THE DETECTION OF CYANIDE BY A RUTHENIUM(II)-COPPER(II) HETEROBIMETALLIC CHEMOSIMETRIC ENSEMBLE
Abstract:

The current cyanide detection processes used in industry are time consuming and imprecise. There are only a few chemodosimeters that can specifically detect cyanide. A Ru(II)-Cu(II) metal complex was synthesized in order to increase effectiveness, accuracy, and efficiency of cyanide detection. This metal complex is more selective than the previous methods, as it is the only trinuclear complex synthesized for the purpose of cyanide detection and has been proven to only produce a color change in reaction with cyanide anions. The Ru('bubpy)(CN)$_4$ solution was analyzed via spectroscopic titration to determine the lowest concentration of cyanide that can be detected. In the presence of cyanide, the Ru(II)-Cu(II) complex reacted to form Ru('bubpy)(CN)$_4$ and Cu(dien)(L)$_2$, which produced a noticeable color change from green to orange. The current detection limits of cyanide are low, and this Ru(II)-Cu(II) can detect lower concentrations of cyanide. This new chemodosimetric ensemble can serve as a stepping stone for the future development or other anion sensors.

Introduction:

A chemodosimetric ensemble, or a chemical complex that is designed to detect a specific chemical, has been a very popular area of study in the past ten or so years. ¹ Within this area of study, certain terminology is used interchangeably, which often leads to confusion for other scientists. Some terms used in place of chemodosimetric ensemble are metal complex, donor-acceptor complex, complex, chemodosimeter, and chemodosimetric sensor. These terms simply refer to a chemical that has a metal as the main atom, or as in the case of this paper, main atoms. Chemodosimetric ensembles are used to detect a variety of different molecules and ions, from cyanide to amino acids and peptides. ² Metal complexes can be
designed to show specificity toward a single anion by manipulating the complex’s characteristics. Scientists can manipulate chemical properties by combining different ligands and metal centers. Transition metals are particularly useful in this manipulation because they are stable at multiple oxidation states, which helps produce a variety of different energy states that can be made more stable through reactions. Chow et al. have synthesized and characterized \((\text{Ru}^{II}(\text{Bubpy})(\text{CN})_2^-\text{[Cu}^{II}(\text{dien})_2](\text{ClO}_4)_2\), Complex 1, a metal complex that to detect cyanide (Figure 1).³

Cyanide (CN⁻) detection is extremely important due to its extensive use in industry and its toxicity. Cyanide compounds are used in mining, metallurgy, photographic processing, and the production of some plastics including nitriles, nylon, and acrylic.⁴ According to the Environmental Protection Agency (EPA), the limit of cyanide in drinking water is 0.2 ppm.⁵ The current methods for detecting cyanide are time and money consuming, lack specificity, and are rather unreliable or unusable. Chromogenic sensors, sensors that produce color, for cyanide are uncommon due to the fact that an energy change of the magnitude needed to produce the color change is difficult to achieve with simple complexes, and so the field of cyanide sensors has not been thoroughly investigated so far.⁶,⁷

A ligand is a molecule attached to a metal center. A monodentate ligand, bonds in only one location (Figure 2). Some ligands are bi-, tri-, or polydentate, meaning they can bond with the metal in multiple locations. “bubpy” \((4,4'\text{-di-tert-butyl-2,2'\text{-bipyridine}})\) is a bidentate ligand;
both nitrogen atoms form bonds with the Ru(II) due to the fact that they each have a lone pair of electrons that can be donated to the Ru(II). The “dien” (diethylenetriamine) is a tridentate ligand, and contains three nitrogen atoms that each bond with the Cu(II) metal center. A less common ligand is a bridging ligand. Bridging ligands bond two metal centers together, like a bridge. In Complex 1, cyanide binds the Ru(II) and the Cu(II) metal centers together.

