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Research Article

Interfacial Mechanisms of O-O Type Chelating Collectors in the Flotation of Copper Minerals: A Density Functional Study

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ABSTRACT

Flotation is a widely used separation technique in mineral processing that relies on surface chemistry to recover valuable metals from low-grade ores. This study presents a theoretical evaluation of O-O type chelating collectors in the selective flotation of copper minerals, emphasizing their interactions at the colloidal and interfacial levels. Using advanced computational methods, key surface chemistry parameters—including adhesion mechanisms, electron density distributions, and binding energies—were analyzed to assess the efficiency and selectivity of these collectors. The findings demonstrate that O-O type chelating collectors establish strong and specific interactions with copper mineral surfaces, enhancing hydrophobicity and improving attachment to air bubbles. Among the studied collectors—Cupferon, Neocupferon, 2-nitroso-1-naphthol, 2,4-pentanedione, Octyl hydroxamate, and 2-Acetyl-acetanalid—Octyl hydroxamate exhibited the highest stability and affinity for Cu^{2+} ions, while 2-Acetyl-acetanalid showed the weakest performance. This study provides fundamental insights into the interfacial mechanisms governing flotation efficiency and offers guidance for optimizing reagent selection. By contributing to the design of more selective and sustainable collectors, these findings support advancements in mineral processing, environmental technologies, and interfacial science.

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INTRODUCTION

Flotation is one of the most common methods of beneficiation, which uses differences in the surface properties of minerals for their separation in water. It is significant in the metal mining and mineral processing industries, especially for the economic recovery of valuable metals from low-grade ores (Atak, 1990; Yekeler and Yekeler, 2005). Flotation is considered one of the most critical processes. developments in mining and metallurgy in the 20th century. This method has enabled the economical processing of solid fuel resources and ores. In addition to the flotation methods widely used in the mining industry for ore and coal beneficiation, flotation methods are also applied in fields such as chemical, food and environmental engineering (Chia et al., 2019). Flotation is widely used in the mineral industry, but it is also used in many other fields (Peleka et al., 2018).

The flotation process allows collectors, known as surfactants, to adsorb on the surface of certain minerals, allowing these minerals to bind to air bubbles and be transported to the surface. This method utilizes the different surface properties of the grains and the air bubbles created in the pulp. Separation of the grains is achieved by the upward movement of the grains that are in contact with the air bubble (hydrophobes) and the downward movement of the grains that are not in contact (hydrophiles) (Hacıfazlıoğlu, 2007; Valderrama and Rubio, 2008). This method has been widely applied for the recovery of copper (Gupta et al., 2023), zinc (Chen at al., 2024), lead (Kee and Shoparwe, 2024) and precious metals (Fuerstenau, 2000).

Chelating agents are organic ligands that form coordination complexes with metal ions and change their solubility, stability and reactivity. O-O-type chelating agents have functional groups containing two oxygen atoms in their structure and form chelate structures by binding to metal ions through these atoms. They are used in purification processes by selective precipitation or complexation of metal ions (Dwyer, 2012). It increases the yield of reactions by acting as a ligand in transition metal catalysts. Some O-O type chelates with antioxidant properties are used in medical treatments and drug design. It is used in the paper, textile and detergent industries to prevent unwanted reactions by binding metal ions (Torres and Kremer, 2023).

Collectors used in the flotation of copper minerals are generally compounds that change the surface chemistry and make the minerals hydrophobic. Collectors are divided into different categories according to their chemical structure. O-O type chelating collectors play a strong and important role in dealing with metal ions. In the future, more selective and efficient chelating agents can be designed by developing O-O type ligands containing new functional groups.

The main feature of such collectors is that they show a high affinity for metal ions and form stable complexes (Brooks and Fleming, 1989). Some of the O-O type chelating collectors are. Cupferone (N-nitrosofenylhydroxylamine) is a selective collector for copper minerals in an acidic solution. Neocupferon acts as a collector with its two aromatic rings in an acidic solution. Another chelating reagent for copper minerals is 2,4-pentanedione. Octyl hydroxamate is a perfect collector for copper oxide and natural copper minerals. The use of this reagent as a collector of copper oxide mineral is because it forms stable copper chelate. High solubility in water. The long chain structure helps to retain the reaction product on the surface (Fuerstenau, 2000). 2-Acetyl-acetanalite is also one of the essential collectors used in the flotation of copper minerals.

The main factors determining flotation efficiency include pH, reagent concentration, solvent medium, temperature and surface-tension relations (Marabini et al., 1988). In particular, the and ionic componentssolvent medium's dielectric constant and ionic composition directly affect the collector-mineral surface interaction (Rai, 2003). Highly efficient flotation processes depend on the collector'scollectors' adhesion force to the mineral surface. The size of the hydrophobic area formed by the collectors on the surface is one of the main parameters that increase flotation efficiency (Ackerman et al., 1999).

