine/$Ag_2$ Complex (**N5**) | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 21.9 | 1.7 | 0.0 | | | |
| | | | 24.4 | 0.8 | 4.4 | | | |
| | | | 73.6 | 0.3 | 0.8 | | | |
| | | | 78.1 | 2.2 | 11.6 | | | |
| | | | 102.7 | 3.2 | 3.6 | | | |
| | | | 191.6 | 10.7 | 41.1 | | | |
| 224.0 | 0.0 | 0.0 | 228.3 | 0.0 | 0.1 | 4.4 | 0.0 | 0.1 |
| 249.1 | 8.1 | 0.2 | 249.3 | 7.1 | 0.0 | 0.2 | -0.9 | -0.1 |
| 429.8 | 1.5 | 0.3 | 439.5 | 4.7 | 0.7 | 9.7 | 3.2 | 0.4 |
| 457.6 | 4.0 | 0.3 | 463.1 | 7.5 | 0.1 | 5.5 | 3.5 | -0.2 |
| 465.3 | 97.7 | 0.4 | 490.1 | 93.9 | 1.0 | 24.8 | -3.8 | 0.6 |
| 572.2 | 3.4 | 5.0 | 580.3 | 10.8 | 4.7 | 8.2 | 7.5 | -0.3 |
| 629.1 | 2.7 | 0.0 | 629.1 | 2.0 | 1.0 | -0.1 | -0.7 | 1.0 |
| 654.9 | 2.5 | 0.9 | 651.9 | 2.9 | 1.0 | -3.0 | 0.4 | 0.1 |
| 661.9 | 0.8 | 6.1 | 661.0 | 1.7 | 8.6 | -0.9 | 1.0 | 2.5 |
| 803.9 | 5.8 | 25.8 | 818.7 | 22.2 | 37.3 | 14.7 | 16.3 | 11.6 |
| 832.7 | 10.4 | 0.0 | 829.1 | 8.0 | 0.4 | -3.6 | -2.3 | 0.3 |
| 901.4 | 12.6 | 0.4 | 911.0 | 10.6 | 0.3 | 9.6 | -2.0 | -0.1 |
| 908.2 | 22.7 | 0.8 | 914.5 | 17.7 | 2.8 | 6.3 | -5.0 | 2.0 |
| 931.1 | 8.2 | 0.4 | 937.6 | 7.5 | 0.3 | 6.5 | -0.8 | -0.2 |
| 944.6 | 2.9 | 5.2 | 947.8 | 5.4 | 9.5 | 3.2 | 2.5 | 4.3 |
| 992.8 | 0.2 | 0.0 | 994.3 | 0.0 | 0.2 | 1.5 | -0.2 | 0.2 |
| 1097.4 | 18.8 | 12.8 | 1101.2 | 25.5 | 11.0 | 3.8 | 6.6 | -1.8 |
| 1134.8 | 6.0 | 16.6 | 1144.4 | 8.1 | 20.7 | 9.6 | 2.1 | 4.1 |
| 1200.5 | 4.2 | 2.8 | 1210.0 | 6.3 | 5.8 | 9.5 | 2.1 | 3.0 |
| 1257.3 | 13.8 | 3.8 | 1262.9 | 3.9 | 8.9 | 5.7 | -10.0 | 5.1 |
| 1290.4 | 39.5 | 25.3 | 1295.6 | 50.5 | 30.6 | 5.2 | 11.0 | 5.3 |
| 1318.7 | 1.6 | 8.6 | 1324.9 | 6.2 | 14.7 | 6.2 | 4.7 | 6.1 |
| 1369.1 | 12.3 | 30.9 | 1366.3 | 53.8 | 39.0 | -2.8 | 41.5 | 8.1 |
| 1402.8 | 152.0 | 44.2 | 1410.9 | 139.8 | 54.3 | 8.1 | -12.2 | 10.1 |
| 1423.3 | 52.5 | 4.3 | 1425.1 | 65.8 | 3.7 | 1.8 | 13.3 | -0.6 |
| 1493.5 | 13.1 | 1.8 | 1492.3 | 38.0 | 5.6 | -1.2 | 24.9 | 3.8 |
| 1524.5 | 39.2 | 28.2 | 1520.3 | 42.9 | 20.3 | -4.2 | 3.7 | -7.9 |
| 1591.9 | 57.2 | 6.8 | 1602.1 | 96.8 | 19.1 | 10.2 | 39.5 | 12.3 |
| 1646.0 | 48.5 | 4.6 | 1647.0 | 48.3 | 11.9 | 1.0 | -0.2 | 7.3 |
| 3145.7 | 18.2 | 120.4 | 3157.5 | 12.8 | 165.1 | 11.8 | -5.4 | 44.8 |
| 3173.1 | 15.1 | 142.6 | 3193.4 | 1.0 | 71.7 | 20.3 | -14.1 | -70.9 |
| 3236.7 | 0.7 | 119.1 | 3242.7 | 1.0 | 125.2 | 6.0 | 0.3 | 6.1 |
| 3639.4 | 72.8 | 150.6 | 3636.0 | 105.4 | 227.1 | -3.4 | 32.6 | 76.5 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-17.3:** Harmonic Vibrational Frequencies for Purine and Purine/$Ag_2$ Complex (**N7**)[a]

| Purine | | | Purine/$Ag_2$ Complex (**N7**) | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 21.1 | 0.9 | 0.1 | | | |
| | | | 22.5 | 1.0 | 2.5 | | | |
| | | | 71.2 | 1.2 | 8.9 | | | |
| | | | 92.9 | 0.6 | 5.2 | | | |
| | | | 103.3 | 7.3 | 2.1 | | | |
| | | | 193.6 | 10.7 | 45.4 | | | |
| 224.0 | 0.0 | 0.0 | 239.1 | 0.1 | 0.4 | 15.2 | 0.1 | 0.4 |
| 249.1 | 8.1 | 0.2 | 251.7 | 8.9 | 0.1 | 2.6 | 0.8 | -0.1 |
| 429.8 | 1.5 | 0.3 | 430.9 | 0.2 | 0.9 | 1.1 | -1.4 | 0.6 |
| 457.6 | 4.0 | 0.3 | 464.2 | 5.3 | 0.9 | 6.6 | 1.3 | 0.7 |
| 465.3 | 97.7 | 0.4 | 483.7 | 93.5 | 0.6 | 18.4 | -4.2 | 0.2 |
| 572.2 | 3.4 | 5.0 | 585.6 | 10.3 | 4.7 | 13.5 | 6.9 | -0.3 |
| 629.1 | 2.7 | 0.0 | 629.8 | 0.9 | 0.7 | 0.7 | -1.8 | 0.7 |
| 654.9 | 2.5 | 0.9 | 651.5 | 1.6 | 0.2 | -3.4 | -0.9 | -0.7 |
| 661.9 | 0.8 | 6.1 | 666.4 | 1.9 | 3.0 | 4.5 | 1.1 | -3.1 |
| 803.9 | 5.8 | 25.8 | 806.5 | 2.9 | 42.8 | 2.6 | -3.0 | 17.0 |
| 832.7 | 10.4 | 0.0 | 832.0 | 9.1 | 0.6 | -0.7 | -1.3 | 0.6 |
| 901.4 | 12.6 | 0.4 | 912.1 | 10.4 | 0.4 | 10.7 | -2.2 | 0.0 |
| 908.2 | 22.7 | 0.8 | 924.8 | 40.9 | 2.3 | 16.6 | 18.2 | 1.5 |
| 931.1 | 8.2 | 0.4 | 937.8 | 8.5 | 2.4 | 6.7 | 0.3 | 2.0 |
| 944.6 | 2.9 | 5.2 | 945.5 | 10.2 | 4.8 | 0.9 | 7.3 | -0.4 |
| 992.8 | 0.2 | 0.0 | 987.7 | 0.2 | 0.2 | -5.1 | 0.0 | 0.2 |
| 1097.4 | 18.8 | 12.8 | 1098.1 | 20.2 | 14.0 | 0.7 | 1.4 | 1.1 |
| 1134.8 | 6.0 | 16.6 | 1127.7 | 58.4 | 28.6 | -7.0 | 52.4 | 12.0 |
| 1200.5 | 4.2 | 2.8 | 1201.6 | 10.2 | 14.3 | 1.1 | 6.0 | 11.5 |
| 1257.3 | 13.8 | 3.8 | 1264.0 | 19.9 | 20.4 | 6.7 | 6.1 | 16.6 |
| 1290.4 | 39.5 | 25.3 | 1291.1 | 46.9 | 42.4 | 0.7 | 7.4 | 17.1 |
| 1318.7 | 1.6 | 8.6 | 1323.2 | 1.7 | 25.3 | 4.5 | 0.1 | 16.7 |
| 1369.1 | 12.3 | 30.9 | 1375.4 | 28.2 | 55.7 | 6.4 | 15.9 | 24.8 |
| 1402.8 | 152.0 | 44.2 | 1408.5 | 190.5 | 77.8 | 5.7 | 38.5 | 33.6 |
| 1423.3 | 52.5 | 4.3 | 1429.8 | 87.8 | 9.1 | 6.5 | 35.2 | 4.8 |
| 1493.5 | 13.1 | 1.8 | 1498.5 | 17.7 | 1.6 | 5.0 | 4.6 | -0.2 |
| 1524.5 | 39.2 | 28.2 | 1526.5 | 51.5 | 82.9 | 2.0 | 12.3 | 54.6 |
| 1591.9 | 57.2 | 6.8 | 1587.1 | 33.2 | 4.8 | -4.8 | -24.0 | -2.0 |
| 1646.0 | 48.5 | 4.6 | 1659.9 | 87.2 | 11.0 | 13.9 | 38.7 | 6.3 |
| 3145.7 | 18.2 | 120.4 | 3173.5 | 9.7 | 60.7 | 27.8 | -8.5 | -59.7 |
| 3173.1 | 15.1 | 142.6 | 3191.0 | 1.2 | 73.8 | 17.9 | -13.9 | -68.8 |
| 3236.7 | 0.7 | 119.1 | 3240.0 | 0.8 | 164.3 | 3.3 | 0.1 | 45.2 |
| 3639.4 | 72.8 | 150.6 | 3634.4 | 86.0 | 147.1 | -5.0 | 13.2 | -3.5 |