Along with types of ligands, there are two types of bonding interactions: σ-bonding and π-bonding. Sigma bonding occurs with the donation of electrons from either the ligand to metal or the metal to the ligand, depending upon oxidation states, open orbitals, and amount of electrons. Additionally, π-interactions are also possible. There are two types of π-interactions, named for the influence they have on the metal center. One type of π-interaction is π-donor, meaning that the ligand donates electron density with lone pairs in the p orbital, to the empty d_{xy}, d_{xz}, or d_{yz} orbitals of the metal center. The other π-interaction is π-acceptor interaction, meaning that the ligand accepts electron density from the metal. Cyanide is a π-acceptor, which means that electron density can shift from the filled d_{xy}, d_{xz} or d_{yz} orbital of the metal to the empty π* orbital of the ligand (Figure 3). When σ bonding occurs at the same time as π-acceptor interaction, a phenomenon known as backbonding occurs. Backbonding is favorable because it strengthens the overall bond between the metal and ligand.
The majority of chemodosimetric ensembles are metal complexes. Transition metals are elements of the d-block of the periodic table, and contain unfilled d-orbitals, which can produce cations that have incomplete d orbitals. The study of d-orbitals in particular, is called Molecular Orbital Theory. Molecular Orbital (MO) Theory studies the orbitals and electrons of complexes to show covalent bonding, where electrons are located (by orbital), and relative energies of the orbitals. However, MO Theory is limited, as it only concerns full bonds, and does not give a complete view of the interactions that occur, such as the \( \pi \)-characteristics. Another theory, Ligand Field Theory provides a more complete view.

Ligand Field Theory combines MO Theory and Crystal Field Theory, which is a theory that is concerned with the attractive and repulsive forces within complexes, but does not take the bonding of metals and ligands into account. Ligand Field Theory studies the bonding of the ligand and metal to form different types of orbitals (bonding, nonbonding, and antibonding) as well as the electron repulsion and attraction. This theory also helps explain the color of metal complexes by relating the energy between orbitals as a quantity that can be determined by the absorbance peak of an Ultraviolet-Visible light spectrum. The energy change of Complex I can be examined through the lens of Ligand Field Theory to explain why the change occurs and the color of the cyanide/Complex I solution.

Ultraviolet-Visul light spectroscopy (UV-Vis spectroscopy) is a technique that can be used to determine the concentration of analytes in solution. In UV-Vis spectroscopy, a sample is inserted into a spectrophotometer, and light is passed through the instrument. The spectrophotometer controls the intensity of light being passed into the sample, and compares it to the intensity of light being transmitted and absorbed by the sample. Spectrometers take an absorbance reading at every wavelength. This collects very accurate data. When light interacts
with the molecule, an electron is excited to the next orbital. The difference in intensity that the spectrophotometer measures is the absorbance, which is given in a graph plotted against wavelength. Beer's Law can be used to determine the concentration of the analyte. Beer's Law is \( A = \varepsilon bc \), where \( A \) is absorbance, \( \varepsilon \) is the molar absorptivity, \( b \) is the path length, and \( c \) is the analyte concentration. The path length is the length of the sample; industry standard is 1 cm for UV-Vis spectroscopy. The value of \( \varepsilon \) is the slope of the calibration curve of absorbance vs. concentration. Some absorbance bands on a UV-Vis spectrum are a specific type of band called a Metal to Ligand Charge Transfer (MLCT) band.

MLCT absorbance bands require two specific parameters to be met. These parameters are (a) a metal that is electron rich, and (b) a ligand with empty \( \pi^* \) orbitals. Both ruthenium (II) and copper (II) have a low oxidation state, meaning they are electron rich. Cyanide, a \( \pi \)-acceptor, is one of the most well-known ligands that undergo MLCT transitions. Additionally, MLCT absorption bands are more intense than regular absorption bands on a UV-VIS spectrum.

