Hartree-Fock methods analysis protonated rhodochrosite crystal and potential in the elimination of cancer cells through synchrotron radiation using Small–Angle X–Ray Scattering (SAXS), Ultra–Small Angle X–Ray Scattering (USAXS), Fluctuation X–Ray Scattering (FXS), Wide–Angle X–Ray Scattering (WAXS), Grazing–Incidence Small–Angle X–Ray Scattering (GISAXS), Grazing–Incidence Wide–Angle X–Ray Scattering (GIWAXS) and Small–Angle Neutron Scattering (SANS)

ABSTRACT

The rhodochrosite (MnCO3) shows complete solid solution with siderite (FeCO3), and it may contain substantial amounts of Zn, Mg, Co, and Ca. The electric charge that accumulates in certain solid materials, such as crystals, certain ceramics, and biological matter such as bone, DNA and various proteins in response to applied mechanical stress, phenomenon called piezoelectricity. There is no precedent in the literature on the treatment of tumor tissues by eliminating these affected tissues, using rhodochrosite crystals in tissue absorption and eliminating cancerous tissues by synchrotron radiation. An in-depth study is necessary to verify the absorption by the tumoral and non-tumoral tissues of rhodochrosite, before and after irradiating of synchrotron radiation using Small–Angle X–Ray Scattering (SAXS), Ultra–Small Angle X–Ray Scattering (USAXS), Fluctuation X–Ray Scattering (FXS), Wide–Angle X–Ray Scattering (WAXS), Grazing–Incidence Small–Angle X–Ray Scattering (GISAXS), Grazing–Incidence Wide–Angle X–Ray Scattering (GIWAXS), Small–Angle Neutron Scattering (SANS), Grazing–Incidence Small–Angle Neutron Scattering (GISANS), X–Ray Diffraction (XRD), Powder X–Ray Diffraction (PXRD), Wide–Angle X–Ray Diffraction (WAXD), Grazing–Incidence X–Ray Diffraction (GIXD) and Energy–Dispersive X–Ray Diffraction (EDXRD). Later studies could check the advantages and disadvantages of rhodochrosite in the treatment of cancer through synchrotron radiation, such as one oscillator crystal. The studies that are found are research papers of this team. Through an unrestricted Hartree-Fock (UHF) computational simulation, Compact effective potentials (CEP), the infrared spectrum of the protonated rhodochrosite crystal, CH19Mn6O8, and the load distribution by the unit molecule by two widely used methods, Atomic Polar Tensor (APT) and Mulliken, were studied. The rhodochrosite crystal unit cell of structure CMn6O8, where the load distribution by the molecule was verified in the UHF CEP-4G (Effective core potential (ECP) minimal basis), UHF CEP-31G (ECP split valance) and UHF CEP-121G (ECP triple-split basis). The largest load variation in the APT and Mulliken methods were obtained in the CEP-121G basis set, with δ = 2.922 and δ = 2.650 u. a., respectively, being δAPT > δMulliken. The maximum absorbance peaks in the CEP-4G, CEP-31G and CEP-121G basis set are present at the frequencies 2172.23 cm⁻¹, with a normalized intensity of 0.65; 2231.4 cm⁻¹ and 0.454; and 2177.24 cm⁻¹ and 1.0, respectively. Studying the sites of rhodochrosite action may lead to a better understanding of its absorption by healthy and/or tumor tissues, thus leading to a better application of synchrotron radiation to the tumors to eliminate them.

KEYWORDS: Rhodochrosite, Quartz Crystal, Hartree-Fock Methods, APT, Mulliken, Effective core potential, Synchrotron Radiation, Cancer, Tumoral Tissues.

INTRODUCTION:

1. Introduction

The rhodochrosite (MnCO₃) shows complete solid solution with siderite (FeCO₃), and it may contain substantial amounts of Zn, Mg, Co, and Ca. The electric charge that accumulates in certain solid materials, such as crystals, certain ceramics, and biological matter such as bone, DNA and various proteins in response to applied mechanical stress, phenomenon called piezoelectricity. [1-12]

Through an unrestricted Hartree-Fock (UHF) computational simulation, Compact effective potentials (CEP), the infrared spectrum of the protonated rhodochrosite crystal, CH₁₉Mn₆O₈, and the load distribution by the unit molecule by two widely used methods, Atomic Polar Tensor (APT) and Mulliken, were studied. The rhodochrosite crystal unit cell of structure CMn₆O₈, where the load distribution by the molecule was verified in the UHF CEP-4G (Effective core potential (ECP) minimal basis), UHF CEP-31G (ECP split valance) and UHF CEP-121G (ECP triple-split basis).