Computational chemistry methods are necessaryessential in understanding flotation reagents' effectiveness. Density Functional Theory (DFT) has emerged as a reliable method to determine chemical systems electronic and structural properties (Zhang et al., 2022).

In this study, the flotation efficiency of O-O type chelators were investigated using DFT. Calculations at the B3LYP/6-31G** level and then the frequency values of the O-O type chelators optimized with the

B3PW91/LANL2DZ basis set calculated were calculated in this study. The complex structures formed by O-O type chelators with Cu+2 were optimized with the B3PW91/LANL2DZ basis set, and parameters such as frequency values, relative energy (ΔE), atomic charges, and parameters such as frequency values, relative energy (ΔE), atomic charges, and HOMO-LUMO energies were evaluated.

The main objective of this study is to determine the effectiveness of O-O type chelating collectors in the flotation of copper minerals and to theoretically investigate their usability in the flotation of copper minerals. The results obtained will contribute to optimizing the choice of reagents in flotation processes, the development ofoptimizing the choice of reagents in flotation processes, and the development of more environmentally sustainable collectors.

MATERIAL AND METHODS

All calculations of isolated complexes were executed using Gaussian 98W and GaussView 6 program package (Chen et al., 1998). The optimized structures of Cu-complex were found at B3LYP functional in the gas phase. In the study, LANL2DZ and 6-311++G(d,p) basis sets were used for Cu atom and rest atoms in complexes, respectively. Geometric optimization was performed using Becke's three-parameter hybrid three-parameter exchange function (B3LYP) within the Density Functional Theory (DFT) framework. This function, which considers electron correlation and exchange interactions, is recognized as an effective method to accurately describe the electronic structure of chemical systems (Becke, 1993).

In the calculations, the 6-31G basis set was used to provide sufficient accuracy to represent the wave function of the system. To verify whether the optimized molecular structures reach a stable minimum energy conformation, the harmonic vibrational frequencies were calculated at the same level. This analysis was performed to determine whether each optimization point is a true minimum energy configuration and to detect virtual frequencies, if any.

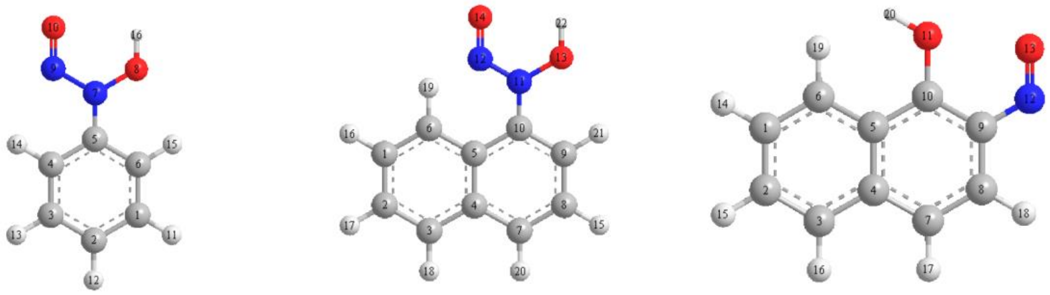
In addition, zero-point vibrational energy (ZPE) corrections were calculated and their contribution to the total relative energy (ΔE) values was evaluated. For the ZPE corrections, a scaling factor of 0.9804, which is widely used in the literature (Tantirungrotechai et al., 2006), was applied to improve the agreement between theoretical calculations and experimental data.

To better understand the reactivity and electron distribution properties of molecules, Mulliken charge analysis was performed. The atomic charge values calculated using the Mulliken scheme (Mulliken, 1955) provide an important reference for evaluating the electrostatic properties, bond formation mechanisms and chemical reactivity of molecules.

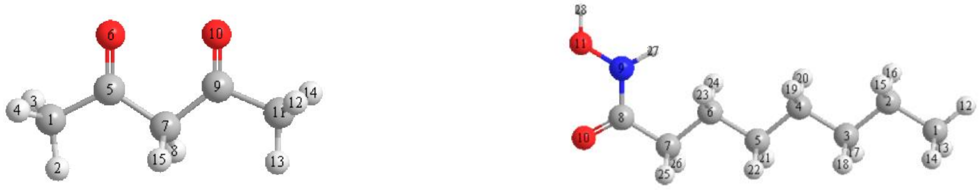
These calculations are a reliable method for understanding molecular systems' electronic and geometrical structures and provide a fundamental source of data for predicting the interaction of flotation agents with metal surfaces.