[a] Frequencies ($\omega$) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

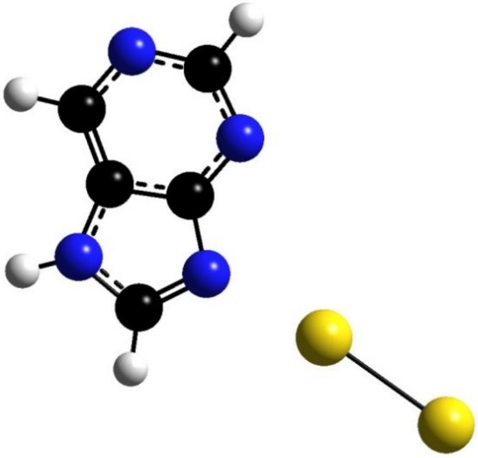


**Figure A-17.1:** Purine/$Ag_2$ Complex (**N3**)

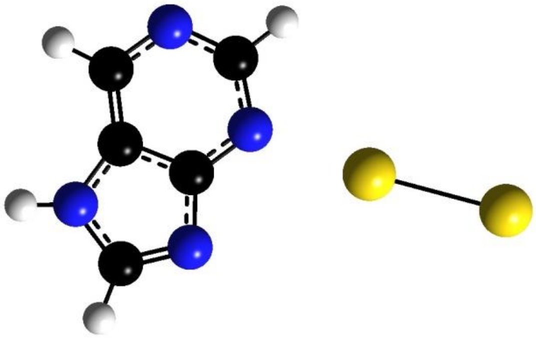


**Figure A-17.2:** Purine/$Ag_2$ Complex (**N5**)

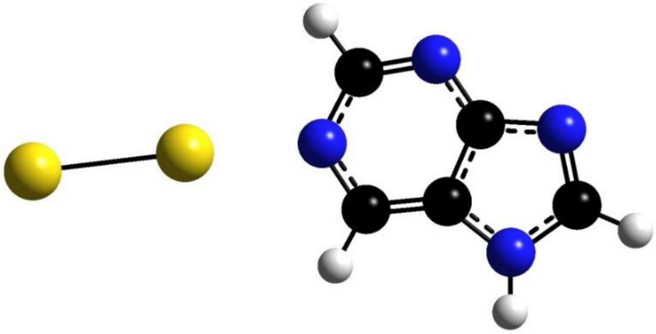


**Figure A-17.3:** Purine/$Ag_2$ Complex (**N7**)

**Table A-18:** Harmonic Vibrational Frequencies for Quinoline and Quinoline/$Ag_2$ Complex[a]

| Quinoline | | | Quinoline/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 23.3 | 0.2 | 0.2 | | | |
| | | | 24.1 | 0.0 | 5.3 | | | |
| | | | 69.1 | 0.0 | 10.4 | | | |
| | | | 83.5 | 0.9 | 1.6 | | | |
| | | | 110.2 | 1.9 | 7.0 | | | |
| 174.4 | 4.5 | 0.1 | 179.2 | 3.0 | 0.3 | 4.8 | -1.5 | 0.2 |
| 183.4 | 0.1 | 0.0 | 190.0 | 0.1 | 0.3 | 6.6 | 0.0 | 0.3 |
| | | | 194.2 | 11.2 | 36.6 | | | |
| 383.6 | 4.4 | 0.2 | 395.3 | 10.0 | 0.4 | 11.7 | 5.6 | 0.2 |
| 404.3 | 1.7 | 1.4 | 406.7 | 0.5 | 1.0 | 2.5 | -1.2 | -0.5 |
| 483.2 | 0.1 | 0.0 | 483.4 | 0.4 | 0.5 | 0.2 | 0.3 | 0.5 |
| 492.8 | 8.0 | 0.0 | 500.5 | 9.3 | 0.0 | 7.6 | 1.3 | 0.0 |
| 529.3 | 0.1 | 13.8 | 529.3 | 0.9 | 11.6 | 0.0 | 0.9 | -2.2 |
| 531.5 | 0.2 | 8.1 | 535.6 | 1.4 | 12.2 | 4.1 | 1.2 | 4.1 |
| 627.5 | 5.8 | 0.1 | 639.9 | 10.7 | 1.4 | 12.4 | 4.9 | 1.3 |
| 650.2 | 0.8 | 0.1 | 648.9 | 0.1 | 0.3 | -1.3 | -0.7 | 0.2 |
| 751.6 | 9.1 | 0.7 | 755.1 | 6.3 | 0.1 | 3.5 | -2.7 | -0.6 |
| 772.3 | 2.0 | 46.6 | 780.1 | 11.4 | 46.2 | 7.8 | 9.5 | -0.4 |
| 812.0 | 27.5 | 0.0 | 812.2 | 36.0 | 0.1 | 0.3 | 8.5 | 0.1 |
| 825.7 | 62.4 | 0.1 | 829.6 | 44.3 | 0.5 | 3.9 | -18.1 | 0.4 |
| 832.5 | 0.9 | 0.1 | 831.0 | 0.9 | 0.6 | -1.5 | 0.0 | 0.5 |
| 894.6 | 0.1 | 0.2 | 898.4 | 0.4 | 0.6 | 3.7 | 0.3 | 0.4 |
| 956.6 | 3.6 | 0.4 | 965.1 | 11.3 | 2.0 | 8.5 | 7.7 | 1.6 |
| 974.2 | 0.0 | 0.3 | 980.7 | 0.0 | 0.8 | 6.4 | 0.0 | 0.5 |
| 983.9 | 1.5 | 0.9 | 988.8 | 0.5 | 1.4 | 4.9 | -1.0 | 0.4 |
| 1009.2 | 1.6 | 0.1 | 1014.6 | 0.7 | 0.1 | 5.4 | -0.9 | -0.1 |
| 1013.8 | 0.0 | 0.3 | 1020.3 | 0.1 | 1.1 | 6.4 | 0.0 | 0.8 |
| 1036.6 | 2.9 | 10.6 | 1042.0 | 4.2 | 20.7 | 5.4 | 1.3 | 10.1 |
| 1053.9 | 3.6 | 28.7 | 1069.3 | 2.7 | 26.8 | 15.4 | -0.9 | -1.8 |
| 1144.4 | 8.3 | 3.1 | 1151.7 | 11.9 | 2.3 | 7.3 | 3.7 | -0.8 |
| 1165.7 | 2.2 | 5.8 | 1170.3 | 1.9 | 10.3 | 4.6 | -0.2 | 4.5 |
| 1173.0 | 0.7 | 1.0 | 1179.4 | 1.7 | 4.7 | 6.4 | 1.0 | 3.7 |
| 1237.5 | 0.3 | 0.6 | 1239.5 | 3.3 | 2.7 | 2.0 | 3.0 | 2.0 |

[a] Frequencies ($\omega$) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-18 Continued**[a]

| Quinoline | | | Quinoline/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | Δ ω | Δ IR | Δ Raman |
| 1263.0 | 0.8 | 1.6 | 1264.8 | 11.5 | 5.7 | 1.7 | 10.7 | 4.1 |
| 1287.6 | 0.6 | 3.7 | 1292.8 | 2.2 | 13.0 | 5.2 | 1.6 | 9.3 |
| 1359.2 | 7.8 | 4.0 | 1356.5 | 21.2 | 23.6 | -2.7 | 13.4 | 19.6 |
| 1387.3 | 4.7 | 125.2 | 1391.4 | 10.8 | 158.6 | 4.1 | 6.1 | 33.4 |
| 1423.0 | 2.2 | 20.0 | 1428.7 | 5.5 | 8.3 | 5.6 | 3.3 | -11.7 |
| 1470.3 | 5.4 | 70.6 | 1475.1 | 1.4 | 46.8 | 4.8 | -4.0 | -23.8 |
| 1501.8 | 1.6 | 8.0 | 1502.2 | 15.2 | 10.4 | 0.3 | 13.6 | 2.4 |
| 1540.0 | 25.7 | 3.4 | 1544.9 | 48.3 | 4.9 | 4.8 | 22.7 | 1.6 |
| 1603.4 | 13.3 | 32.5 | 1611.8 | 23.2 | 46.8 | 8.5 | 9.9 | 14.3 |
| 1639.6 | 12.5 | 3.4 | 1637.3 | 4.6 | 5.0 | -2.3 | -7.9 | 1.6 |
| 1660.1 | 7.5 | 12.9 | 1660.7 | 8.5 | 13.6 | 0.6 | 1.0 | 0.8 |
| 3138.2 | 22.6 | 149.8 | 3167.0 | 3.1 | 74.6 | 28.8 | -19.5 | -75.1 |
| 3161.8 | 0.8 | 23.2 | 3168.5 | 2.3 | 20.9 | 6.7 | 1.5 | -2.3 |
| 3165.5 | 8.4 | 99.1 | 3171.7 | 0.3 | 141.2 | 6.2 | -8.1 | 42.0 |
| 3174.0 | 9.3 | 101.1 | 3174.7 | 3.6 | 167.2 | 0.7 | -5.7 | 66.1 |
| 3188.4 | 16.2 | 130.9 | 3185.2 | 10.8 | 47.2 | -3.2 | -5.4 | -83.7 |
| 3192.6 | 15.9 | 230.2 | 3197.4 | 13.2 | 353.7 | 4.8 | -2.6 | 123.5 |
| 3199.1 | 8.8 | 230.1 | 3203.6 | 10.1 | 293.1 | 4.5 | 1.2 | 63.0 |

[a] Frequencies ($\omega$) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

**Table A-19:** Harmonic Vibrational Frequencies for Phenazine and Phenazine/$Ag_2$ Complex[a]

| Phenazine | | | Phenazine/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 20.8 | 0.0 | 0.7 | | | |
| | | | 23.0 | 0.0 | 9.0 | | | |
| | | | 55.5 | 0.9 | 9.5 | | | |
| | | | 81.4 | 1.9 | 5.8 | | | |
| | | | 84.1 | 0.2 | 0.1 | | | |
| 95.4 | 3.1 | 0.0 | 102.5 | 1.6 | 1.7 | 7.1 | -1.5 | 1.7 |
| 110.7 | 0.0 | 0.0 | 109.3 | 0.0 | 0.0 | -1.3 | 0.0 | 0.0 |
| | | | 190.5 | 7.8 | 40.3 | | | |
| 242.9 | 0.0 | 1.3 | 242.4 | 0.0 | 1.4 | -0.5 | 0.0 | 0.2 |
| 247.0 | 4.9 | 0.0 | 256.3 | 18.9 | 0.2 | 9.4 | 14.0 | 0.2 |
| 281.7 | 0.0 | 0.4 | 288.7 | 0.5 | 0.2 | 7.0 | 0.5 | -0.2 |
| 405.2 | 5.9 | 0.0 | 403.8 | 2.7 | 1.0 | -1.4 | -3.1 | 1.0 |
| 418.7 | 0.0 | 24.7 | 420.4 | 0.0 | 27.6 | 1.6 | 0.0 | 2.9 |
| 452.9 | 0.0 | 8.6 | 455.6 | 0.3 | 11.9 | 2.8 | 0.3 | 3.3 |
| 497.1 | 0.1 | 0.0 | 501.0 | 0.0 | 1.3 | 3.9 | -0.1 | 1.3 |
| 501.3 | 0.0 | 2.2 | 508.0 | 0.0 | 0.1 | 6.7 | 0.0 | -2.2 |
| 510.7 | 0.0 | 0.0 | 509.9 | 0.7 | 1.0 | -0.8 | 0.7 | 1.0 |
| 538.0 | 0.0 | 6.3 | 544.6 | 0.0 | 7.1 | 6.6 | 0.0 | 0.8 |
| 604.1 | 0.0 | 0.6 | 600.2 | 0.3 | 0.1 | -3.8 | 0.3 | -0.5 |
| 611.4 | 17.7 | 0.0 | 611.8 | 15.4 | 0.2 | 0.5 | -2.3 | 0.2 |
| 627.5 | 0.0 | 5.9 | 636.4 | 0.4 | 4.9 | 8.9 | 0.4 | -1.0 |
| 667.2 | 5.2 | 0.0 | 669.5 | 11.9 | 0.2 | 2.3 | 6.7 | 0.2 |
| 745.4 | 0.0 | 78.8 | 752.8 | 4.3 | 63.5 | 7.4 | 4.3 | -15.3 |
| 772.3 | 147.0 | 0.0 | 771.5 | 119.5 | 1.9 | -0.8 | -27.5 | 1.9 |
| 778.3 | 0.0 | 0.0 | 775.9 | 0.0 | 0.1 | -2.3 | 0.0 | 0.1 |
| 788.3 | 0.0 | 0.3 | 789.0 | 0.0 | 0.0 | 0.7 | 0.0 | -0.3 |
| 823.2 | 0.0 | 0.0 | 822.1 | 0.8 | 0.2 | -1.1 | 0.8 | 0.2 |
| 836.4 | 15.4 | 0.0 | 843.2 | 15.7 | 2.4 | 6.8 | 0.4 | 2.4 |
| 890.2 | 0.0 | 0.0 | 890.5 | 0.0 | 0.2 | 0.3 | 0.0 | 0.2 |
| 904.0 | 0.0 | 0.2 | 902.9 | 0.9 | 1.9 | -1.1 | 0.9 | 1.7 |
| 919.0 | 2.1 | 0.0 | 923.0 | 6.7 | 0.6 | 3.9 | 4.6 | 0.6 |
| 943.7 | 0.0 | 0.4 | 942.8 | 0.0 | 0.1 | -0.9 | 0.0 | -0.3 |
| 993.2 | 1.7 | 0.0 | 996.1 | 0.2 | 1.4 | 2.9 | -1.5 | 1.4 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-19 Continued**[a]

| Phenazine | | | Phenazine/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| 995.2 | 0.0 | 3.4 | 998.6 | 0.0 | 3.9 | 3.4 | 0.0 | 0.5 |
| 1015.7 | 0.0 | 1.2 | 1020.0 | 0.0 | 0.1 | 4.3 | 0.0 | -1.1 |
| 1015.7 | 0.0 | 0.0 | 1020.0 | 0.3 | 3.4 | 4.3 | 0.3 | 3.4 |
| 1020.3 | 7.5 | 0.0 | 1026.3 | 6.7 | 3.6 | 6.1 | -0.8 | 3.6 |
| 1023.2 | 0.0 | 74.5 | 1028.4 | 1.6 | 76.8 | 5.2 | 1.6 | 2.3 |
| 1145.0 | 0.0 | 5.5 | 1148.4 | 0.6 | 11.1 | 3.4 | 0.6 | 5.6 |
| 1151.2 | 14.0 | 0.0 | 1155.1 | 20.1 | 1.2 | 3.9 | 6.1 | 1.2 |
| 1163.9 | 11.1 | 0.0 | 1169.8 | 6.7 | 1.7 | 5.9 | -4.4 | 1.7 |
| 1181.1 | 0.0 | 3.7 | 1189.2 | 0.0 | 22.2 | 8.0 | 0.0 | 18.5 |
| 1230.8 | 0.0 | 12.5 | 1236.1 | 0.1 | 36.9 | 5.3 | 0.1 | 24.4 |
| 1248.9 | 0.4 | 0.0 | 1253.0 | 1.8 | 0.3 | 4.0 | 1.4 | 0.3 |
| 1294.3 | 0.5 | 0.0 | 1299.6 | 3.9 | 10.6 | 5.4 | 3.4 | 10.6 |
| 1312.8 | 0.0 | 26.8 | 1313.5 | 4.8 | 50.4 | 0.7 | 4.8 | 23.7 |
| 1343.2 | 0.0 | 0.0 | 1343.3 | 1.5 | 0.9 | 0.1 | 1.5 | 0.9 |
| 1374.0 | 27.0 | 0.0 | 1374.7 | 37.0 | 16.7 | 0.7 | 10.0 | 16.7 |
| 1419.9 | 0.0 | 2.6 | 1420.7 | 0.0 | 0.0 | 0.8 | 0.0 | -2.6 |
| 1422.5 | 0.0 | 870.2 | 1424.9 | 3.1 | 755.0 | 2.4 | 3.1 | -115.2 |
| 1470.0 | 5.3 | 0.0 | 1471.7 | 18.9 | 0.6 | 1.7 | 13.6 | 0.6 |
| 1512.6 | 6.3 | 0.0 | 1510.6 | 30.9 | 19.5 | -2.0 | 24.7 | 19.5 |
| 1514.7 | 0.0 | 165.5 | 1515.5 | 1.5 | 146.4 | 0.7 | 1.5 | -19.0 |
| 1557.1 | 44.1 | 0.0 | 1559.6 | 46.6 | 0.1 | 2.5 | 2.4 | 0.1 |
| 1570.7 | 0.0 | 2.9 | 1565.5 | 0.6 | 17.6 | -5.2 | 0.6 | 14.7 |
| 1588.4 | 0.0 | 62.6 | 1590.9 | 0.0 | 60.3 | 2.5 | 0.0 | -2.3 |
| 1646.3 | 0.0 | 5.4 | 1647.6 | 2.0 | 1.4 | 1.3 | 2.0 | -4.0 |
| 1675.0 | 0.7 | 0.0 | 1674.8 | 3.7 | 1.4 | -0.2 | 3.1 | 1.4 |
| 3171.9 | 4.8 | 0.0 | 3165.6 | 0.8 | 250.8 | -6.3 | -4.1 | 250.8 |
| 3172.0 | 0.0 | 99.4 | 3165.7 | 0.2 | 49.7 | -6.3 | 0.2 | -49.7 |
| 3183.4 | 8.6 | 0.0 | 3180.7 | 7.2 | 59.1 | -2.8 | -1.4 | 59.1 |
| 3183.5 | 0.0 | 315.1 | 3180.7 | 0.3 | 89.4 | -2.8 | 0.3 | -225.6 |
| 3195.8 | 0.0 | 129.4 | 3193.2 | 10.0 | 6.0 | -2.6 | 10.0 | -123.4 |
| 3196.0 | 17.3 | 0.0 | 3193.3 | 1.7 | 358.9 | -2.7 | -15.6 | 358.9 |
| 3200.2 | 31.5 | 0.0 | 3203.9 | 15.1 | 86.0 | 3.8 | -16.4 | 86.0 |
| 3200.7 | 0.0 | 704.8 | 3204.2 | 6.3 | 618.8 | 3.6 | 6.3 | -86.0 |