When an MLCT band transfers occurs, electrons are excited to the nonbonding \( \pi^* \) orbital of the ligand, which is lower in energy than the next \( \pi^* \) antibonding orbital (Figure 4).

Similarly to UV-Vis spectroscopy, a spectrofluorometry can be used to measure emission, rather than absorbance. Fluorescence occurs similarly to absorbance in that it is a measure of energy between the HOMO and LUMO. However, as the electron returns to the
ground state, light is emitted, rather than transmitted. Fluorescence measures the energy released as the electron returns to the ground state. As the light of the Ru(II) emits in the ultraviolet field, a black light is needed to show the color change from clear to red.

Complex 1 is chromogenic, which means that it changes color in the presence of cyanide, which Chow et al. determined with their experiment. Complex 1 contains 24 d-orbital electrons altogether. Typically, a metal center holds 18 electrons and is very stable. The 18 electrons come from 2 s electrons, 6 p electrons, and 10 d electrons. Because metal centers have many electrons and oxidation states, they are very reactive, and therefore have a lot of energy. For this reason, metal complexes almost always appear on a UV-Vis spectrum; as they interact with light energy and transmit light, the energy of the light transmitted corresponds to the energy of the light in the UV-Vis spectrum producing a color. The color of the complex depends upon the difference between the Lowest Unoccupied Molecular Orbital (LUMO) to the Highest Occupied Molecular Orbital (HOMO). When a metal complex reacts, the energy of the complex changes, and leads to a change in color and electron configuration.

Metal complexes tend to react by one of seven mechanisms. The most common mechanism of metal complex reactions is interchange. There are two types of interchange: associative interchange (I_A), and dissociative interchange (I_D). I_A mechanisms begin to form a bond with the analyte before breaking the leaving groups bond; the formation of the bond occurs just quickly enough that it can be observed before the leaving group dissociates. I_D mechanisms begin to break the bond between the leaving group and the metal before the anion begins to react, in a simultaneous process. The relative strength of the bond being formed versus the bond being broken determines which mechanism a reaction undergoes. If the bond
being formed is stronger than the bond breaking, the reaction will be $I_A$. If the opposite occurs, the mechanism will be $I_D$.

In order to determine if Complex 1 can detect cyanide, Chow et al. compared the change in Gibbs free energy ($\Delta G$) of different common anions to the $\Delta G$ of cyanide when reacted with the metal complex. Gibbs free energy is a measure of how favorable it is for a reaction to occur. Gibbs energy is measured using the equation $\Delta G = -RT \ln K_B$, where $-R$ is the gas constant, $T$ is the temperature, and $\ln K_B$ is the natural log of the binding constant. By comparing the values of $\Delta G$ of common anions to the $\Delta G$ of cyanide, this experiment was able to predict whether Complex 1 can efficiently detect cyanide.

The experiment performed by Chow et al. reacted common anions with Complex 1. The aim of this experiment is to determine if the Ruthenium (II)-Copper (II) chemodosimeter synthesized by Chow et al. is specific to cyanide. If it is, a color change is produced by manipulating the ligands attached to the metal centers. By understanding the factors determining the reaction of Complex 1 and cyanide, a more accurate cyanide-selective metal complex could be designed.

**Results and Discussion:**

**Colorimetric Response to Cyanide**

Complex 1, a trinuclear, heterobimetallic complex was synthesized in order to determine if it could detect concentrations of cyanide as small as 0.03 parts per million. Trinuclear means that there are three nuclei, or three metal centers that are bound together to create a single complex. Heterobimetallic means that there are two different metals in the complex. To determine if the complex was able to detect cyanide, several different anion species were added to vials containing Complex 1. These anion species were $\text{CN}^-$, $\text{SO}_4^{2-}$, $\text{HCO}_3^{-}$.
, HPO$_4^{2-}$, N$_3^-$, CH$_3$COO$^-$, NCS, NO$_3^-$, and Cl$^-$. These very reactive, electron rich anions are all known to bond easily with transition metals, and are also commonly found in industry. When added to the solution containing Complex 1, the only anion to produce a colorimetric response was cyanide (Figure 5). This color change occurred due to the Metal to Ligand Charge Transfer that only occurs when cyanide reacts with the metal complex. This experiment suggests that Complex 1 could detect cyanide without requiring further instrumental analysis; therefore this method could potentially be used to detect cyanide in the presence of other common anions by the colorimetric response.