RESULTS AND DISCUSSION

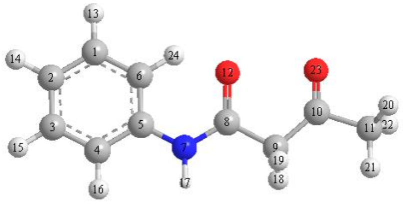
Developing and designing new chemical reagents for froth flotation remains an active area of research aimed at improving the efficiency of mineral separation processes. The use of selective, economical and highly efficient reagents plays a critical role in optimizing flotation processes. In this context, Marabini et al synthesized new compounds with chelating properties for flotation studies. The effectiveness of new flotation reagents is based on evaluating donor-acceptor interactions between donor atoms (N, S, O, etc.) in functional groups in the reagent molecule and metal surfaces. The structures of some O-O type chelating collectors Cupferon, Neocupferon, 2-nitroso-1-naphthol, 2,4-pentanedione, Octyl hydroxamate and 2-Acetyl-acetanalide are given in Fig. 1.



Cupferon Neocupferon 2-nitroso-1-naphthol



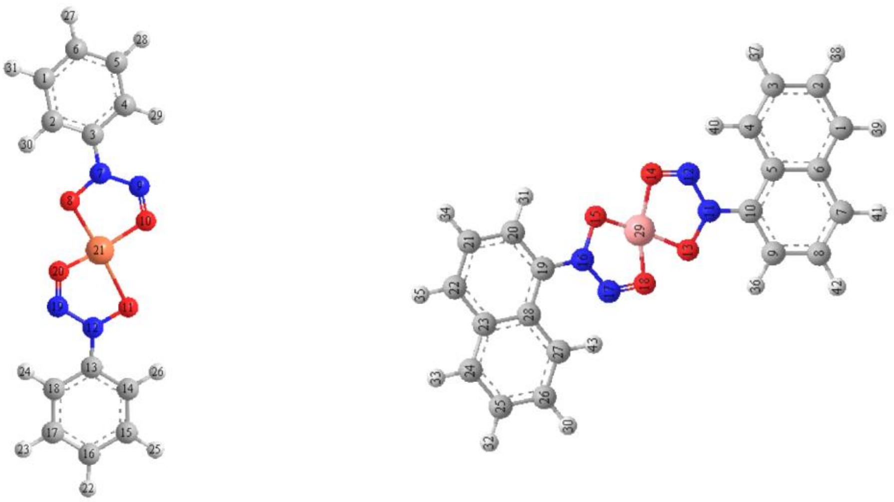
2,4-pentanedione Octyl hydroxamate



2-Acetyl-acetanalide

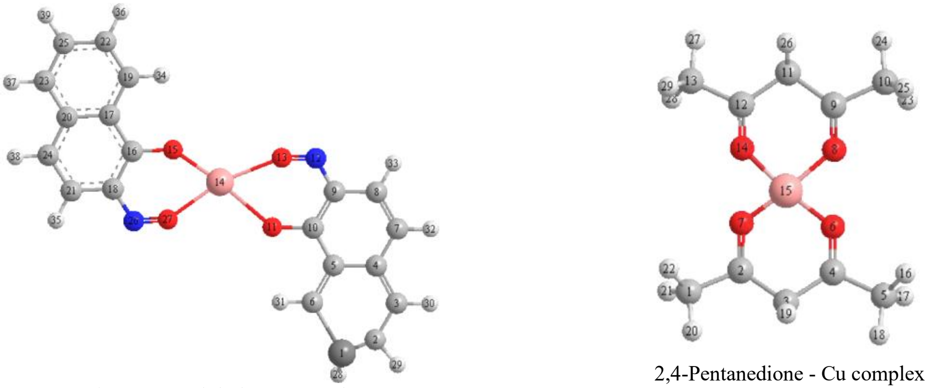
Figure 1. *Structures of Cupferon, Neocupferon, 2-nitroso-1-naphthol, 2,4-pentanedione, Octyl hydroxamate and 2-Acetyl-acetanilide*

Chelate rings are ringed structures formed by a multi-toothed ligand bonded to the central metal with at least two donor atoms. Chelate compounds show high selectivity and efficiency in flotation. For a ligand to form a chelate with a metal, it must have appropriate functional groups and form a closed heterocyclic structure with the metal through N, O, S or P atoms in these groups. The O-O type chelating agents examined in this study, Cupferon Neocupferon, 2-nitroso-1-naphthol, 2,4-pentanedione, octyl hydroxamate and 2-acetyl-acetanalide form ring complexes with Cu^{2+} ion via oxygen atoms. The efficiency of an organic compound as a flotation collector varies depending on the chemical and structural properties of the layer formed on the metal surface. The complex structures formed by O-O type chelating agents with copper minerals are given in Fig. 2.