[a] Frequencies (*ω*) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

**Table A-20:** Harmonic Vibrational Frequencies for Quinoxaline and Quinoxaline/Ag$_2$ Complex[a]

| Quinoxaline | | | Quinoxaline/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 22.2 | 0.0 | 0.1 | | | |
| | | | 23.4 | 0.0 | 5.7 | | | |
| | | | 68.3 | 0.7 | 9.8 | | | |
| | | | 79.8 | 1.0 | 1.3 | | | |
| | | | 105.4 | 2.7 | 4.8 | | | |
| 173.4 | 0.0 | 0.2 | 180.7 | 3.6 | 0.1 | 7.3 | 3.6 | -0.2 |
| 183.7 | 5.4 | 0.1 | 187.8 | 1.3 | 0.5 | 4.1 | -4.1 | 0.3 |
| | | | 193.1 | 9.6 | 40.2 | | | |
| 400.9 | 5.2 | 0.0 | 411.8 | 13.2 | 0.1 | 10.9 | 8.1 | 0.1 |
| 416.1 | 10.9 | 1.9 | 419.0 | 6.1 | 2.0 | 2.9 | -4.8 | 0.1 |
| 483.1 | 0.0 | 0.0 | 481.0 | 0.0 | 0.2 | -2.1 | 0.0 | 0.2 |
| 502.6 | 0.0 | 0.0 | 512.5 | 0.2 | 0.4 | 9.9 | 0.2 | 0.4 |
| 537.0 | 0.0 | 13.1 | 538.5 | 0.2 | 13.0 | 1.5 | 0.2 | -0.1 |
| 544.5 | 0.2 | 7.7 | 545.5 | 1.7 | 9.0 | 1.0 | 1.5 | 1.3 |
| 618.7 | 3.0 | 0.3 | 630.3 | 3.1 | 0.7 | 11.6 | 0.1 | 0.4 |
| 659.0 | 0.0 | 0.3 | 657.0 | 0.3 | 0.1 | -1.9 | 0.3 | -0.2 |
| 771.6 | 4.4 | 45.8 | 776.5 | 8.1 | 50.3 | 4.9 | 3.7 | 4.4 |
| 777.0 | 56.4 | 0.5 | 779.1 | 46.4 | 0.3 | 2.1 | -10.0 | -0.2 |
| 823.3 | 0.0 | 0.0 | 821.3 | 0.3 | 0.2 | -1.9 | 0.3 | 0.1 |
| 852.5 | 1.0 | 0.1 | 850.3 | 0.6 | 0.5 | -2.3 | -0.4 | 0.4 |
| 888.7 | 29.1 | 0.4 | 887.0 | 25.2 | 0.5 | -1.7 | -4.0 | 0.1 |
| 906.2 | 0.0 | 0.0 | 906.3 | 2.2 | 0.6 | 0.1 | 2.2 | 0.6 |
| 968.0 | 17.2 | 0.7 | 974.4 | 31.4 | 1.0 | 6.4 | 14.1 | 0.3 |
| 993.6 | 3.2 | 0.8 | 996.4 | 0.4 | 1.2 | 2.8 | -2.9 | 0.3 |
| 996.3 | 0.0 | 0.0 | 997.3 | 0.9 | 0.8 | 1.1 | 0.9 | 0.8 |
| 1018.1 | 0.0 | 0.2 | 1022.9 | 0.1 | 0.8 | 4.8 | 0.1 | 0.5 |
| 1031.7 | 0.8 | 13.7 | 1035.8 | 2.1 | 25.1 | 4.1 | 1.3 | 11.4 |
| 1049.1 | 22.0 | 15.4 | 1060.4 | 19.4 | 12.6 | 11.4 | -2.6 | -2.9 |
| 1150.9 | 8.6 | 2.7 | 1156.3 | 8.5 | 10.2 | 5.4 | -0.1 | 7.5 |
| 1163.0 | 1.9 | 2.7 | 1167.8 | 6.6 | 1.6 | 4.8 | 4.7 | -1.0 |
| 1238.7 | 3.0 | 1.8 | 1238.0 | 15.5 | 15.3 | -0.6 | 12.5 | 13.5 |
| 1239.2 | 0.6 | 7.2 | 1243.0 | 5.7 | 5.1 | 3.8 | 5.2 | -2.0 |
| 1294.9 | 0.1 | 0.6 | 1298.3 | 1.3 | 15.4 | 3.3 | 1.2 | 14.8 |

[a] Frequencies (*ω*) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^{4}$ amu$^{-1}$

**Table A-20 Continued**[a]

| Quinoxaline | | | Quinoxaline/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | Δ ω | Δ IR | Δ Raman |
| 1326.2 | 0.0 | 2.7 | 1326.2 | 4.6 | 10.9 | 0.0 | 4.6 | 8.3 |
| 1381.2 | 16.9 | 92.1 | 1382.1 | 27.8 | 143.5 | 1.0 | 11.0 | 51.4 |
| 1415.1 | 2.0 | 0.1 | 1417.5 | 2.0 | 2.9 | 2.4 | 0.1 | 2.9 |
| 1452.8 | 1.7 | 125.3 | 1456.8 | 3.3 | 86.3 | 4.0 | 1.6 | -39.0 |
| 1503.6 | 2.7 | 2.0 | 1503.4 | 13.0 | 4.2 | -0.2 | 10.2 | 2.3 |
| 1533.1 | 27.9 | 3.9 | 1536.6 | 44.3 | 5.2 | 3.5 | 16.4 | 1.2 |
| 1601.7 | 2.8 | 34.1 | 1601.6 | 2.8 | 14.5 | -0.1 | 0.0 | -19.7 |
| 1607.2 | 0.0 | 8.0 | 1608.8 | 0.4 | 32.7 | 1.6 | 0.4 | 24.8 |
| 1656.3 | 0.5 | 6.2 | 1656.0 | 1.7 | 6.8 | -0.2 | 1.2 | 0.7 |
| 3139.2 | 3.1 | 86.4 | 3157.7 | 6.0 | 129.1 | 18.5 | 2.9 | 42.7 |
| 3156.2 | 42.0 | 305.0 | 3170.8 | 0.2 | 144.0 | 14.6 | -41.7 | -161.0 |
| 3172.6 | 1.7 | 49.2 | 3177.3 | 14.2 | 179.8 | 4.7 | 12.5 | 130.6 |
| 3184.1 | 4.6 | 116.4 | 3181.9 | 3.5 | 69.5 | -2.3 | -1.2 | -46.9 |
| 3195.5 | 8.6 | 33.6 | 3194.5 | 5.2 | 127.5 | -0.9 | -3.4 | 93.9 |
| 3200.3 | 10.0 | 314.8 | 3204.2 | 7.9 | 329.2 | 4.0 | -2.1 | 14.4 |

[a] Frequencies ($\omega$) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-21:** Harmonic Vibrational Frequencies for Acridine and Acridine/Ag$_2$ Complex[a]

| Acridine | | | Acridine/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 21.3 | 0.1 | 1.1 | | | |
| | | | 23.6 | 0.0 | 8.5 | | | |
| | | | 54.4 | 0.1 | 9.9 | | | |
| | | | 84.6 | 1.8 | 7.1 | | | |
| | | | 87.8 | 0.1 | 0.0 | | | |
| 92.8 | 2.0 | 0.0 | 100.6 | 1.1 | 1.5 | 7.7 | -0.9 | 1.5 |
| 114.6 | 0.0 | 0.0 | 112.2 | 0.0 | 0.0 | -2.4 | 0.0 | 0.0 |
| | | | 190.6 | 8.8 | 38.0 | | | |
| 239.1 | 0.0 | 1.5 | 238.4 | 0.0 | 1.7 | -0.8 | 0.0 | 0.2 |
| 241.4 | 2.8 | 0.0 | 253.1 | 15.8 | 0.3 | 11.7 | 13.0 | 0.3 |
| 275.6 | 1.6 | 0.1 | 282.8 | 0.6 | 0.6 | 7.2 | -1.0 | 0.5 |
| 396.6 | 1.4 | 0.1 | 395.7 | 0.3 | 0.3 | -0.9 | -1.0 | 0.2 |
| 409.0 | 0.0 | 26.1 | 410.7 | 0.0 | 28.5 | 1.7 | 0.0 | 2.4 |
| 424.0 | 0.2 | 5.7 | 427.9 | 0.0 | 8.1 | 3.9 | -0.1 | 2.5 |
| 484.4 | 8.7 | 0.1 | 488.7 | 0.0 | 0.9 | 4.3 | -8.7 | 0.8 |
| 490.8 | 0.0 | 1.5 | 494.9 | 10.9 | 0.0 | 4.1 | 10.9 | -1.5 |
| 514.3 | 0.0 | 0.2 | 513.9 | 0.0 | 0.0 | -0.4 | 0.0 | -0.1 |
| 536.0 | 2.4 | 8.4 | 542.4 | 2.6 | 9.6 | 6.4 | 0.2 | 1.3 |
| 601.6 | 0.0 | 0.3 | 598.3 | 0.4 | 0.0 | -3.3 | 0.4 | -0.3 |
| 616.4 | 10.4 | 0.0 | 617.9 | 8.4 | 0.0 | 1.5 | -2.0 | 0.0 |
| 634.8 | 2.7 | 2.8 | 642.8 | 5.0 | 2.7 | 8.0 | 2.3 | -0.1 |
| 666.0 | 3.0 | 0.2 | 671.1 | 10.7 | 2.2 | 5.1 | 7.7 | 2.0 |
| 754.3 | 0.3 | 78.7 | 756.3 | 80.0 | 0.4 | 2.0 | 79.7 | -78.3 |
| 755.4 | 98.2 | 0.1 | 764.7 | 7.7 | 60.0 | 9.3 | -90.5 | 59.9 |
| 770.5 | 0.0 | 0.1 | 770.4 | 0.0 | 0.2 | -0.2 | 0.0 | 0.1 |
| 782.8 | 0.0 | 0.7 | 783.1 | 0.0 | 0.2 | 0.3 | 0.0 | -0.4 |
| 813.0 | 7.7 | 0.1 | 813.3 | 11.4 | 0.0 | 0.2 | 3.7 | -0.1 |
| 828.8 | 1.6 | 0.6 | 837.8 | 1.7 | 0.2 | 8.9 | 0.1 | -0.5 |
| 881.7 | 18.1 | 0.2 | 883.1 | 7.8 | 2.0 | 1.4 | -10.3 | 1.8 |
| 882.6 | 0.0 | 0.0 | 884.5 | 0.0 | 0.1 | 1.9 | 0.0 | 0.1 |
| 920.3 | 0.0 | 2.0 | 924.6 | 1.5 | 0.9 | 4.3 | 1.5 | -1.0 |
| 938.3 | 1.3 | 0.0 | 937.9 | 2.0 | 0.2 | -0.4 | 0.7 | 0.2 |
| 940.6 | 14.7 | 0.1 | 950.8 | 16.2 | 0.7 | 10.2 | 1.5 | 0.7 |
| 987.6 | 0.0 | 3.4 | 991.3 | 0.0 | 3.6 | 3.7 | 0.0 | 0.2 |

[a] Frequencies (*ω*) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^{4}$ amu$^{-1}$