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2. Methods

2.1 Hartree-Fock Methods

The molecular Hartree-Fock [15-21] wave function is written as an antisymmetrized product (Slater determinant) of spin-orbitals, each spin-orbital being a product of a spatial orbital \( \phi_i \) and a spin function (either \( \sigma \) or \( \beta \)).

The expression for the Hartree-Fock molecular electronic energy \( E_{HF} \) is given by the variation theorem as

\[
E_{HF} = \langle \phi' | H_{el} + V_{NC} | \phi' \rangle = \langle \phi' | H_{el} | \phi' \rangle + \langle \phi' | V_{NC} | \phi' \rangle
\]

Since \( V_{NC} \) does not involve electronic coordinates and \( D \) is normalized, we have \( \langle \phi' | V_{NC} | \phi' \rangle = V_{NN} (D | D) = V_{NN} \). The operator \( \tilde{H} \) is the sum of one-electron operators \( \tilde{f}_i \) and two-electron operators \( \tilde{g}_{ij} \); we have \( \tilde{H} = \sum_i \tilde{f}_i + \sum_{i>j} \tilde{g}_{ij} \), where

\[
\tilde{f}_i = -\frac{1}{2} \sum \alpha \sum \alpha' \gamma_{\alpha \alpha'} r_{i\alpha}^2
\]

where \( \gamma_{\alpha \alpha'} \) is negative. The Hamiltonian \( \tilde{H} \) is the same as the Hamiltonian \( \hat{H} \) for an atom except that \( \sum \alpha \gamma_{\alpha \alpha'} r_{i\alpha}^2 \) replaces \( Z/r_i \) in \( \tilde{f}_i \).

Therefore, the Hartree-Fock energy of a diatomic or polyatomic molecule with only closed shells is

\[
E_{HF} = 2 \sum_{i=1}^{n/2} H_i^{\text{core}} + \sum_{j=1}^{n/2} \sum_{i=1}^{n/2} (2J_{ij} - K_{ij}) + V_{NN}
\]

where

\[
H_i^{\text{core}} \equiv \langle \phi_i(1)| \tilde{H}_{\text{core}}(1) | \phi_i(1) \rangle = \langle \phi_i(1)| -\frac{1}{2} \sum \gamma_{\alpha \alpha'} r_{i\alpha}^2 | \phi_i(1) \rangle
\]

and

\[
J_{ij} \equiv \langle \phi_i(1) \phi_j(2)| 1/r_{i2} | \phi_i(1) \phi_j(2) \rangle
\]

and

\[
K_{ij} \equiv \langle \phi_i(1) \phi_j(2)| 1/r_{i2} | \phi_i(1) \phi_j(2) \rangle
\]

where the one-electron-operator symbol was changed from \( \tilde{f}_i \) to \( \tilde{H}_{\text{core}}(1) \). [5]
3. Results and Discussion

The Figure (3) show on cell structure of a protonated rhodochrosite crystal of structure Stoichiometric is CH$_{19}$Mn$_6$O$_{18}$, obtained after molecular dynamics via unrestricted Hartree-Fock method, in basis set CEP-4G, CEP-31G and CEP-121G. [32, 97]

The rhodochrosite crystal unit cell of structure CMn$_6$O$_{18}$, where the load distribution by the molecule was verified in the unrestricted Hartee-Fock method, UHF CEP-4G (Effective core potential (ECP) minimal basis), UHF CEP-31G (ECP split valance) and UHF CEP-121G (ECP triple-split basis), through the analysis of APT and Mulliken loads [98-107].

The rhodochrosite unit cell was protonated, then presented the structure CH$_{19}$Mn$_6$O$_{18}$ for the study with ab initio methods with +4 multiplicity. The displacement of charges by the molecule was analyzed to verify the site of molecular action.