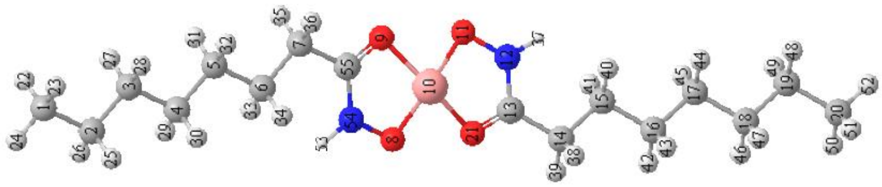
Cupferon-Cu complex

Neocupferon-Cu complex

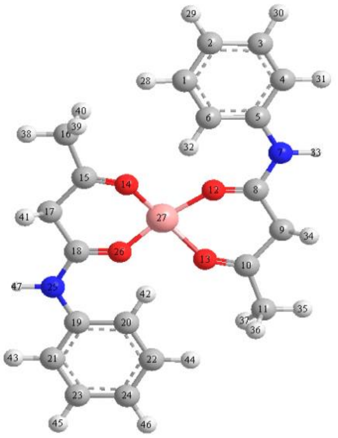


2-nitroso-1-naphthol - Cu complex

2,4-Pentanedione - Cu complex



Octyl hydroxamate - Cu complex



2-Acetyl-acetanalide - Cu complex

Figure 2. *Complex structures formed by Cupferon, Neocupferon, 2-nitroso-1-naphthol, 2,4-pentane-dione, Octyl hydroxamate and 2-Acetyl-acetanilide with copper mineral*

The calculated bond lengths for the 2-nitroso-1-naphthol molecule, one of the O-O type chelators, were determined as C-O 1.276 Å, N-O 1.290 Å and C-C-N-O tetrahedral angle 0.001°, respectively. have measured in experimental studies as 1.238 Å, 1.362 Å, and 0.6°. In this study, the calculated structural parameters of the Cu-2-nitroso-1-naphthol complex were Cu-O_1 1.924 Å, Cu-O_2 1.975 Å, C-O 1.299 Å and O-C-Cu bond angle 129.308°. The experimental data were reported as 1.927 Å, 1.975 Å, 1.305 Å and 127.090°, respectively (Odabaşoğlu et al., 2006).

The calculated bond lengths for another O-O type chelating agent, 2,4-pentanedione molecule, were determined as O-C 1.279 Å, C-C 1.429 Å and O_2-C_2 1.279 Å. Experimental studies showed these values as 1.295 Å, 1.411 Å and 1.282 Å, respectively. In the Cu-2,4-pentanedione complex, Cu-O bond lengths were equal and calculated as 1.941 Å, while experimental studies measured 1.93 Å (Hummel et al., 2009).

For octyl hydroxamate, another O-O type chelating agent, the bond lengths calculated in this study were C=O 1.285 Å, C-N 1.355 Å and N-O 1.373 Å. While the experimental data are 1.22 Å, 1.37 Å and 1.37 Å, ab initio calculations are reported as 1.22 Å, 1.34 Å and 1.44 Å, respectively. In experimental studies, these values were 1.285 Å, 1.355 Å and 1.373 Å.

All these data show that the calculated values largely agree with the experimental findings. The efficiency of flotation reagents can be related to certain quantum chemical parameters. Among these, the energy of the highest occupied molecular orbital (HOMO), which determines the electron-donating capacity of a molecule, stands out as an important parameter. The HOMO and LUMO orbitals are referred to as boundary molecular orbitals and play a critical role in determining chemical reactivity. ZPE, ΔE, ΔH, ΔG, HOMO-LUMO energy values and dipole moment values of O-O type chelators are given in Table 1.

Table 1. *ZPE, ΔE, ΔH, ΔG, HOMO-LUMO energy values and dipole moment values of Cupferon, Neocupferon, 2-nitroso-1-naphthol, 2,4-pentane-dione, Octyl hydroxamate and 2-Acetyl-acetanilide*

	B3PW91/LANL2DZ					B3LYP/6-31G**				
	Dipol moment	HOMO	LUMO	ΔE	ZPE	Dipol moment	HOMO	LUMO	ΔE	ZPE
Cupferon	9.339	-0.263	-0.173	-491.150	0.105	3.192	0.008	0.125	-491.399	0.105
Neocupferon	11.047	-0.263	-0.197	-644.66	0.153	3.281	-0.004	0.0851	- 644.995	0.151
2-nitroso-1-naphthol	9.497	-0.266	-0.203	-589.41	0.136	4.307	-0.013	0.0929	- 589.726	0.135
2,4-pentanedione	5.912	-0.316	-0.161	-344.93	0.109	5.014	-0.004	0.179	- 345.107	0.108
Octyl hydroxamate	20.864	-0.307	-0.100	-519.161	0.237	3.208	0.055	0.166	-519.436	0.235
2-Acetyl-acetanalide	9.912	-0.298	-0.164	-591.840	0.181	3.400	-0.022	0.120	-592.155	0.179

Since chemical bond formation is usually shaped by the interactions of valence electrons (Zhang et al., 2009), the HOMO orbital, which determines the spatial distribution of these electrons, is considered an important indicator in identifying regions prone to electrophilic attacks. Since flotation agents act as electron-donating species (Mohammadi-Jam et al., 2014), especially HOMO orbitals are considered in this study. The HOMO plots are given in Figure 3 and it is seen that the charge density is generally on the functional groups. However, the charge density is also distributed in the annular structure for some molecules. This is due to the participation of π electrons in the resonance in the annular structure.