**Table A-21 Continued**[a]

| Acridine | | | Acridine/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| 991.2 | 5.7 | 0.1 | 995.4 | 3.2 | 0.2 | 4.2 | -2.4 | 0.0 |
| 1012.3 | 0.0 | 0.2 | 1017.6 | 0.0 | 0.5 | 5.3 | 0.0 | 0.4 |
| 1012.5 | 0.2 | 1.1 | 1017.7 | 0.1 | 4.0 | 5.3 | -0.1 | 2.9 |
| 1024.6 | 6.8 | 0.0 | 1033.1 | 5.7 | 4.8 | 8.5 | -1.1 | 4.8 |
| 1028.4 | 0.0 | 74.2 | 1035.7 | 2.9 | 74.8 | 7.2 | 2.9 | 0.5 |
| 1136.3 | 0.4 | 1.3 | 1139.7 | 0.5 | 4.0 | 3.4 | 0.1 | 2.7 |
| 1158.0 | 3.0 | 0.0 | 1163.8 | 6.3 | 0.1 | 5.8 | 3.2 | 0.1 |
| 1167.4 | 9.6 | 0.2 | 1177.9 | 4.8 | 1.9 | 10.5 | -4.8 | 1.7 |
| 1187.3 | 0.0 | 5.7 | 1193.4 | 0.0 | 22.3 | 6.1 | 0.0 | 16.6 |
| 1196.0 | 1.5 | 11.1 | 1202.3 | 1.1 | 23.2 | 6.3 | -0.4 | 12.0 |
| 1237.2 | 0.5 | 11.6 | 1246.1 | 0.0 | 27.5 | 8.9 | -0.5 | 15.9 |
| 1291.8 | 0.1 | 3.2 | 1292.9 | 8.3 | 9.4 | 1.1 | 8.2 | 6.2 |
| 1303.4 | 1.0 | 42.8 | 1308.6 | 7.1 | 83.2 | 5.1 | 6.0 | 40.4 |
| 1335.5 | 2.8 | 1.8 | 1329.6 | 2.5 | 0.3 | -5.9 | -0.3 | -1.6 |
| 1342.5 | 0.7 | 23.4 | 1343.1 | 0.0 | 22.0 | 0.7 | -0.7 | -1.4 |
| 1389.9 | 3.1 | 1.1 | 1397.2 | 8.2 | 9.8 | 7.2 | 5.1 | 8.7 |
| 1421.6 | 5.8 | 844.0 | 1424.0 | 2.3 | 2.0 | 2.5 | -3.5 | -842.0 |
| 1424.0 | 0.2 | 1.6 | 1425.3 | 2.4 | 691.3 | 1.3 | 2.2 | 689.7 |
| 1477.0 | 0.7 | 0.3 | 1479.2 | 6.5 | 0.1 | 2.2 | 5.8 | -0.2 |
| 1501.2 | 4.1 | 8.6 | 1499.3 | 29.4 | 22.8 | -1.8 | 25.3 | 14.1 |
| 1517.8 | 1.5 | 130.2 | 1520.0 | 14.2 | 112.1 | 2.2 | 12.7 | -18.1 |
| 1558.8 | 45.8 | 0.2 | 1560.3 | 54.2 | 0.3 | 1.5 | 8.4 | 0.1 |
| 1589.1 | 8.8 | 70.2 | 1593.9 | 18.6 | 70.0 | 4.9 | 9.8 | -0.2 |
| 1620.8 | 9.8 | 8.2 | 1620.4 | 8.8 | 18.4 | -0.5 | -1.0 | 10.3 |
| 1655.4 | 19.5 | 1.1 | 1656.6 | 31.8 | 0.3 | 1.1 | 12.3 | -0.8 |
| 1673.8 | 3.0 | 1.1 | 1674.6 | 0.9 | 4.1 | 0.9 | -2.1 | 3.0 |
| 3155.2 | 5.8 | 40.4 | 3162.4 | 1.7 | 182.5 | 7.2 | -4.1 | 142.1 |
| 3162.4 | 0.7 | 1.7 | 3163.1 | 4.5 | 85.2 | 0.7 | 3.8 | 83.6 |
| 3163.0 | 6.5 | 127.8 | 3163.3 | 0.0 | 51.0 | 0.3 | -6.5 | -76.9 |
| 3173.5 | 0.9 | 144.0 | 3170.3 | 0.2 | 1.0 | -3.2 | -0.7 | -143.0 |
| 3173.6 | 18.3 | 89.2 | 3170.9 | 5.4 | 337.2 | -2.7 | -12.9 | 248.0 |
| 3188.7 | 22.4 | 60.4 | 3184.1 | 0.2 | 127.2 | -4.6 | -22.2 | 66.8 |
| 3188.8 | 13.3 | 365.3 | 3184.1 | 20.8 | 18.4 | -4.7 | 7.6 | -346.9 |
| 3199.2 | 20.8 | 27.0 | 3197.0 | 28.5 | 54.3 | -2.2 | 7.7 | 27.3 |

[a] Frequencies (*ω*) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

**Table A-22:** Harmonic Vibrational Frequencies for Isoquinoline and Isoquinoline/Ag$_2$ Complex[a]

| Isoquinoline | | | Isoquinoline/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 19.9 | 0.1 | 0.3 | | | |
| | | | 22.1 | 0.0 | 2.6 | | | |
| | | | 67.9 | 0.0 | 11.2 | | | |
| | | | 88.8 | 0.9 | 4.9 | | | |
| | | | 104.3 | 2.0 | 2.8 | | | |
| 171.8 | 0.1 | 0.1 | 178.6 | 1.0 | 0.0 | 6.9 | 0.9 | 0.0 |
| 186.0 | 0.9 | 0.1 | 193.9 | 11.2 | 49.2 | 7.9 | 10.4 | 49.1 |
| | | | 200.3 | 0.0 | 0.5 | | | |
| 362.7 | 0.1 | 0.1 | 371.8 | 0.7 | 0.2 | 9.1 | 0.6 | 0.1 |
| 389.5 | 0.4 | 0.8 | 393.6 | 0.2 | 1.3 | 4.1 | -0.2 | 0.6 |
| 474.2 | 1.2 | 0.0 | 480.1 | 4.1 | 0.1 | 5.9 | 2.9 | 0.1 |
| 496.7 | 19.9 | 0.1 | 496.8 | 13.8 | 0.3 | 0.1 | -6.2 | 0.2 |
| 512.0 | 1.1 | 11.9 | 529.5 | 5.5 | 19.7 | 17.6 | 4.4 | 7.8 |
| 531.9 | 0.4 | 11.0 | 532.4 | 3.6 | 4.9 | 0.5 | 3.2 | -6.1 |
| 657.4 | 5.3 | 0.9 | 657.4 | 11.2 | 0.6 | -0.1 | 5.9 | -0.3 |
| 658.0 | 4.7 | 0.1 | 657.7 | 1.9 | 0.6 | -0.3 | -2.8 | 0.5 |
| 757.6 | 28.2 | 0.5 | 761.7 | 27.8 | 0.5 | 4.1 | -0.4 | 0.0 |
| 793.1 | 0.8 | 44.3 | 793.8 | 0.0 | 61.1 | 0.8 | -0.8 | 16.8 |
| 803.9 | 1.3 | 0.1 | 804.3 | 0.2 | 0.2 | 0.4 | -1.1 | 0.0 |
| 814.4 | 3.9 | 0.1 | 827.5 | 10.2 | 0.7 | 13.1 | 6.3 | 0.6 |
| 849.5 | 44.3 | 0.0 | 852.3 | 41.3 | 0.2 | 2.8 | -3.0 | 0.2 |
| 885.2 | 7.4 | 0.1 | 890.1 | 8.5 | 0.1 | 4.9 | 1.1 | 0.0 |
| 957.9 | 0.6 | 0.1 | 962.1 | 0.9 | 0.2 | 4.2 | 0.3 | 0.0 |
| 960.4 | 8.9 | 0.2 | 970.1 | 15.1 | 2.7 | 9.7 | 6.2 | 2.5 |
| 984.7 | 1.5 | 1.3 | 988.8 | 0.6 | 3.1 | 4.0 | -0.9 | 1.8 |
| 1001.8 | 1.2 | 0.2 | 1002.7 | 2.1 | 0.3 | 0.8 | 0.8 | 0.2 |
| 1013.6 | 0.0 | 0.3 | 1021.1 | 0.0 | 0.3 | 7.5 | 0.0 | 0.0 |
| 1039.0 | 4.2 | 18.5 | 1040.0 | 7.0 | 23.4 | 1.0 | 2.7 | 4.8 |
| 1065.0 | 3.5 | 17.3 | 1067.2 | 36.2 | 31.1 | 2.2 | 32.7 | 13.8 |
| 1162.1 | 1.5 | 3.2 | 1165.6 | 1.7 | 5.1 | 3.5 | 0.2 | 1.8 |
| 1169.1 | 2.3 | 1.5 | 1174.7 | 2.2 | 2.5 | 5.5 | -0.1 | 1.0 |
| 1206.7 | 0.8 | 2.2 | 1209.0 | 15.9 | 4.4 | 2.4 | 15.2 | 2.3 |
| 1243.4 | 5.4 | 3.9 | 1244.6 | 21.2 | 6.2 | 1.2 | 15.9 | 2.3 |

[a] Frequencies (*ω*) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

**Table A-22 Continued**[a]

| Isoquinoline | | | Isoquinoline/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | Δ ω | Δ IR | Δ Raman |
| 1282.2 | 1.0 | 5.2 | 1285.5 | 1.5 | 3.9 | 3.3 | 0.6 | -1.3 |
| 1293.6 | 14.8 | 2.0 | 1298.3 | 18.5 | 3.6 | 4.6 | 3.6 | 1.6 |
| 1367.2 | 0.1 | 16.2 | 1366.9 | 3.4 | 15.1 | -0.3 | 3.4 | -1.1 |
| 1400.9 | 4.4 | 134.3 | 1406.5 | 12.5 | 255.6 | 5.6 | 8.2 | 121.3 |
| 1413.4 | 6.4 | 13.8 | 1418.6 | 13.6 | 4.8 | 5.2 | 7.3 | -8.9 |
| 1469.4 | 1.4 | 19.5 | 1474.2 | 1.6 | 51.5 | 4.8 | 0.1 | 32.0 |
| 1495.0 | 0.9 | 39.6 | 1498.4 | 7.7 | 80.4 | 3.4 | 6.8 | 40.8 |
| 1537.6 | 9.9 | 5.8 | 1539.4 | 6.0 | 1.8 | 1.8 | -3.9 | -3.9 |
| 1607.9 | 7.3 | 26.4 | 1607.1 | 2.0 | 25.0 | -0.8 | -5.3 | -1.4 |
| 1626.4 | 19.9 | 7.4 | 1635.5 | 25.9 | 10.5 | 9.1 | 5.9 | 3.0 |
| 1665.8 | 20.6 | 12.9 | 1668.5 | 39.2 | 31.6 | 2.7 | 18.5 | 18.6 |
| 3125.5 | 19.5 | 94.0 | 3158.3 | 5.4 | 40.1 | 32.8 | -14.1 | -53.8 |
| 3161.4 | 6.9 | 83.1 | 3170.9 | 0.7 | 16.7 | 9.5 | -6.2 | -66.4 |
| 3164.7 | 1.7 | 16.0 | 3175.9 | 0.1 | 92.9 | 11.2 | -1.6 | 76.9 |
| 3169.6 | 0.7 | 118.8 | 3181.4 | 0.7 | 74.5 | 11.8 | -0.1 | -44.3 |
| 3181.0 | 5.5 | 170.9 | 3186.8 | 13.1 | 104.4 | 5.9 | 7.6 | -66.5 |
| 3182.0 | 38.3 | 94.0 | 3197.6 | 12.0 | 260.9 | 15.6 | -26.3 | 166.9 |
| 3193.4 | 13.9 | 313.6 | 3198.9 | 14.5 | 282.1 | 5.5 | 0.6 | -31.5 |

[a] Frequencies ($\omega$) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

**Table A-23:** Harmonic Vibrational Frequencies for 3-Methylquinoline and 3-Methylquinoline/Ag$_2$ Complex[a]

| 3-Methylquinoline | | | 3-Methylquinoline/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 23.1 | 0.0 | 6.1 | | | |
| | | | 23.5 | 0.2 | 0.0 | | | |
| | | | 65.4 | 0.2 | 5.1 | | | |
| 74.7 | 0.6 | 0.1 | 77.0 | 0.1 | 5.4 | 2.3 | -0.5 | 5.4 |
| | | | 82.9 | 0.9 | 1.0 | | | |
| | | | 98.0 | 1.3 | 6.4 | | | |
| 115.6 | 1.6 | 1.3 | 119.8 | 1.0 | 0.8 | 4.1 | -0.6 | -0.4 |
| 183.9 | 0.1 | 0.0 | 187.3 | 0.4 | 0.0 | 3.5 | 0.2 | 0.0 |
| | | | 192.7 | 9.4 | 37.9 | | | |
| 262.8 | 1.4 | 0.6 | 268.6 | 7.8 | 0.6 | 5.9 | 6.4 | 0.0 |
| 287.2 | 0.2 | 0.1 | 289.0 | 0.0 | 0.5 | 1.9 | -0.2 | 0.3 |
| 418.4 | 1.4 | 1.7 | 424.2 | 0.3 | 1.3 | 5.8 | -1.1 | -0.5 |
| 429.9 | 2.6 | 0.2 | 440.8 | 5.8 | 0.5 | 10.9 | 3.2 | 0.3 |
| 456.8 | 0.0 | 14.4 | 459.0 | 0.3 | 15.1 | 2.2 | 0.2 | 0.6 |
| 492.8 | 7.2 | 0.1 | 499.6 | 9.1 | 0.1 | 6.8 | 1.9 | 0.0 |
| 513.1 | 0.1 | 0.1 | 511.6 | 0.0 | 0.3 | -1.5 | -0.1 | 0.1 |
| 537.6 | 0.2 | 9.7 | 538.5 | 2.1 | 10.8 | 1.0 | 1.9 | 1.1 |
| 628.9 | 4.5 | 0.6 | 634.2 | 4.4 | 2.1 | 5.3 | -0.1 | 1.5 |
| 653.3 | 1.8 | 0.1 | 651.6 | 0.7 | 0.3 | -1.7 | -1.0 | 0.2 |
| 715.5 | 3.6 | 4.8 | 733.1 | 12.8 | 0.6 | 17.6 | 9.2 | -4.2 |
| 768.8 | 46.7 | 0.4 | 771.6 | 39.0 | 0.1 | 2.8 | -7.7 | -0.3 |
| 784.2 | 1.3 | 40.3 | 788.3 | 8.3 | 43.5 | 4.1 | 7.0 | 3.2 |
| 811.7 | 8.9 | 0.0 | 813.7 | 9.2 | 0.2 | 2.0 | 0.3 | 0.2 |
| 887.1 | 9.6 | 0.2 | 890.1 | 5.2 | 0.6 | 3.0 | -4.4 | 0.4 |
| 904.2 | 0.0 | 0.3 | 906.8 | 0.9 | 0.3 | 2.6 | 0.9 | 0.0 |
| 913.9 | 13.4 | 0.1 | 921.4 | 12.7 | 0.3 | 7.6 | -0.7 | 0.2 |
| 967.0 | 0.0 | 0.1 | 974.3 | 0.2 | 0.7 | 7.3 | 0.2 | 0.6 |
| 985.8 | 3.2 | 0.7 | 990.0 | 1.4 | 1.2 | 4.3 | -1.9 | 0.5 |
| 992.3 | 9.4 | 6.2 | 1001.3 | 12.4 | 4.6 | 9.0 | 3.0 | -1.6 |
| 1012.1 | 0.1 | 0.2 | 1018.3 | 0.0 | 1.0 | 6.2 | 0.0 | 0.8 |
| 1023.8 | 12.2 | 0.1 | 1027.5 | 12.4 | 1.0 | 3.7 | 0.3 | 0.9 |
| 1040.7 | 2.3 | 30.7 | 1046.0 | 4.7 | 42.3 | 5.3 | 2.4 | 11.6 |