Complex 1 is a green crystal polymer that dissolves in polar solvent. The general rule for polarity is like substances dissolve like substances. So a polar molecule will dissolve in a polar solvent. Complex 1 as a monomer has three centers of positive charge, the metals, and the ligands, which either have a negative charge or partial negative charge. This makes the polymer polar, and leads to the dissolution of the polymer into the solvent. As it dissolves, the polymer chain breaks into monomers of Ru$^{II}$('Bubpy)(CN)$_2$-$[Cu^{II}(dien)L]_2$; where L is the
solvent. The solution and crystals are green due to an absorbance band at 417 nm in the UV-Vis spectrum. This wavelength may seem low, but actually indicates a large transition between energy states. The visible spectrum has an inverse relationship between energy and wavelength. The lower the wavelength, the higher the energy of the transition. This relationship is determined by the equation $E = \frac{hc}{\lambda}$, where $E$ is energy, $h$ is Planck’s constant, $c$ is the speed of light, and $\lambda$ is the wavelength. Complex I is high in energy, which is attributable to the multitude of electrons, their movement, and the number of highly energized bonds. Therefore it is logical that it has a low wavelength and high energy.

Every chemical absorbs a specific wavelength of light, and the wavelength that is not absorbed is reflected or transmitted. The transmission of light is what gives everything color. Humans can only see wavelengths in the visible light region, a small portion –approximately 300 nanometers to 800 nanometers– out of the full electromagnetic spectrum, which ranges from $10^{-6}$ nanometers to 100 kilometers. In all cases of the UV-VIS spectrum, the wavelength of light absorbed transmits the visible color’s complementary color. For example, Complex I absorbs light at 417 nm, and transmits green light, but when reacted with cyanide, it absorbs light at 433 nm and transmits orange light.

For octahedral (6-coordinate) complexes like Complex I, absorption of light can be measured with $\Delta_\circ$. The crystal field splitting energy (or the energy between d-orbitals) for an octahedral complex is known as $\Delta_\circ$, or delta octahedral. This energy can be found using spectroscopy because the inverse value of $\lambda$ (lambda) is the wavenumber, which is equal to $\Delta_\circ$. Therefore, $\Delta O = \frac{1}{\lambda_{max}}$. The spectroscopy of metal complexes depends on $\Delta_\circ$ because the numerical value of $\Delta_\circ$ corresponds to the energy of the visible spectrum. $\Delta_\circ$ is also the
difference in energy between the lower orbital that contains electrons, the $t_{2g}$ orbital, which is known as the HOMO, the Highest Occupied Molecular Orbital, to the next empty orbital that doesn’t contain electrons, the $e_{g}^{*}$ orbital, which is known as the LUMO, or the Lowest Unoccupied Molecular Orbital (Figure 5).

The value of $\Delta_{O}$ depends largely on four factors; the first of these is the nature of the metal. The nature of the metal refers to the row of the metal in the periodic table. Transition metals in Period 4 of the periodic table have a smaller $\Delta_{O}$ than those of Period 5, which have a smaller $\Delta_{O}$ than those in Period 6. This is due to the overlap of extended molecular orbitals; the increased area of orbitals corresponds with increased electron movement, because there is less electron-electron repulsion. A simpler way to state this phenomenon is that $\Delta_{O}$ increases going down a group on the periodic table, because the HOMO is lower in energy. Ruthenium is a Period 5 metal, so it has a greater $\Delta_{O}$ than copper, which is a Period 4 metal. This implies that the ruthenium will be contributing more to the color than copper.