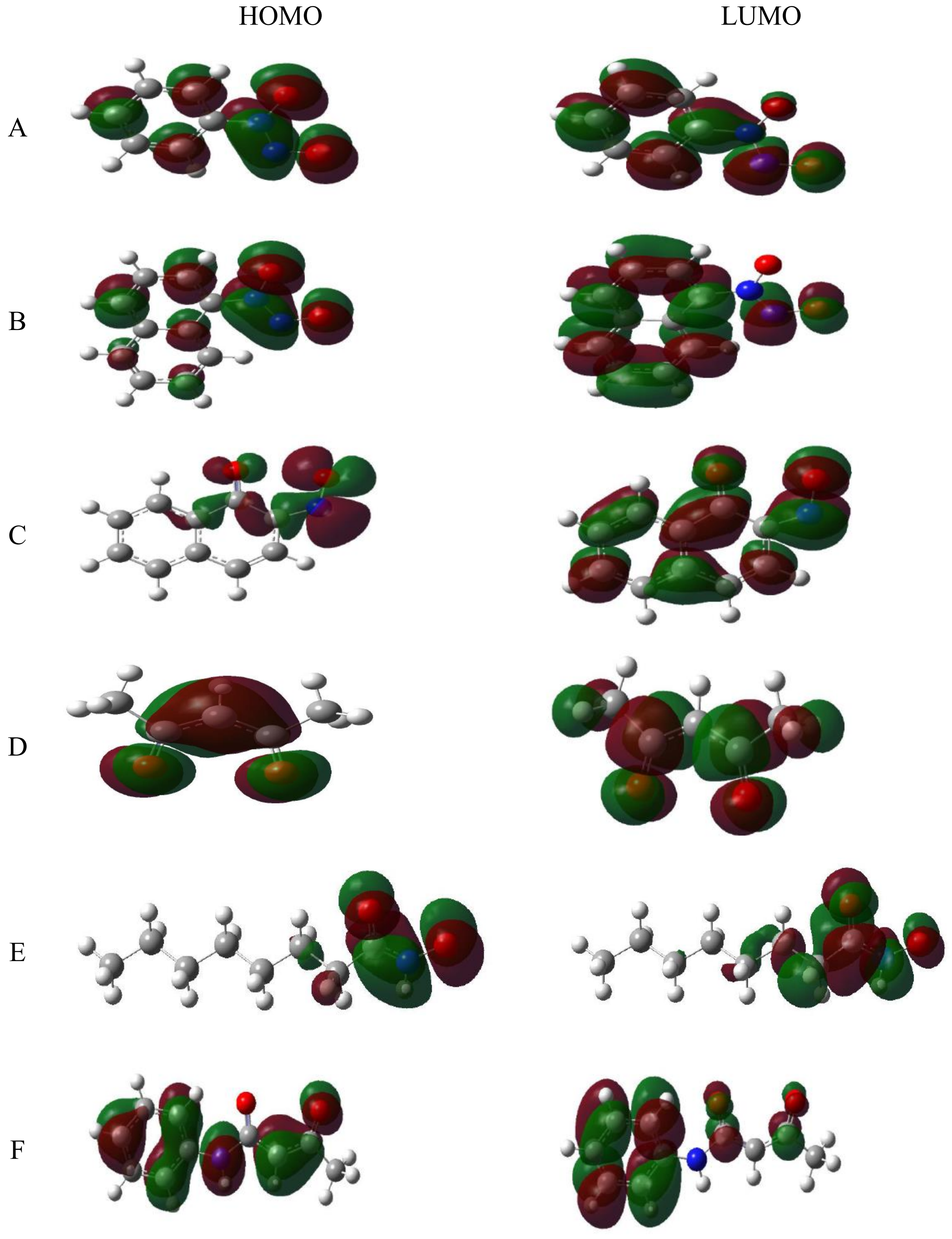


Figure 3. *HOMO-LUMO structures of Cupferon (A), Neocupferon (B), 2-nitroso-1-naphthol (C), 2,4-pentane-dione (D), Octyl hydroxamate (E) and 2-Acetyl-acetanilide (F).*

By looking at the Mulliken charge densities, we can predict which atoms the metal atom will prefer for complex formation (Lu et al., 2006). Moreover, since chemical reactions take place with valence electrons, the HOMO and LUMO orbitals, their shape and energy values in molecules also provide information about the activity of molecules. The chelating capacity of a molecule is directly related to the electronic charge distribution of the donor atoms on the ligand. Since metal atoms are electrophilic, the electron density of the electron donor atoms in the ligand compound is important for chelation. Since metal atoms are electrophilic, they prefer to bind to atoms with high electron density. The electronegativity of the O atom significantly affects the formation of the complex. Therefore, Mulliken population analysis was performed to determine the atomic charge distributions and relevant parameters were evaluated to better understand ligand-metal interactions.