[a] Frequencies ($\omega$) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

**Table A-23 Continued[a]**

| 3-Methylquinoline | | | 3-Methylquinoline/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| 1071.4 | 2.7 | 0.6 | 1073.8 | 2.6 | 0.5 | 2.4 | -0.1 | 0.0 |
| 1149.6 | 5.8 | 4.2 | 1156.8 | 5.1 | 6.6 | 7.2 | -0.7 | 2.5 |
| 1164.6 | 1.8 | 1.3 | 1171.7 | 3.8 | 2.0 | 7.1 | 2.0 | 0.6 |
| 1198.1 | 1.3 | 7.7 | 1202.4 | 1.0 | 12.5 | 4.3 | -0.3 | 4.8 |
| 1232.1 | 0.8 | 3.6 | 1234.6 | 7.6 | 5.0 | 2.4 | 6.8 | 1.4 |
| 1263.4 | 1.4 | 1.9 | 1267.1 | 12.1 | 7.4 | 3.8 | 10.7 | 5.5 |
| 1301.8 | 3.2 | 1.2 | 1307.0 | 4.1 | 11.4 | 5.3 | 0.9 | 10.2 |
| 1374.5 | 12.3 | 18.3 | 1372.9 | 28.5 | 3.6 | -1.6 | 16.2 | -14.7 |
| 1392.2 | 0.2 | 135.4 | 1393.9 | 6.1 | 197.6 | 1.7 | 5.9 | 62.2 |
| 1400.5 | 2.1 | 1.6 | 1405.4 | 1.6 | 0.5 | 4.9 | -0.4 | -1.1 |
| 1419.3 | 0.4 | 26.8 | 1422.7 | 0.4 | 26.2 | 3.4 | 0.0 | -0.6 |
| 1451.5 | 4.9 | 77.8 | 1453.5 | 7.8 | 39.4 | 2.0 | 2.9 | -38.4 |
| 1483.7 | 6.2 | 6.8 | 1484.2 | 7.2 | 7.1 | 0.5 | 1.1 | 0.4 |
| 1490.7 | 10.6 | 47.1 | 1492.5 | 7.9 | 39.1 | 1.8 | -2.6 | -8.0 |
| 1503.4 | 0.7 | 6.9 | 1504.1 | 4.1 | 6.3 | 0.7 | 3.4 | -0.6 |
| 1535.8 | 26.7 | 4.4 | 1539.9 | 56.7 | 6.5 | 4.1 | 30.0 | 2.1 |
| 1602.3 | 9.1 | 32.9 | 1609.4 | 17.5 | 40.2 | 7.1 | 8.4 | 7.3 |
| 1651.9 | 2.9 | 3.1 | 1651.3 | 2.9 | 5.2 | -0.6 | 0.0 | 2.1 |
| 1661.3 | 0.8 | 41.2 | 1661.6 | 2.2 | 40.8 | 0.4 | 1.4 | -0.4 |
| 3027.6 | 28.3 | 361.9 | 3032.7 | 20.2 | 343.5 | 5.0 | -8.1 | -18.4 |
| 3073.2 | 12.8 | 109.2 | 3080.3 | 8.9 | 92.4 | 7.1 | -3.9 | -16.8 |
| 3107.0 | 12.8 | 60.9 | 3113.4 | 12.7 | 77.7 | 6.4 | -0.1 | 16.8 |
| 3119.1 | 31.1 | 155.8 | 3150.7 | 6.0 | 60.9 | 31.6 | -25.0 | -94.9 |
| 3153.6 | 11.3 | 67.9 | 3161.4 | 9.6 | 97.5 | 7.9 | -1.7 | 29.6 |
| 3161.5 | 5.1 | 73.1 | 3167.7 | 4.2 | 29.3 | 6.2 | -0.9 | -43.8 |
| 3173.6 | 9.3 | 98.9 | 3171.3 | 1.3 | 264.0 | -2.3 | -8.0 | 165.1 |
| 3187.3 | 16.8 | 154.6 | 3184.5 | 12.3 | 53.5 | -2.8 | -4.4 | -101.1 |
| 3198.5 | 11.2 | 235.3 | 3196.8 | 13.9 | 373.3 | -1.6 | 2.7 | 138.1 |

[a] Frequencies (*ω*) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

**Table A-24:** Harmonic Vibrational Frequencies for Phenanthridine and Phenanthridine/$Ag_2$ Complex[a]

| Phenanthridine | | | Phenanthridine/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 19.4 | 0.0 | 0.5 | | | |
| | | | 21.8 | 0.0 | 5.8 | | | |
| | | | 59.0 | 0.1 | 11.1 | | | |
| | | | 82.1 | 1.0 | 0.5 | | | |
| | | | 86.6 | 1.4 | 6.5 | | | |
| 96.6 | 0.9 | 0.2 | 97.8 | 0.4 | 0.0 | 1.1 | -0.5 | -0.2 |
| 102.7 | 0.5 | 0.3 | 108.4 | 0.4 | 1.2 | 5.7 | -0.1 | 0.9 |
| | | | 191.5 | 10.0 | 46.7 | | | |
| 229.5 | 0.2 | 0.8 | 243.6 | 2.0 | 0.1 | 14.1 | 1.8 | -0.7 |
| 242.8 | 0.7 | 3.7 | 248.5 | 4.6 | 2.5 | 5.6 | 3.9 | -1.2 |
| 248.5 | 0.9 | 1.1 | 249.5 | 0.1 | 1.2 | 1.0 | -0.8 | 0.1 |
| 417.8 | 1.1 | 0.7 | 421.0 | 0.4 | 1.4 | 3.2 | -0.8 | 0.7 |
| 419.9 | 0.2 | 18.5 | 421.3 | 0.1 | 19.8 | 1.4 | 0.0 | 1.2 |
| 440.7 | 5.4 | 0.2 | 440.1 | 4.7 | 0.1 | -0.6 | -0.7 | -0.1 |
| 455.4 | 2.5 | 4.3 | 463.2 | 9.1 | 2.6 | 7.8 | 6.6 | -1.7 |
| 511.1 | 1.9 | 0.0 | 510.7 | 2.1 | 0.1 | -0.4 | 0.3 | 0.1 |
| 512.5 | 1.1 | 1.7 | 522.6 | 4.5 | 2.0 | 10.1 | 3.4 | 0.3 |
| 554.0 | 0.9 | 0.2 | 555.7 | 0.3 | 0.4 | 1.8 | -0.6 | 0.2 |
| 559.5 | 0.3 | 5.8 | 569.4 | 3.3 | 5.0 | 10.0 | 3.0 | -0.7 |
| 620.5 | 1.1 | 0.1 | 620.4 | 0.2 | 0.5 | -0.2 | -0.9 | 0.4 |
| 631.1 | 5.6 | 1.1 | 631.4 | 5.0 | 1.2 | 0.3 | -0.6 | 0.1 |
| 725.3 | 0.8 | 32.8 | 728.1 | 3.9 | 41.8 | 2.8 | 3.2 | 9.1 |
| 742.4 | 6.1 | 7.5 | 748.6 | 8.8 | 4.4 | 6.2 | 2.7 | -3.1 |
| 745.3 | 19.1 | 0.0 | 746.9 | 21.2 | 0.2 | 1.6 | 2.1 | 0.2 |
| 766.2 | 90.6 | 0.2 | 769.5 | 76.4 | 0.2 | 3.3 | -14.2 | 0.1 |
| 787.6 | 9.6 | 1.6 | 788.4 | 9.5 | 1.1 | 0.9 | -0.1 | -0.4 |
| 818.2 | 0.9 | 0.3 | 819.8 | 1.6 | 0.4 | 1.6 | 0.7 | 0.1 |
| 846.8 | 0.1 | 5.2 | 850.0 | 4.4 | 6.1 | 3.2 | 4.3 | 0.9 |
| 882.1 | 0.0 | 0.2 | 885.1 | 0.4 | 0.7 | 3.0 | 0.3 | 0.5 |
| 902.5 | 12.5 | 3.9 | 914.0 | 27.4 | 5.5 | 11.5 | 14.9 | 1.5 |
| 903.8 | 1.6 | 0.1 | 908.2 | 0.7 | 0.3 | 4.3 | -0.9 | 0.2 |
| 956.1 | 5.2 | 0.5 | 962.0 | 4.4 | 0.0 | 5.9 | -0.8 | -0.5 |

[a] Frequencies ($\omega$) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

**Table A-24 Continued**[a]

| Phenanthridine | | | Phenanthridine/Ag$_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| 980.4 | 0.2 | 0.8 | 983.8 | 0.0 | 1.0 | 3.4 | -0.2 | 0.2 |
| 989.4 | 5.9 | 0.0 | 993.2 | 3.5 | 0.7 | 3.9 | -2.4 | 0.7 |
| 1010.8 | 0.1 | 0.0 | 1015.8 | 0.0 | 0.3 | 5.0 | 0.0 | 0.3 |
| 1013.5 | 0.0 | 0.0 | 1018.9 | 0.0 | 0.1 | 5.4 | 0.0 | 0.1 |
| 1023.9 | 2.0 | 1.4 | 1024.2 | 1.4 | 6.4 | 0.3 | -0.7 | 5.0 |
| 1057.3 | 2.0 | 56.7 | 1059.9 | 3.6 | 54.0 | 2.6 | 1.6 | -2.7 |
| 1059.2 | 5.7 | 14.0 | 1062.9 | 5.2 | 32.8 | 3.6 | -0.5 | 18.8 |
| 1125.3 | 0.6 | 0.8 | 1129.3 | 0.5 | 1.9 | 3.9 | -0.1 | 1.1 |
| 1160.0 | 3.5 | 12.5 | 1167.0 | 7.0 | 4.4 | 7.0 | 3.4 | -8.1 |
| 1171.7 | 1.7 | 23.0 | 1176.0 | 2.4 | 23.9 | 4.3 | 0.7 | 0.9 |
| 1189.5 | 0.4 | 4.7 | 1192.8 | 0.3 | 6.2 | 3.4 | -0.1 | 1.5 |
| 1219.2 | 1.9 | 35.1 | 1220.0 | 4.0 | 33.6 | 0.8 | 2.0 | -1.5 |
| 1252.0 | 0.8 | 36.4 | 1256.2 | 4.4 | 39.8 | 4.2 | 3.6 | 3.4 |
| 1265.3 | 15.8 | 31.0 | 1268.9 | 30.9 | 19.4 | 3.6 | 15.0 | -11.5 |
| 1309.4 | 0.4 | 3.4 | 1314.8 | 0.5 | 8.5 | 5.4 | 0.2 | 5.1 |
| 1321.0 | 1.9 | 13.6 | 1324.2 | 0.4 | 8.5 | 3.1 | -1.5 | -5.1 |
| 1364.9 | 2.6 | 186.7 | 1368.0 | 4.6 | 153.8 | 3.2 | 2.0 | -32.9 |
| 1377.8 | 3.0 | 176.7 | 1382.4 | 8.1 | 247.0 | 4.6 | 5.1 | 70.4 |
| 1426.3 | 1.8 | 76.0 | 1427.9 | 8.2 | 121.3 | 1.6 | 6.4 | 45.3 |
| 1439.5 | 1.5 | 55.1 | 1445.6 | 1.8 | 67.1 | 6.2 | 0.4 | 12.0 |
| 1482.6 | 7.0 | 96.1 | 1481.9 | 23.0 | 92.2 | -0.7 | 15.9 | -4.0 |
| 1494.3 | 6.9 | 18.7 | 1495.2 | 15.4 | 40.0 | 0.9 | 8.5 | 21.2 |
| 1524.6 | 12.5 | 0.8 | 1527.1 | 18.7 | 3.8 | 2.5 | 6.2 | 3.0 |
| 1565.4 | 7.4 | 63.1 | 1565.9 | 25.7 | 76.0 | 0.6 | 18.3 | 12.9 |
| 1609.6 | 6.6 | 30.6 | 1612.9 | 7.3 | 48.8 | 3.2 | 0.7 | 18.3 |
| 1632.2 | 25.2 | 30.0 | 1631.3 | 28.0 | 29.5 | -0.9 | 2.8 | -0.4 |
| 1648.7 | 7.1 | 80.0 | 1649.5 | 4.7 | 81.9 | 0.9 | -2.4 | 1.9 |
| 1657.5 | 10.0 | 30.0 | 1658.5 | 34.3 | 91.1 | 0.9 | 24.3 | 61.1 |
| 3114.2 | 21.3 | 122.1 | 3146.2 | 2.9 | 56.6 | 32.0 | -18.5 | -65.6 |
| 3165.5 | 3.2 | 58.4 | 3171.8 | 1.1 | 49.9 | 6.2 | -2.1 | -8.5 |
| 3170.2 | 0.2 | 80.5 | 3167.7 | 1.0 | 194.8 | -2.5 | 0.7 | 114.3 |
| 3174.6 | 9.3 | 103.5 | 3178.1 | 0.4 | 179.7 | 3.5 | -8.9 | 76.2 |
| 3182.1 | 11.3 | 62.8 | 3179.8 | 8.6 | 15.0 | -2.3 | -2.7 | -47.8 |
| 3190.0 | 5.8 | 221.0 | 3192.0 | 11.3 | 18.8 | 2.0 | 5.5 | -202.3 |
| 3193.9 | 12.4 | 140.8 | 3196.1 | 2.4 | 467.6 | 2.3 | -10.0 | 326.8 |
| 3199.5 | 17.5 | 120.5 | 3200.5 | 12.5 | 46.0 | 0.9 | -5.0 | -74.6 |
| 3205.1 | 15.4 | 296.5 | 3210.5 | 17.3 | 310.1 | 5.4 | 2.0 | 13.6 |