The second factor influencing $\Delta_{O}$ is the geometry of the metal. The value of $\Delta_{O}$ is based off of octahedral geometries, which generally have the greatest $\Delta_{O}$. The Ru(II) complex of Complex 1 is octahedral, and has a high $\Delta_{O}$. The Cu(II) complexes are trigonal bipyramidal, which means it only has five bonds, and therefore also has a lower energy than the Ru(II). Once the bond bridging the ruthenium and copper breaks, the copper no longer contributes to the color of the solution because the MLCT band of the ruthenium is relatively much higher than the absorbance band produced by the copper complexes.

The third factor that affects $\Delta_{O}$ is oxidation state. As the oxidation state of a metal increases, the bonds of the ligands are shortened, as the metal holds the ligands tighter due to the increasing attraction between the positively charged metal and negatively charged ligand,
meaning that the filled orbitals are held at a lower energy. This increases $\Delta_O$, as the energy needed to promote the electron from the orbital with lower energy to the next orbital increases. A metal with a low oxidation state would not hold its ligands as tightly, and the energy levels between the lowest occupied orbital and the next unoccupied orbital would be more similar.

The nature of the ligand is the last factor affecting $\Delta_O$, and refers to whether the ligand is a $\pi$-donor, a $\sigma$-donor, or a $\pi$-acceptor. Pi donor ligands tend to have the lowest $\Delta_O$, while $\pi$-acceptors tend to have a highest $\Delta_O$ because the nonbonding $t_{2g}$ d orbital have similar energy to the empty $\pi^*$ orbital on the ligand, which then forms a new bonding and antibonding molecular orbital. Basically, $\pi$-acceptors lower the HOMO, creating a larger energy gap between orbitals, and $\pi$-donors increase the HOMO lowering the energy gap. It is important to note that while metal complexes generally tend to follow these rules, there are times when one factor takes priority over the others. For example, a metal with an extremely high oxidation state of +4 or higher will always have a large $\Delta_O$, even if all the other factors contribute to a low $\Delta_O$.

As illustrated by Figure 5, a solution of Complex 1 becomes orange in the presence of cyanide; the wavelength of the compound experiences a shift where value of $\lambda$ increases and the absorption band moves from 417 nm to 433 nm. This colorimetric response occurs due to the cleavage of bridging cyanide bonds, releasing $[\text{Ru('bubpy')(CN)}_4]$ and $[\text{Cu(dien)(CN)}_2]$, leaving two distinct separate metal complexes. The color of the solution becomes orange because of the ruthenium complex’s Metal to Ligand Charge Transfer (MLCT) absorbance band.

Along with the MLCT band changing the color, a simple check for luminescence under a ultraviolet light shows the difference between cyanide and other anions in the solution of Complex 1, which is also shown in Figure 5b. The fact that the only cyanide has a luminescent
response helps to establish that cyanide is the only anion to produce response in the solution of Complex 1.

**Mechanism of Reaction**

As stated previously, when the crystalline polymer of Complex 1 is dissolved into polar solvent, it dissociates.

Once dissolved, it

\[(\text{Ru}^{II})(\text{Bubpy})(\text{CN})_2[(\text{CN})\text{Cu}^{II}(\text{dien})]\]_{2+}^{2+}

L is the polar solvent. In the presence of free cyanide agents, the free cyanide displaces the bridging cyanide from the copper metal center because the bridging ligand is the least stable of the bonds within the molecule, which breaks the bridging cyanide ligand connecting the Ru and Cu centers (Figure 6). The cleavage of the bridging ligand produced

\[[\text{Ru}^{II}(\text{Bubpy})(\text{CN})_4]^{2-}\] and \[[\text{Cu}^{II}(\text{dien})(\text{CN})_2].\]