Table 2. *Mulliken Charge Densities of Cupferon, Neocupferon, 2-nitroso-1-naphthol, 2,4-pentanedione, Octyl hydroxamate and 2-Acetyl-acetanalide*

	Cupferon			**Neocupferon**	
	B3PW91/LANL2DZ	B3LYP/6-31G**		B3PW91/LANL2DZ	B3LYP/6-31G**
7 N	-0.096	-0.106	11 N	-0.105	-0.074
8 O	-0.505	-0.419	12 N	-0.057	0.136
9 N	-0.068	0.155	13 O	-0.485	-0.420
10 O	-0.379	-0.320	14 O	-0.361	-0.426
	2-nitroso-1-naphthol			**2,4-pentanedione**	
	B3PW91/LANL2DZ	B3LYP/6-31G**		B3PW91/LANL2DZ	B3LYP/6-31G**
11 O	-0.334	-0.545	6 O	-0.372	-0.406
12 N	-0.068	-0.090	10 O	-0.372	-0.407
13 O	-0.345	-0.372			
	Octyl hydroxamate			**2-Acetyl-acetanalide**	
	B3PW91/LANL2DZ	B3LYP/6-31G**		B3PW91/LANL2DZ	B3LYP/6-31G**
9 N	-0.274	-0.324	7 N	-0.554	-0.653
10 O	-0.439	-0.464	12 O	-0.366	-0.601
11 O	-0.573	-0.406	23 O	-0.369	-0.532

When the Mulliken charge densities are analyzed, it is seen that the O atom is more electronegative. Mulliken charge values of octyl hydroxamate molecule were calculated as N -0.274 D, O1 -0.439 D, O2 -0.573 D. In the literature, these values were found as -0.305 D, -0.595 D, -0.588 D, respectively [15]. Atoms with a more negative charge generally have a higher electron density and a higher tendency to bond to metal ions. The most negative oxygen and nitrogen atoms have the potential to form strong coordination bonds with metal ions. Octyl hydroxamate molecule has oxygens carrying relatively strong negative charges such as (-0.573, -0.406). This suggests that it can form a stronger coordination bond with Cu^{2+} ions and be more effective in flotation. Octyl hydroxamate may show the highest binding interaction to the metal surface compared to other collectors. Although the most negative charges (-0.653, -0.601, -0.532) in the 2-Acetyl-acetanilide collector appear high for some atoms, the distribution of these values may be less symmetrical compared to Octyl hydroxamate. It is conceivable that the molecule is weak in binding ability and has a lower capacity to form a stable complex with Cu^{2+}. The nitrogen and oxygen charge distributions of Cupferon (-0.505, -0.419, -0.068, 0.155) and Neocupferon (-0.485, -0.420, -0.057, 0.136) are similar. This similarity suggests that the performance of the two compounds in flotation may also be close. 2-Nitroso-1-Naphthol carries relatively low negative charges on its oxygens (-0.334, -0.545, -0.345). 2,4-Pentanedione, on the other hand, has a charge distribution of (-0.372, -0.407) and can interact moderately with metal ions. Although these compounds do not bind as strongly as Octyl hydroxamate, they may show a certain selectivity in the flotation process. Octyl Hydroxamate is the collector that provides the strongest interaction with Cu^{2+} ions. 2-Acetyl-acetanilide was evaluated as the weakest collector. Other collectors (Cupferon, Neocupferon, 2-Nitroso-1-Naphthol, 2,4-Pentanedione) have moderate selectivity and binding capacity. The theoretical calculations agree with the experimental findings and show that computational chemistry can be effectively used in the design of flotation collectors. According to both studies, it is seen that the metal, Cu+2, will form a chelate with the O atom. Because the electron density is even higher. When the structures of the collectors are examined, it can be predicted that this structure will form a chelate with the O atom instead of the N atom. This predicted situation has also been confirmed in the studies.