[a] Frequencies (*ω*) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

**Table A-25.1:** Harmonic Vibrational Frequencies for Cinnoline and Cinnoline/Ag$_2$ Complex (**N1**)[a]

| Cinnoline | | | Cinnoline/Ag$_2$ Complex (**N1**) | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 17.2 | 0.5 | 0.4 | | | |
| | | | 22.2 | 0.2 | 2.6 | | | |
| | | | 68.0 | 0.1 | 12.3 | | | |
| | | | 83.3 | 1.5 | 4.5 | | | |
| | | | 100.8 | 0.8 | 1.3 | | | |
| 174.6 | 3.6 | 0.0 | 177.0 | 3.9 | 0.1 | 2.4 | 2.4 | 0.3 |
| | | | 192.4 | 10.4 | 57.3 | | | |
| 180.8 | 2.9 | 0.2 | 199.9 | 0.2 | 2.0 | 19.0 | 19.0 | -2.7 |
| 379.9 | 3.0 | 0.2 | 387.7 | 4.2 | 0.6 | 7.7 | 7.7 | 1.3 |
| 387.0 | 1.2 | 1.3 | 391.8 | 0.7 | 0.1 | 4.9 | 4.9 | -0.4 |
| 480.9 | 0.2 | 0.1 | 485.7 | 3.8 | 2.1 | 4.8 | 4.8 | 3.6 |
| 487.7 | 7.0 | 0.1 | 489.1 | 2.8 | 0.8 | 1.4 | 1.4 | -4.3 |
| 519.7 | 1.1 | 10.4 | 533.6 | 6.3 | 20.2 | 13.9 | 13.9 | 5.2 |
| 539.9 | 0.8 | 11.5 | 539.4 | 1.3 | 11.9 | -0.6 | -0.6 | 0.5 |
| 650.9 | 2.6 | 0.6 | 651.7 | 5.4 | 0.5 | 0.9 | 0.9 | 2.8 |
| 673.1 | 1.3 | 0.1 | 674.9 | 0.1 | 1.5 | 1.8 | 1.8 | -1.2 |
| 765.8 | 37.3 | 0.4 | 768.6 | 34.0 | 0.0 | 2.9 | 2.9 | -3.3 |
| 786.6 | 1.7 | 41.5 | 787.0 | 6.9 | 58.9 | 0.4 | 0.4 | 5.2 |
| 819.4 | 1.0 | 0.0 | 820.2 | 1.9 | 0.2 | 0.8 | 0.8 | 0.8 |
| 836.5 | 3.1 | 0.9 | 845.1 | 6.0 | 1.6 | 8.6 | 8.6 | 2.9 |
| 862.8 | 45.3 | 0.1 | 866.0 | 43.5 | 0.1 | 3.1 | 3.1 | -1.8 |
| 901.9 | 1.2 | 0.1 | 904.9 | 1.9 | 0.0 | 3.0 | 3.0 | 0.7 |
| 976.8 | 1.2 | 0.1 | 982.7 | 0.8 | 1.0 | 5.9 | 5.9 | -0.4 |
| 991.3 | 1.3 | 1.0 | 995.2 | 0.6 | 2.9 | 3.8 | 3.8 | -0.8 |
| 1003.5 | 0.9 | 0.1 | 1006.6 | 1.5 | 0.7 | 3.2 | 3.2 | 0.6 |
| 1020.2 | 0.0 | 0.3 | 1025.7 | 0.0 | 0.4 | 5.6 | 5.6 | 0.0 |
| 1031.9 | 2.9 | 15.4 | 1032.7 | 3.5 | 20.7 | 0.8 | 0.8 | 0.6 |
| 1054.1 | 0.9 | 19.8 | 1073.3 | 1.2 | 58.6 | 19.2 | 19.2 | 0.3 |
| 1131.9 | 8.9 | 1.3 | 1147.2 | 9.8 | 2.4 | 15.4 | 15.4 | 0.9 |
| 1164.3 | 6.4 | 3.3 | 1166.9 | 10.6 | 2.8 | 2.5 | 2.5 | 4.2 |
| 1192.5 | 1.6 | 2.1 | 1193.3 | 13.3 | 7.1 | 0.8 | 0.8 | 11.7 |
| 1219.2 | 10.8 | 7.4 | 1223.7 | 20.3 | 4.5 | 4.5 | 4.5 | 9.6 |
| 1283.1 | 0.9 | 3.8 | 1286.0 | 1.1 | 5.1 | 2.8 | 2.8 | 0.2 |
| 1297.8 | 5.6 | 10.2 | 1303.0 | 8.0 | 5.5 | 5.2 | 5.2 | 2.4 |
| 1319.0 | 4.2 | 2.4 | 1328.9 | 5.5 | 8.9 | 9.9 | 9.9 | 1.3 |

[a] Frequencies (*ω*) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

**Table A-25.1 Continued**[a]

| Cinnoline | | | Cinnoline/$Ag_2$ Complex (**N1**) | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| 1407.9 | 9.9 | 122.5 | 1412.1 | 19.9 | 244.7 | 4.2 | 10.0 | 122.2 |
| 1452.5 | 3.7 | 15.3 | 1454.3 | 3.6 | 44.9 | 1.8 | -0.1 | 29.6 |
| 1484.3 | 4.3 | 24.0 | 1487.4 | 5.5 | 60.5 | 3.0 | 1.2 | 36.5 |
| 1529.8 | 7.3 | 8.4 | 1534.0 | 6.8 | 7.9 | 4.3 | -0.5 | -0.5 |
| 1581.2 | 0.1 | 23.9 | 1581.4 | 2.7 | 20.1 | 0.2 | 2.7 | -3.8 |
| 1619.5 | 11.1 | 16.1 | 1623.6 | 12.2 | 46.3 | 4.1 | 1.2 | 30.2 |
| 1661.8 | 2.4 | 6.1 | 1661.3 | 2.9 | 19.1 | -0.6 | 0.4 | 13.0 |
| 3166.9 | 0.6 | 32.8 | 3173.5 | 0.3 | 42.4 | 6.6 | -0.3 | 9.6 |
| 3170.3 | 3.2 | 96.3 | 3182.7 | 0.6 | 71.9 | 12.4 | -2.6 | -24.4 |
| 3178.7 | 8.7 | 101.9 | 3184.4 | 8.8 | 159.6 | 5.7 | 0.1 | 57.7 |
| 3190.7 | 11.1 | 128.8 | 3195.2 | 8.7 | 237.7 | 4.5 | -2.4 | 109.0 |
| 3192.9 | 16.1 | 209.1 | 3207.1 | 4.4 | 128.9 | 14.2 | -11.8 | -80.2 |
| 3202.1 | 6.5 | 225.4 | 3207.8 | 7.0 | 217.0 | 5.6 | 0.5 | -8.4 |
| 1407.9 | 9.9 | 122.5 | 1412.1 | 19.9 | 244.7 | 4.2 | 10.0 | 122.2 |
| 1452.5 | 3.7 | 15.3 | 1454.3 | 3.6 | 44.9 | 1.8 | -0.1 | 29.6 |
| 1484.3 | 4.3 | 24.0 | 1487.4 | 5.5 | 60.5 | 3.0 | 1.2 | 36.5 |
| 1529.8 | 7.3 | 8.4 | 1534.0 | 6.8 | 7.9 | 4.3 | -0.5 | -0.5 |
| 1581.2 | 0.1 | 23.9 | 1581.4 | 2.7 | 20.1 | 0.2 | 2.7 | -3.8 |
| 1619.5 | 11.1 | 16.1 | 1623.6 | 12.2 | 46.3 | 4.1 | 1.2 | 30.2 |
| 1661.8 | 2.4 | 6.1 | 1661.3 | 2.9 | 19.1 | -0.6 | 0.4 | 13.0 |
| 3166.9 | 0.6 | 32.8 | 3173.5 | 0.3 | 42.4 | 6.6 | -0.3 | 9.6 |
| 3170.3 | 3.2 | 96.3 | 3182.7 | 0.6 | 71.9 | 12.4 | -2.6 | -24.4 |
| 3178.7 | 8.7 | 101.9 | 3184.4 | 8.8 | 159.6 | 5.7 | 0.1 | 57.7 |
| 3190.7 | 11.1 | 128.8 | 3195.2 | 8.7 | 237.7 | 4.5 | -2.4 | 109.0 |
| 3192.9 | 16.1 | 209.1 | 3207.1 | 4.4 | 128.9 | 14.2 | -11.8 | -80.2 |
| 3202.1 | 6.5 | 225.4 | 3207.8 | 7.0 | 217.0 | 5.6 | 0.5 | -8.4 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

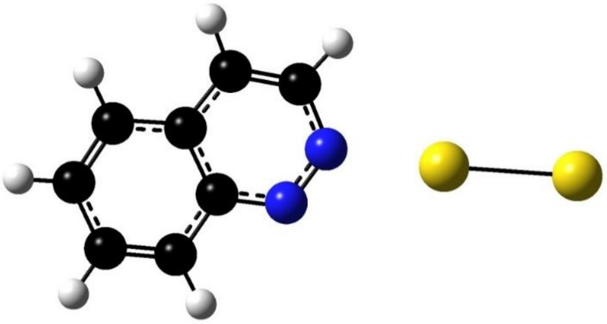


**Figure A-25.1:** Cinnoline/$Ag_2$ Complex (**N1**)

**Table A-25.2:** Harmonic Vibrational Frequencies for Cinnoline and Cinnoline/$Ag_2$ Complex (**N2**)[a]

| Cinnoline | | | Cinnoline/$Ag_2$ Complex (**N2**) | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 23.2 | 0.6 | 0.5 | | | |
| | | | 24.6 | 0.4 | 5.0 | | | |
| | | | 70.6 | 0.1 | 10.8 | | | |
| | | | 80.3 | 0.1 | 0.6 | | | |
| | | | 104.5 | 4.2 | 5.0 | | | |
| 174.6 | 3.6 | 0.0 | 178.4 | 0.3 | 0.2 | 3.8 | -3.4 | 0.1 |
| | | | 190.1 | 3.4 | 1.5 | 9.3 | 3.4 | 1.5 |
| 180.8 | 2.9 | 0.2 | 192.5 | 11.4 | 41.0 | | | |
| 379.9 | 3.0 | 0.2 | 390.8 | 4.7 | 0.3 | 10.9 | 1.7 | 0.0 |
| 387.0 | 1.2 | 1.3 | 392.8 | 0.2 | 1.3 | 5.9 | -0.9 | -0.1 |
| 480.9 | 0.2 | 0.1 | 482.9 | 0.2 | 0.1 | 1.9 | 0.0 | 0.0 |
| 487.7 | 7.0 | 0.1 | 494.0 | 7.7 | 0.1 | 6.3 | 0.6 | 0.0 |
| 519.7 | 1.1 | 10.4 | 519.7 | 2.2 | 12.7 | 0.0 | 1.1 | 2.2 |
| 539.9 | 0.8 | 11.5 | 542.0 | 1.8 | 12.7 | 2.0 | 1.0 | 1.2 |
| 650.9 | 2.6 | 0.6 | 659.6 | 2.0 | 0.9 | 8.7 | -0.6 | 0.3 |
| 673.1 | 1.3 | 0.1 | 674.1 | 2.6 | 0.4 | 1.0 | 1.3 | 0.3 |
| 765.8 | 37.3 | 0.4 | 767.6 | 28.6 | 0.6 | 1.8 | -8.7 | 0.2 |
| 786.6 | 1.7 | 41.5 | 793.7 | 6.1 | 48.6 | 7.1 | 4.4 | 7.1 |
| 819.4 | 1.0 | 0.0 | 821.0 | 2.7 | 0.1 | 1.6 | 1.6 | 0.1 |
| 836.5 | 3.1 | 0.9 | 835.1 | 4.1 | 1.7 | -1.4 | 1.0 | 0.7 |
| 862.8 | 45.3 | 0.1 | 868.8 | 37.1 | 0.3 | 5.9 | -8.2 | 0.2 |
| 901.9 | 1.2 | 0.1 | 906.0 | 4.9 | 1.2 | 4.2 | 3.7 | 1.1 |
| 976.8 | 1.2 | 0.1 | 984.0 | 1.5 | 0.1 | 7.2 | 0.3 | 0.0 |
| 991.3 | 1.3 | 1.0 | 996.0 | 0.3 | 2.1 | 4.6 | -1.0 | 1.1 |
| 1003.5 | 0.9 | 0.1 | 1009.0 | 0.3 | 0.0 | 5.6 | -0.6 | -0.1 |
| 1020.2 | 0.0 | 0.3 | 1026.4 | 0.1 | 1.9 | 6.2 | 0.0 | 1.5 |
| 1031.9 | 2.9 | 15.4 | 1035.9 | 3.8 | 22.4 | 4.1 | 0.9 | 7.0 |
| 1054.1 | 0.9 | 19.8 | 1073.7 | 0.5 | 21.2 | 19.7 | -0.3 | 1.5 |
| 1131.9 | 8.9 | 1.3 | 1142.0 | 20.1 | 6.1 | 10.1 | 11.3 | 4.8 |
| 1164.3 | 6.4 | 3.3 | 1170.3 | 2.7 | 10.6 | 5.9 | -3.7 | 7.3 |
| 1192.5 | 1.6 | 2.1 | 1197.8 | 5.4 | 3.4 | 5.3 | 3.8 | 1.3 |
| 1219.2 | 10.8 | 7.4 | 1225.7 | 9.4 | 6.3 | 6.5 | -1.3 | -1.1 |
| 1283.1 | 0.9 | 3.8 | 1289.0 | 0.6 | 10.6 | 5.9 | -0.3 | 6.8 |
| 1297.8 | 5.6 | 10.2 | 1299.2 | 9.9 | 22.0 | 1.5 | 4.3 | 11.8 |