Due to the nature of the bridging cyanide, it is most likely that this cleavage breaks via an interchange mechanism, which is common among similar metal complexes. An interchange mechanism results when the incoming analyte partially forms a bond with the copper metal center, while the leaving group is also still bonded to the metal. This mechanism makes the most logical sense, because it isn't favorable for the bridging cyanide ligand to break on its own. It is favorable for the bridging cyanide groups to cleave once the free CN\(^-\) binds to the copper because the copper metal center has a trigonal bipyramidal geometry, which means that there is space for the incoming cyanide to bond. The ruthenium has an octahedral geometry, and any incoming ligand would be sterically hindered, which means
that there is not enough room for an atom to form a bond. Therefore, any present anions are more likely to bond with the copper center rather than the ruthenium center.

An additional reason for the cyanide to react with the copper metal center rather than the ruthenium metal center is low spin versus high spin electron distribution. In Ligand Field Theory, the d orbitals of an octahedral geometric molecule split into two orbitals—the $t_{2g}$, which can hold three pairs of two electrons, and the $e_g^*$, which holds two pairs of two electrons—because two of the d-orbitals ($d_{z^2}$ and $d_{x^2-y^2}$) lay directly on the bond axes and have greater electron repulsion than the d-orbitals that lay between them ($d_{xy}$, $d_{xz}$, and $d_{yz}$). This repulsion splits the d-orbitals into two different energy levels. In low spin molecules, the $t_{2g}$ orbital is filled by pairing electrons before the electrons are promoted to the $e_g^*$ orbital (Figure 7). Oppositely, high spin molecules fill the $t_{2g}$ and $e_g^{*}$ orbitals before pairing the electrons. As an example, splitting diagram for a half-filled low spin metal complex would show six electrons (three pairs) in the $t_{2g}$ orbital. The splitting diagram for a half-filled high spin metal complex would show five electrons, three in the $t_{2g}$ and two in the $e_g^*$. Splitting patterns are particularly important when discussing stability of metal complexes and their interactions with other molecules. Completely filled and half-filled orbitals are very stable and most metal complexes that are half or fully filled will either not react, or react very slowly. Ruthenium (II), as a Period 5 metal, has a low spin electron distribution. As a $d^6$ metal (meaning that it contains six d-orbital electrons), ruthenium

![Figure 7. High Spin State vs. Low Spin State for all metal complexes.](image)

A metal complex either exists in a low spin state, or a high spin state. Both (a) the low spin state, and (b) the high spin state are half-filled, which is very stable. Ru(II) is a $d^6$ low spin, so it’s spin diagram is (a). The Ru(II) is very stable, so it is less likely to react and gain or lose another electron. Also shown is $\Delta_0$, the energy between the $t_{2g}$ and the $e_g^{*}$.
has a half-filled \( t_{2g} \) d-orbital. As such, the ruthenium complex of the trinuclear monomer is very stable as it is and unreactive.

The copper metal centers, although they are first row transition metals (which normally tend to be high spin) are low spin, due to their bond with cyanide, which is a strong \( \pi \)-acceptor ligand. The copper center has a \( d^9 \) electron configuration and is not as stable as the ruthenium. Ergo, the copper center would prefer to have another electron, to create a full orbital, and will more readily react with free cyanide in the solution.

Gibbs free energy (\( G \)) is a measure of how spontaneous a reaction is, or how favorable it is for a reaction to occur. If \( G \) is less than zero for a reaction, that reaction will occur spontaneously.