The energy values required for complex formation of O-O type chelating agents are Cupferon (-646,6064966 kcal/mol), Neocupferon (-640,8290166 kcal/mol), 2 -Nitroso-1-naphthol (-632, 3733261 kcal/mol), 2,4-Pentanedione (-668,263732 kcal/mol), Octyl hydroxamate (-677,0413349 kcal/mol), 2-Acetyl-acetanalide (-

654,6166554 kcal/mol). When the energy values are ranked from higher to lower, we can say that 2-Nitroso-1-naphthol, Neocupferon, cupferon, 2-acetyl-acetanalide, 2,4-pentanedione and octyl hydroxamate are ranked. Octyl Hydroxamate (-677.0413 kcal/mol) stands out as the collector that forms the most stable complex with Cu^{2+} ions as it has the lowest (most negative) energy value. This result means it has a high electron density and exhibits strong chelation ability. It can be said that Octyl Hydroxamate will show high efficiency and selectivity in the flotation process. 2,4-Pentanedione (-668.2637 kcal/mol) and 2-Acetyl-Acetanalide (-654.6167 kcal/mol) 2,4-Pentanedione has a stability close to Octyl Hydroxamate and its flotation efficiency can be high. 2-Acetyl-Acetanalide was reported as the weakest collector in this study but its energy value is intermediate with -654,6167 kcal/mol. This indicates that it can form stable complexes in some cases but will be less effective than other collectors. Octyl hydroxamate has the strongest binding and highest flotation efficiency. 2,4-Pentanedione and 2-Acetyl-Acetanalide can form moderately stable complexes. Theoretical calculations show that Octyl hydroxamate is the best collector for flotation and provides the strongest binding to metal ions.Considering this ranking, the octyl hydroxamate collector with low energy value has a more stable structure. In the experimental study, the activity order was found to be octyl hydroxamate, cupferon, Neocupferon and 2,4- pentanedione in the order from largest to smallest. In this study, we see that the ranking between the energy values for these four collectors agrees with the experimental study.

When attention is paid to the molecules examined, five- or six-membered rings are formed during chelate formation. Cupferon, Neocupferon and octyl hydroxamate formed five-membered rings, while 2-nitroso-1-naphthol, 2,4-pentanedione and 2-acetyl-acetanalide formed six-membered rings. Accordingly, we would expect the stability of Cupferon and Neocupferon molecules to be higher, but this is not the case. Because in case of resonance in the chelate ring, the six-membered ring gives a more stable complex. For Cupferon and Neocupferon complexes forming five-ring chelates, Cupferon is more stable. Because π electrons resonate on a single benzene ring in Cupferon and on a double benzene ring in Neocupferon. Therefore, Cupferon will be more active than Neocupferon. Among the O-O type chelators, octyl hydroxamate and 2-acetyl-acetanalide contain similar functional groups. In the 2-acetyl-acetanalide molecule, electrons on the O atom will be attracted due to the resonance effect. In octyl hydroxamate, the electron density of O atoms will increase due to the inductive effect. Therefore, we expect octyl hydroxamate to be more stable than 2-acetyl-acetanalide. This shows that the values calculated in this study agree with those in the experimental studies.

CONCLUSION

This study provides a theoretical framework for understanding the interfacial mechanisms governing the flotation efficiency of O-O type chelating collectors in the selective recovery of copper minerals. By employing computational approaches, key chemical parameters—including HOMO energies, atomic charges, and binding energies—were analyzed to evaluate the stability and selectivity of different collectors. The results demonstrate that Octyl hydroxamate exhibits the highest reactivity and strongest interaction with Cu^{2+} ions, forming a stable chelate, whereas 2-Acetyl-acetanilid shows the weakest binding affinity. The strong correlation between theoretical predictions and experimental findings highlights computational techniques' reliability in characterizing flotation reagents' activity. These insights contribute to the rational design of more effective and environmentally sustainable collectors, aligning with colloid and interface science advancements, adsorption processes, and interfacial chemistry. The ability to predict and optimize collector performance at the molecular level offers valuable implications for industrial flotation processes, mineral beneficiation, and broader applications in catalysis, environmental remediation, and nanomaterials. Future studies can further refine these approaches by integrating experimental validations with advanced molecular dynamics simulations, expanding the scope of computational chemistry in optimizing reagent selection and improving flotation technologies.

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CONFLICT OF INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

AUTHOR CONTRIBUTION

Adem Necip: Writing – review & editing, Writing – original draft, Methodology, Investigation, Conceptualization. Hülya Yekeler: Writing – review & editing, Methodology, Investigation, Data curation Conceptualization.

REFERENCES

Ackerman, P., Harris, G., Klimpel, R., & Aplan, F. (1999). Use of chelating agents as collectors in the flotation of copper sulfides and pyrite. *Mining, Metallurgy & Exploration, 16*(1), 27–35.

Atak, S. (1990). *Flotasyon ilkeleri ve uygulaması*. ĐTÜ Vakfı.

Becke, A. D. (1993). Density-functional thermochemistry. III. The role of exact exchange. *The Journal of Chemical Physics, 98*(7), 5648–5652.

Brooks, M., & Fleming, I. (1989). Modernization of the Nchanga Flotation plant: A comparison of flotation cells and columns. *Mining Magazine, 160*(7), 34–35.

Chen, W., Wong, M., Andres, J., Head-Gordon, M., Replogle, E., & Pople, J. (1998). *Gaussian 98, revision A.7*. Gaussian, Inc.