[a] Frequencies ($\omega$) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-25.2 Continued**[a]

| Cinnoline | | | Cinnoline/$Ag_2$ Complex (**N2**) | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| 1407.9 | 9.9 | 122.5 | 1412.0 | 14.9 | 126.2 | 4.0 | 5.0 | 3.7 |
| 1452.5 | 3.7 | 15.3 | 1455.8 | 6.3 | 13.3 | 3.3 | 2.7 | -2.0 |
| 1484.3 | 4.3 | 24.0 | 1484.0 | 12.0 | 21.9 | -0.4 | 7.7 | -2.1 |
| 1529.8 | 7.3 | 8.4 | 1531.9 | 16.9 | 12.7 | 2.1 | 9.6 | 4.4 |
| 1581.2 | 0.1 | 23.9 | 1586.0 | 3.1 | 22.4 | 4.7 | 3.0 | -1.4 |
| 1619.5 | 11.1 | 16.1 | 1616.9 | 15.3 | 37.4 | -2.5 | 4.2 | 21.2 |
| 1661.8 | 2.4 | 6.1 | 1661.5 | 0.3 | 3.9 | -0.3 | -2.1 | -2.2 |
| 3166.9 | 0.6 | 32.8 | 3171.2 | 0.4 | 106.1 | 4.3 | -0.3 | 73.3 |
| 3170.3 | 3.2 | 96.3 | 3175.7 | 1.1 | 137.0 | 5.4 | -2.1 | 40.8 |
| 3178.7 | 8.7 | 101.9 | 3179.6 | 1.5 | 131.6 | 0.8 | -7.3 | 29.7 |
| 3190.7 | 11.1 | 128.8 | 3188.1 | 7.6 | 60.2 | -2.6 | -3.5 | -68.5 |
| 3192.9 | 16.1 | 209.1 | 3199.2 | 10.8 | 320.1 | 6.3 | -5.3 | 110.9 |
| 3202.1 | 6.5 | 225.4 | 3201.6 | 11.8 | 296.1 | -0.6 | 5.3 | 70.6 |
| 1407.9 | 9.9 | 122.5 | 1412.0 | 14.9 | 126.2 | 4.0 | 5.0 | 3.7 |
| 1452.5 | 3.7 | 15.3 | 1455.8 | 6.3 | 13.3 | 3.3 | 2.7 | -2.0 |
| 1484.3 | 4.3 | 24.0 | 1484.0 | 12.0 | 21.9 | -0.4 | 7.7 | -2.1 |
| 1529.8 | 7.3 | 8.4 | 1531.9 | 16.9 | 12.7 | 2.1 | 9.6 | 4.4 |
| 1581.2 | 0.1 | 23.9 | 1586.0 | 3.1 | 22.4 | 4.7 | 3.0 | -1.4 |
| 1619.5 | 11.1 | 16.1 | 1616.9 | 15.3 | 37.4 | -2.5 | 4.2 | 21.2 |
| 1661.8 | 2.4 | 6.1 | 1661.5 | 0.3 | 3.9 | -0.3 | -2.1 | -2.2 |
| 3166.9 | 0.6 | 32.8 | 3171.2 | 0.4 | 106.1 | 4.3 | -0.3 | 73.3 |
| 3170.3 | 3.2 | 96.3 | 3175.7 | 1.1 | 137.0 | 5.4 | -2.1 | 40.8 |
| 3178.7 | 8.7 | 101.9 | 3179.6 | 1.5 | 131.6 | 0.8 | -7.3 | 29.7 |
| 3190.7 | 11.1 | 128.8 | 3188.1 | 7.6 | 60.2 | -2.6 | -3.5 | -68.5 |
| 3192.9 | 16.1 | 209.1 | 3199.2 | 10.8 | 320.1 | 6.3 | -5.3 | 110.9 |
| 3202.1 | 6.5 | 225.4 | 3201.6 | 11.8 | 296.1 | -0.6 | 5.3 | 70.6 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

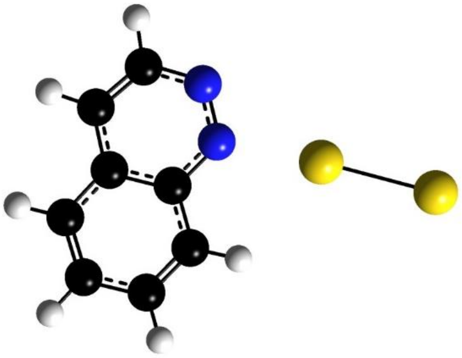


**Figure A-25.2:** Cinnoline/$Ag_2$ Complex (**N2**)

**Table A-26:** Harmonic Vibrational Frequencies for Phthalazine and Phthalazine/$Ag_2$ Complex[a]

| Phthalazine | | | Phthalazine/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 18.3 | 0.1 | 0.6 | | | |
| | | | 22.1 | 0.4 | 2.8 | | | |
| | | | 65.5 | 0.0 | 11.0 | | | |
| | | | 85.9 | 0.0 | 2.6 | | | |
| | | | 98.6 | 4.1 | 1.9 | | | |
| 168.6 | 2.2 | 0.3 | 174.1 | 0.5 | 0.2 | 5.4 | -1.7 | -0.2 |
| 174.8 | 0.0 | 0.0 | 192.3 | 11.6 | 53.2 | 17.5 | 11.6 | 53.2 |
| | | | 194.3 | 0.0 | 0.9 | | | |
| 355.9 | 0.4 | 0.0 | 364.4 | 1.0 | 0.3 | 8.5 | 0.5 | 0.3 |
| 388.1 | 5.7 | 0.3 | 392.8 | 3.5 | 2.2 | 4.7 | -2.2 | 1.9 |
| 462.1 | 0.0 | 0.0 | 470.6 | 0.0 | 0.4 | 8.5 | 0.0 | 0.3 |
| 486.9 | 18.8 | 0.0 | 487.0 | 17.4 | 0.1 | 0.0 | -1.4 | 0.1 |
| 517.9 | 0.4 | 14.1 | 522.6 | 2.0 | 17.1 | 4.6 | 1.6 | 3.0 |
| 529.3 | 0.4 | 6.8 | 540.6 | 1.4 | 11.1 | 11.3 | 1.0 | 4.3 |
| 669.2 | 0.0 | 0.0 | 670.5 | 12.1 | 2.2 | 1.2 | 12.1 | 2.1 |
| 669.5 | 6.9 | 1.7 | 671.5 | 0.4 | 0.5 | 2.0 | -6.5 | -1.2 |
| 768.6 | 49.4 | 0.2 | 771.8 | 47.0 | 0.2 | 3.2 | -2.4 | 0.0 |
| 812.3 | 0.0 | 0.1 | 810.8 | 0.0 | 0.5 | -1.4 | 0.0 | 0.4 |
| 813.1 | 1.3 | 39.3 | 812.6 | 1.0 | 55.4 | -0.4 | -0.3 | 16.1 |
| 825.2 | 1.1 | 0.3 | 835.8 | 0.4 | 0.4 | 10.5 | -0.8 | 0.1 |
| 888.8 | 0.0 | 0.2 | 891.6 | 0.0 | 0.2 | 2.8 | 0.0 | 0.0 |
| 933.1 | 14.8 | 0.2 | 941.6 | 14.8 | 0.1 | 8.5 | 0.0 | -0.1 |
| 970.2 | 13.4 | 0.1 | 970.5 | 16.4 | 0.6 | 0.3 | 3.0 | 0.5 |
| 972.2 | 0.0 | 0.0 | 976.8 | 0.1 | 0.4 | 4.7 | 0.1 | 0.4 |
| 976.4 | 2.4 | 0.1 | 993.0 | 17.3 | 0.5 | 16.6 | 14.8 | 0.5 |
| 993.5 | 3.5 | 0.4 | 998.2 | 3.3 | 0.6 | 4.7 | -0.1 | 0.3 |
| 1020.1 | 0.0 | 0.2 | 1025.7 | 0.0 | 0.2 | 5.6 | 0.0 | -0.1 |
| 1040.3 | 1.9 | 24.6 | 1041.9 | 1.2 | 35.5 | 1.6 | -0.7 | 10.9 |
| 1162.6 | 0.6 | 3.0 | 1164.6 | 0.6 | 2.2 | 1.9 | 0.1 | -0.9 |
| 1178.1 | 3.4 | 1.4 | 1183.0 | 6.3 | 5.6 | 5.0 | 2.9 | 4.2 |
| 1233.5 | 4.6 | 13.3 | 1239.9 | 8.8 | 27.0 | 6.3 | 4.2 | 13.8 |
| 1283.7 | 4.5 | 4.6 | 1287.5 | 5.4 | 5.0 | 3.7 | 0.8 | 0.4 |
| 1294.8 | 16.0 | 2.4 | 1297.1 | 12.6 | 1.9 | 2.3 | -3.3 | -0.5 |
| 1332.1 | 0.0 | 18.9 | 1340.9 | 4.0 | 41.4 | 8.8 | 4.0 | 22.5 |
| 1343.0 | 1.7 | 0.6 | 1347.6 | 4.5 | 1.2 | 4.6 | 2.8 | 0.6 |
| 1403.5 | 12.2 | 112.0 | 1405.1 | 29.4 | 223.7 | 1.5 | 17.2 | 111.8 |
| 1458.4 | 5.3 | 60.5 | 1467.8 | 9.3 | 180.6 | 9.4 | 4.0 | 120.2 |
| 1468.9 | 0.4 | 2.9 | 1473.2 | 1.6 | 10.5 | 4.3 | 1.2 | 7.7 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-26 Continued**[a]

| Phthalazine | | | Phthalazine/$Ag_2$ Complex | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| $\omega$ | IR | Raman | $\omega$ | IR | Raman | Δ ω | Δ IR | Δ Raman |
| 1524.6 | 3.3 | 12.4 | 1527.0 | 6.4 | 17.4 | 2.4 | 3.1 | 4.9 |
| 1601.7 | 5.2 | 0.4 | 1608.1 | 2.8 | 27.1 | 6.4 | -2.4 | 26.7 |
| 1615.3 | 2.6 | 18.7 | 1616.2 | 2.9 | 20.3 | 1.0 | 0.2 | 1.6 |
| 1661.3 | 1.4 | 9.2 | 1660.8 | 2.7 | 69.2 | -0.5 | 1.3 | 60.0 |
| 3143.9 | 23.2 | 17.5 | 3157.2 | 8.2 | 116.3 | 13.3 | -15.0 | 98.8 |
| 3145.8 | 0.4 | 199.2 | 3167.7 | 2.0 | 77.7 | 21.9 | 1.6 | -121.5 |
| 3169.4 | 1.0 | 21.4 | 3175.1 | 0.2 | 20.9 | 5.7 | -0.7 | -0.4 |
| 3174.7 | 0.6 | 133.0 | 3180.7 | 0.3 | 123.1 | 6.0 | -0.3 | -10.0 |
| 3185.2 | 15.4 | 59.4 | 3190.2 | 8.9 | 82.6 | 5.0 | -6.5 | 23.3 |
| 3195.9 | 11.3 | 295.7 | 3199.9 | 9.8 | 372.0 | 4.0 | -1.5 | 76.3 |