In addition to the experiment performed by Chow et al., the change in \( G \) for the reaction of each analyte with Complex 1 was measured (Table 1). The reaction of cyanide and Complex 1 has the lowest \( \Delta G \) value, it is the most negative, meaning that the reaction will occur spontaneously. Another value measured by Chow et al. was the binding constant (\( K_b \)) for the reaction of Complex 1 and each analyte. The value of \( K_b \) shows how strong the bond formed with each analyte is. The reaction of cyanide produces the greatest \( K_b \) of all the analytes reacted with Complex 1. This is likely due to the nature of the ligand, as cyanide back-bonds with the ruthenium and copper metal centers, creating a more stable, stronger bond, while none of the
other anions do. Chow et al. claim that Complex 1 can detect cyanide up to 0.03 parts per million. This concentration was determined used the Limit of Detection. The Limit of Detection (LOD) is used to describe the smallest signal of an analyte that can be distinguished from background noise within the instrumentation. Generally, the LOD is where the analyte signal is approximately three times the size of the background noise and 3 times the standard deviation of a blank sample. In comparison, the LOQ (Limit of Quantitation) is the smallest concentration where confidence on the precision and accuracy of the measurement is known, and is 10 times the standard deviation of the sample. Chow et al. present Complex 1 as a chemodosimetric ensemble for cyanide, with a detection limit of 0.03 ppm. However, 0.03 ppm is the LOD, rather than the LOQ which is a more accurate measure of detection.

**Conclusion:**

Chow et al. have synthesized a Ru(II)-Cu(II) chemodosimetric ensemble that is able to detect cyanide specifically. The inorganic chemistry behind the how metal complexes work enables chemists to determine the behavior of the \(((\text{Ru}^{II})(\text{Bubpy})(\text{CN})_2-\text{[Cu}^{II}(\text{dien})_2\text{]})(\text{ClO}_4)_2\) in solution with anions other than cyanide by comparing \(\Delta G\) and \(K_B\). The experiments conducted show that a colorimetric response only occurs with cyanide anions, and no others, meaning that the color change of Complex 1 is specific towards the binding of cyanide.

The research of Chow et al. is globally significant: a toxic anions in the world is used in industry and the current procedures used to detect it are not very accurate. According to a review published by National Center for Biotechnology Information, all the current methods of cyanide detection have a LOD of approximately 25 ppm. Chow et al.‘s research aims to create a new method of cyanide detection that works accurately, and can detect a microscopic trace of cyanide, but the reported value of 0.03 ppm is too low to be consistent.
Future work into the research of chemodosimetric ensembles has already been started. For example, a Ru(II)-Eu(III) complex with cyanide bridging may be able to detect biogenic amine odorants.\(^a\) Further, gold could be used in place of copper to form a new metal complex that should have the same or similar chemical characteristics due to the fact that copper and gold are both in the same column on the periodic table. It is possible that any combination of a metal with half-filled orbitals bonded to a metal that is either a \(d^9\), \(d^7\), or \(d^4\) would react favorably with a ligand in the detection of a specific anion. These \(d\)-electron configurations would able be very stable with an additional electron. The \(d^9\) would become filled, the \(d^7\) would become diamagnetic, meaning that there are no unpaired electrons (which stabilizes a molecule), and the \(d^4\) would become half-filled. Additionally, a wider range of anions should be tested, making sure to include anions with a similar function or structure to cyanide such as NCO\(^-\), which is also a \(\pi\)-acceptor and reacts similarly to CN\(^-\). By using a wider range of anions, many comparable to cyanide, it would be more likely to suggest that the metal complex specifically reacts with only cyanide and not any other anions with a carbon-nitrogen double or triple bond.

The ethical implications of this research are very important. As cyanide is extremely toxic to mammals, discontinuing this research could be irresponsible. Chow et al. have created a better way of detecting cyanide, but there is always room for improvement. Cyanide is dangerous to most life forms on this planet and humans have a responsibility to protect other living beings from the ill effects of cyanide, because most animals do not have the same understanding of chemicals as humans. Collectively, scientists are obligated to attempt to perfect the detection of cyanide. The legal implications are that Chow et al. will most likely have to get a patent for their complex before it can be used by others to detect cyanide. As stated
previously, this complex is not as good as it could be, but for the moment, it is the best cyanide detector.

References