Chen, Y., Sun, Y., & Han, Y. (2024). Efficient flotation separation of lead–zinc oxide ores using mineral sulfidation reconstruction technology: A review. *Green and Smart Mining Engineering*, *1*(2), 175–189.

Chia, S. R., Mak, K. Y., Khaw, Y. J., Suhaidi, N., Chew, K. W., & Show, P. L. (2019). An efficient and rapid method to extract and purify protein–Liquid triphasic flotation system. *Bioresource Technology, 294*, 122158.

Dwyer, F. (2012). *Chelating agents and metal chelates*. Elsevier.

Fuerstenau, D., Herrera-Urbina, R., & McGlashan, D. (2000). Studies on the applicability of chelating agents as universal collectors for copper minerals. *International Journal of Mineral Processing, 58*(1–4), 15–33.

Gupta, M., Huang, K., Noble, A., & Yoon, R.-H. (2023). Improving the performance of a low-grade porphyry copper ore flotation plant using a simulator that can predict grade vs. recovery curves. *Minerals Engineering*, *202*, 108243.

Hacıfazlıoğlu, H. (2007). Alternatif flotasyon yöntemlerinin tanıtılması. *Bilimsel Madencilik Dergisi*, *46(3)*, 23-41.

Hummel, M., Rubatscher, E., Wurst, K., Laus, G., Jaitner, P., & Schottenberger, H. (2009). Crystal structure of 3-(4-azidophenyl) pentane-2, 4-dione, C11H11N3O2. *Zeitschrift für Kristallographie-New Crystal Structures, 224*(1–4), 699–701.

Kee, L. C., & Shoparwe, N. F. (2024). Advances in membrane technology for gold extraction: A comprehensive review. *Malaysian Journal of Bioengineering and Technology*, *1*(2), 121–129.

Lu, H., Dai, D., Yang, P., & Li, L. (2006). Atomic orbitals in molecules: General electronegativity and improvement of Mulliken population analysis. *Physical Chemistry Chemical Physics, 8*(3), 340–346.

Marabini, A., Alesse, V., & Barbaro, M. (1988). New synthetic collectors for selective flotation of zinc and lead oxidized minerals. In *XVI International Mineral Processing Congress* (pp. 1197–1208). Elsevier.

Mohammadi-Jam, S., Burnett, D., & Waters, K. (2014). Surface energy of minerals–Applications to flotation. *Minerals Engineering*, *66*, 112–118.

Mulliken, R. S. (1955). Electronic population analysis on LCAO–MO molecular wave functions. I. *The Journal of Chemical Physics, 23*(10), 1833–1840.

Odabaşoğlu, C. M., Albayrak, O., & Büyükgüngör, O. (2005). 2,6-Dimethyl-1,4-benzoquinone 4-monooxime. *Crystal Structure Communications, 61*(4), o240–o242.

Peleka, E. N., Gallios, G. P., & Matis, K. A. (2018). A perspective on flotation: A review. *Journal of Chemical Technology & Biotechnology*, *93*(3), 615–623.

Rai, B. (2003). Molecular modeling and rational design of flotation reagents. *International Journal of Mineral Processing, 72*(1–4), 95–110.

Tantirungrotechai, Y., Phanasant, K., Roddecha, S., Surawatanawong, P., Sutthikhum, V., & Limtrakul, J. (2006). Scaling factors for vibrational frequencies and zero-point vibrational energies of some recently developed exchange-correlation functionals. *Journal of Molecular Structure: THEOCHEM*, *760*(1–3), 189–192.

Torres, J., & Kremer, C. (2023). Coordination chemistry of lanthanide ions with X-(CH2-COO-)2 (X= O, NH, S) ligands: The leading role of X as carboxylate-connecting group. *Coordination Chemistry Reviews, 494*, 215347.

Valderrama, L., & Rubio, J. (2008). Unconventional column flotation of low-grade gold fine particles from tailings. *International Journal of Mineral Processing, 86*(1–4), 75–84.

Yekeler, M., & Yekeler, H. (2005). Molecular modeling study on the relative stabilities of the flotation products for arsenic-containing minerals: Dixanthogens and arsenic (III) xanthates. *Journal of Colloid and Interface Science, 284*(2), 694–697.

Zhang, H., Sun, W., Zhang, C., He, J., Chen, D., & Zhu, Y. (2022). Adsorption performance and mechanism of the commonly used collectors with oxygen-containing functional group on the ilmenite surface: A DFT study. *Journal of Molecular Liquids, 346*, 117829.

Zhang, L., Ying, F., Wu, W., Hiberty, P. C., & Shaik, S. (2009). Topology of electron charge density for chemical bonds from valence bond theory: A probe of bonding types. *Chemistry–A European Journal, 15*(12), 2979–2989.