[a] Frequencies ($\omega$) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-27.1:** Harmonic Vibrational Frequencies for Quinazoline and Quinazoline /Ag$_2$ Complex (**N1**)[a]

| Quinazoline | | | Quinazoline /Ag$_2$ Complex (**N1**) | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 19.4 | 0.0 | 0.3 | | | |
| | | | 21.5 | 0.1 | 2.4 | | | |
| | | | 65.9 | 0.1 | 11.4 | | | |
| | | | 87.0 | 0.7 | 4.9 | | | |
| | | | 100.1 | 3.3 | 2.2 | | | |
| 172.3 | 0.1 | 0.2 | 180.8 | 0.0 | 0.0 | 8.6 | -0.1 | -0.1 |
| | | | 193.0 | 10.5 | 51.5 | | | |
| 180.0 | 0.2 | 0.0 | 193.1 | 2.0 | 0.8 | 13.1 | 1.8 | 0.8 |
| 380.7 | 1.5 | 0.1 | 389.4 | 3.4 | 0.5 | 8.7 | 1.9 | 0.4 |
| 395.8 | 0.6 | 1.1 | 400.6 | 1.1 | 1.8 | 4.8 | 0.5 | 0.6 |
| 466.8 | 0.1 | 0.0 | 471.0 | 0.1 | 0.4 | 4.2 | 0.0 | 0.3 |
| 501.1 | 10.6 | 0.2 | 500.3 | 7.1 | 0.2 | -0.8 | -3.5 | 0.0 |
| 523.5 | 1.0 | 12.1 | 537.7 | 5.8 | 20.5 | 14.2 | 4.8 | 8.3 |
| 542.0 | 0.3 | 8.7 | 542.4 | 3.6 | 4.8 | 0.4 | 3.3 | -3.9 |
| 650.5 | 11.1 | 0.9 | 649.2 | 22.0 | 0.7 | -1.3 | 11.0 | -0.1 |
| 661.6 | 5.3 | 0.2 | 660.1 | 2.5 | 0.7 | -1.5 | -2.9 | 0.5 |
| 770.3 | 47.9 | 0.3 | 773.1 | 45.9 | 0.4 | 2.7 | -2.0 | 0.1 |
| 788.5 | 3.3 | 41.9 | 788.6 | 2.6 | 58.7 | 0.1 | -0.8 | 16.8 |
| 818.7 | 15.3 | 0.2 | 818.5 | 13.3 | 0.1 | -0.2 | -2.0 | -0.2 |
| 838.6 | 3.0 | 0.3 | 848.9 | 6.3 | 0.4 | 10.3 | 3.3 | 0.0 |
| 896.7 | 6.6 | 0.1 | 899.8 | 5.7 | 0.1 | 3.1 | -0.9 | -0.1 |
| 952.0 | 5.4 | 0.0 | 957.1 | 6.3 | 0.3 | 5.0 | 0.9 | 0.3 |
| 959.5 | 8.2 | 0.8 | 970.2 | 18.5 | 3.1 | 10.7 | 10.2 | 2.3 |
| 992.3 | 3.6 | 0.8 | 995.2 | 2.3 | 1.5 | 2.9 | -1.3 | 0.7 |
| 1013.4 | 0.3 | 0.1 | 1009.0 | 1.2 | 0.4 | -4.4 | 0.9 | 0.3 |
| 1019.4 | 0.1 | 0.2 | 1025.4 | 0.1 | 0.2 | 6.0 | 0.0 | 0.0 |
| 1034.9 | 3.0 | 19.9 | 1035.5 | 3.9 | 25.4 | 0.7 | 0.8 | 5.6 |
| 1106.5 | 7.9 | 8.6 | 1096.0 | 24.3 | 26.2 | -10.5 | 16.4 | 17.6 |
| 1160.9 | 7.4 | 4.8 | 1161.7 | 8.2 | 8.6 | 0.8 | 0.9 | 3.8 |
| 1177.6 | 9.3 | 3.4 | 1179.7 | 27.8 | 3.8 | 2.1 | 18.5 | 0.5 |
| 1238.9 | 5.8 | 10.3 | 1241.9 | 23.1 | 12.6 | 3.0 | 17.3 | 2.3 |
| 1268.8 | 0.7 | 2.6 | 1273.0 | 0.2 | 8.4 | 4.2 | -0.5 | 5.8 |
| 1294.0 | 0.2 | 3.7 | 1296.2 | 0.9 | 2.9 | 2.2 | 0.8 | -0.8 |
| 1345.9 | 9.1 | 10.3 | 1351.0 | 3.9 | 10.9 | 5.1 | -5.2 | 0.6 |
| 1395.3 | 19.9 | 83.4 | 1397.9 | 41.7 | 139.1 | 2.6 | 21.8 | 55.7 |

[a] Frequencies (*ω*) in cm$^{-1}$, IR intensities in km mol$^{-1}$, and Raman scattering activities in A$^4$ amu$^{-1}$

**Table A-27.1 Continued**[a]

| **Quinazoline** | | | Quinazoline /$Ag_2$ Complex (**N1**) | | | **Differences** | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| 1416.7 | 16.6 | 1.0 | 1421.4 | 19.6 | 2.9 | 4.7 | 3.0 | 1.8 |
| 1441.4 | 12.1 | 77.7 | 1445.8 | 4.5 | 176.8 | 4.4 | -7.6 | 99.1 |
| 1492.0 | 1.2 | 7.2 | 1496.3 | 2.1 | 7.3 | 4.3 | 0.8 | 0.1 |
| 1527.2 | 37.0 | 9.9 | 1526.6 | 32.9 | 19.6 | -0.5 | -4.1 | 9.7 |
| 1599.4 | 45.5 | 24.9 | 1601.2 | 35.6 | 30.8 | 1.8 | -9.9 | 5.9 |
| 1620.4 | 63.5 | 2.6 | 1628.8 | 123.7 | 16.6 | 8.4 | 60.3 | 14.0 |
| 1660.3 | 33.4 | 8.2 | 1660.1 | 64.0 | 39.2 | -0.2 | 30.7 | 31.0 |
| 3125.7 | 18.2 | 102.2 | 3155.4 | 6.5 | 43.5 | 29.6 | -11.7 | -58.7 |
| 3165.2 | 20.7 | 153.1 | 3172.9 | 0.6 | 41.4 | 7.6 | -20.2 | -111.6 |
| 3166.1 | 1.2 | 67.0 | 3181.2 | 5.2 | 102.5 | 15.1 | 3.9 | 35.5 |
| 3176.1 | 7.3 | 94.0 | 3182.6 | 1.7 | 82.6 | 6.5 | -5.6 | -11.4 |
| 3191.7 | 12.2 | 147.9 | 3196.2 | 8.9 | 201.6 | 4.5 | -3.4 | 53.7 |
| 3201.5 | 6.4 | 209.9 | 3205.7 | 5.3 | 253.9 | 4.2 | -1.0 | 44.1 |

[a] Frequencies ($\omega$) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

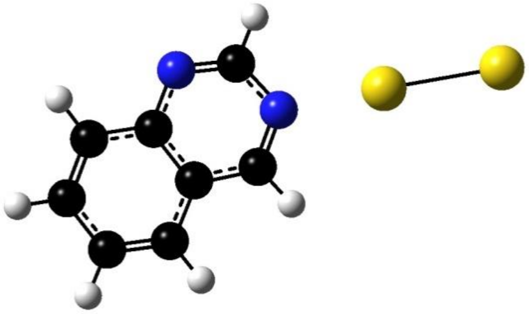


**Figure A-27.1:** Quinazoline /$Ag_2$ Complex (**N1**)

**Table A-27.2:** Harmonic Vibrational Frequencies for Quinazoline and Quinazoline /$Ag_2$ Complex (**N3**)[a]

| Quinazoline | | | Quinazoline /$Ag_2$ Complex (**N3**) | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| | | | 23.1 | 0.0 | 0.2 | | | |
| | | | 23.6 | 0.2 | 4.8 | | | |
| | | | 69.7 | 0.0 | 10.8 | | | |
| | | | 81.4 | 0.4 | 1.6 | | | |
| | | | 106.2 | 3.9 | 5.9 | | | |
| 180.0 | 0.2 | 0.0 | 178.3 | 0.1 | 0.3 | -1.6 | -0.1 | 0.3 |
| 172.3 | 0.1 | 0.2 | 184.4 | 0.3 | 0.5 | 12.1 | 0.2 | 0.3 |
| | | | 193.5 | 10.8 | 37.4 | | | |
| 380.7 | 1.5 | 0.1 | 391.4 | 3.5 | 0.7 | 10.8 | 2.0 | 0.6 |
| 395.8 | 0.6 | 1.1 | 399.0 | 0.0 | 0.7 | 3.2 | -0.6 | -0.4 |
| 466.8 | 0.1 | 0.0 | 467.6 | 0.1 | 0.3 | 0.8 | 0.0 | 0.2 |
| 501.1 | 10.6 | 0.2 | 504.4 | 12.5 | 0.2 | 3.3 | 1.9 | -0.1 |
| 523.5 | 1.0 | 12.1 | 527.1 | 1.4 | 12.2 | 3.6 | 0.5 | 0.0 |
| 542.0 | 0.3 | 8.7 | 542.1 | 3.2 | 9.4 | 0.1 | 2.9 | 0.7 |
| 650.5 | 11.1 | 0.9 | 659.4 | 16.3 | 2.2 | 8.9 | 5.2 | 1.3 |
| 661.6 | 5.3 | 0.2 | 659.9 | 3.5 | 0.5 | -1.7 | -1.9 | 0.3 |
| 770.3 | 47.9 | 0.3 | 773.1 | 39.0 | 0.1 | 2.8 | -8.9 | -0.2 |
| 788.5 | 3.3 | 41.9 | 796.8 | 18.0 | 42.8 | 8.3 | 14.6 | 0.9 |
| 818.7 | 15.3 | 0.2 | 818.6 | 15.6 | 0.5 | -0.1 | 0.3 | 0.3 |
| 838.6 | 3.0 | 0.3 | 837.6 | 2.3 | 1.5 | -0.9 | -0.7 | 1.2 |
| 896.7 | 6.6 | 0.1 | 899.1 | 2.7 | 0.9 | 2.4 | -3.9 | 0.8 |
| 952.0 | 5.4 | 0.0 | 958.8 | 5.7 | 0.0 | 6.8 | 0.4 | 0.0 |
| 959.5 | 8.2 | 0.8 | 967.2 | 8.8 | 3.6 | 7.7 | 0.5 | 2.8 |
| 992.3 | 3.6 | 0.8 | 996.3 | 1.4 | 1.1 | 4.0 | -2.3 | 0.3 |
| 1013.4 | 0.3 | 0.1 | 1017.9 | 0.6 | 0.0 | 4.5 | 0.3 | 0.0 |
| 1019.4 | 0.1 | 0.2 | 1027.0 | 0.0 | 0.9 | 7.6 | -0.1 | 0.7 |
| 1034.9 | 3.0 | 19.9 | 1040.0 | 4.6 | 30.6 | 5.2 | 1.5 | 10.7 |
| 1106.5 | 7.9 | 8.6 | 1124.3 | 5.7 | 6.7 | 17.8 | -2.2 | -1.9 |
| 1160.9 | 7.4 | 4.8 | 1166.4 | 4.2 | 8.8 | 5.5 | -3.2 | 4.0 |
| 1177.6 | 9.3 | 3.4 | 1184.2 | 9.6 | 2.8 | 6.6 | 0.3 | -0.6 |
| 1238.9 | 5.8 | 10.3 | 1240.4 | 16.9 | 24.4 | 1.6 | 11.1 | 14.2 |
| 1268.8 | 0.7 | 2.6 | 1273.7 | 2.0 | 9.1 | 4.9 | 1.4 | 6.5 |
| 1294.0 | 0.2 | 3.7 | 1296.5 | 3.7 | 11.2 | 2.5 | 3.6 | 7.5 |
| 1345.9 | 9.1 | 10.3 | 1343.1 | 34.0 | 42.3 | -2.7 | 24.9 | 32.0 |
| 1395.3 | 19.9 | 83.4 | 1398.7 | 26.7 | 112.8 | 3.4 | 6.8 | 29.4 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

**Table A-27.2 Continued**[a]

| Quinazoline | | | Quinazoline /$Ag_2$ Complex (**N3**) | | | Differences | | |
|---|---|---|---|---|---|---|---|---|
| *ω* | IR | Raman | *ω* | IR | Raman | Δ ω | Δ IR | Δ Raman |
| 1416.7 | 16.6 | 1.0 | 1422.1 | 26.8 | 3.9 | 5.4 | 10.3 | 2.8 |
| 1441.4 | 12.1 | 77.7 | 1444.7 | 7.0 | 45.9 | 3.3 | -5.1 | -31.8 |
| 1492.0 | 1.2 | 7.2 | 1492.6 | 8.3 | 10.0 | 0.6 | 7.0 | 2.8 |
| 1527.2 | 37.0 | 9.9 | 1531.5 | 91.7 | 11.2 | 4.3 | 54.7 | 1.3 |
| 1599.4 | 45.5 | 24.9 | 1605.4 | 61.2 | 32.0 | 6.0 | 15.7 | 7.0 |
| 1620.4 | 63.5 | 2.6 | 1615.4 | 40.8 | 2.5 | -5.0 | -22.7 | -0.1 |
| 1660.3 | 33.4 | 8.2 | 1659.5 | 31.6 | 9.8 | -0.8 | -1.8 | 1.6 |
| 3125.7 | 18.2 | 102.2 | 3137.4 | 14.5 | 138.7 | 11.7 | -3.7 | 36.5 |
| 3165.2 | 20.7 | 153.1 | 3172.4 | 1.1 | 32.0 | 7.1 | -19.6 | -121.1 |
| 3166.1 | 1.2 | 67.0 | 3176.4 | 1.3 | 245.0 | 10.3 | 0.1 | 177.9 |
| 3176.1 | 7.3 | 94.0 | 3182.9 | 1.4 | 72.2 | 6.8 | -5.9 | -21.8 |
| 3191.7 | 12.2 | 147.9 | 3187.6 | 6.5 | 32.8 | -4.0 | -5.7 | -115.1 |
| 3201.5 | 6.4 | 209.9 | 3199.3 | 10.7 | 367.8 | -2.2 | 4.3 | 157.9 |

[a] Frequencies (*ω*) in $cm^{-1}$, IR intensities in km $mol^{-1}$, and Raman scattering activities in $A^4$ $amu^{-1}$

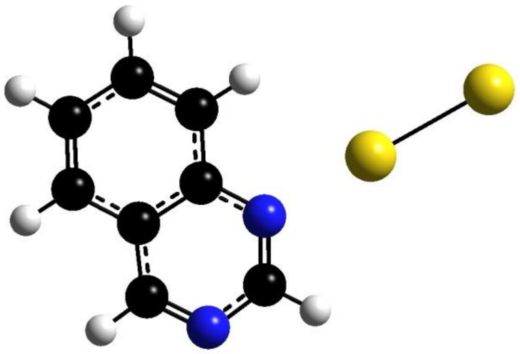


**Figure A-27.2:** Quinazoline /$Ag_2$ Complex (**N3**)