The load distribution by the protonated crystal is evaluated in Table (1), and its vibrational frequencies in Table (2).

Table 1. Load shifting on given basis sets of the Mulliken and APT method.

| Basis Sets | Mulliken | APT |
|------------|----------|-----|
|            | Charge*  | δ   | Charge*  | δ   |
| CEP-4G     | -1.064   | 2.128 | -1.366  | 2.732 |
| CEP-31G    | -1.034   | 2.068 | -1.362  | 2.724 |

The largest load variation in the APT and Mulliken methods were obtained in the CEP-121G base set, with δ = 2.922 e δ = 2.650, respectively, being δ_{APT} > δ_{Mulliken}, in all sets of calculated bases, Table (1).

Table 2. Peaks maximum absorption intensity by the frequency given. Absorbance frequency as a function of vibrational frequencies of protonated rhodochrosite crystal for UHF-CEP-4G basis set, UHF-CEP-31G and UHF-CEP-121G.

|          | ν (cm$^{-1}$) | I (%)   | ν (cm$^{-1}$) | I (%)   | ν (cm$^{-1}$) | I (%)   |
|----------|--------------|---------|--------------|---------|--------------|---------|
| CEP-4G   | 217          | 64.9    | 204          | 67.1    | 219          | 60.8    |
| CEP-31G  | 223          | 45.3    | 189          | 207.7   | 202          | 978.4   |
| CEP-121G | 217          | 100     | 226          | 194.7   | 194          | 83.1    |

The Table (2) show the maximum absorbance peaks in the CEP-4G, CEP-31G and CEP-121G set basis are present at the frequencies 2172.23 cm$^{-1}$, with a normalized intensity of 65%; 2231.4 cm$^{-1}$ and 45.4%; and 2177.24 cm$^{-1}$ and 100%, respectively.

4. Analisys

The Mulliken load method in the UHF-CEP-4G base set; UHF-CEP-31G and UHF-CEP-121G are sufficient to show that the sites of action of the rhodochrosite crystal structure are found in three Oxygen-linked Manganese atoms, which are attached to the central Carbon atom, as well as these. Oxygen atoms and the central Carbon.

These Manganese atoms show a slight negative to neutral load shift in the CEP-4G set basis, neutral to positive in the CEP-31G and CEP-121G set basis at the Mulliken charges.

The charge displacement is strong in the oxygen atoms, especially those near the central carbon, with negative load in all set basis studied, both in the APT and Mulliken charges.

The central carbon atom on all set basis is positively charged in both APT and Mulliken load, except Milliken in CEP-31G, which is neutral.

As might be expected from the charges by APT, the strong positive load manganese atoms, the strong negative load oxygen, the...
positively charged carbon atom. The manganese atom farthest from the carbon atom has a slight positive to neutral load shift.

The Mulliken load method presents a better result when compared to the APT, in the studied set basis, for protonated rhodochrosite crystal, with a smaller load variation \( \delta = 2.650 \) u.a for CEP-121G.

The absorption peaks are in a Gaussian between the frequencies 1620 cm\(^{-1}\) and 2520 cm\(^{-1}\), Figure 3D.

The largest load variation in the APT and Mulliken methods were obtained in the CEP-121G base set, with \( \delta = 2.922 \) and \( \delta = 2.650 \), respectively, being \( \delta_{\text{APT}} > \delta_{\text{Mulliken}} \), in all sets of calculated basis, Table (1).

The Figure (1) is one photography the Rhodochrosite stone from China.

The Figure (2) is one photography the Rhodochrosite with Fluorite, Quartz and Pyrite stone, some cut and used with semi-precious jewelry. Sweet Home Mine, main stope, Mount Bross, Alma District, Park County, Colorado USA (1993) Specimen size:

\[
8.1 \times 7 \times 3.6 \text{ cm} = 3.2'' \times 2.8'' \times 1.4''
\]

Main crystal size: 1.2 \( \times \) 1.2 cm = 0.5\(^{\circ}\) \( \times \) 0.5\(^{\circ}\) [14]

The Figure (3) represented a Cell structure of a protonated rhodochrosite crystal. Represented in red the oxygen; silver in color Manganese; in gray color Hydrogen; in light see green color the Carbon. Stoichiometry not protonated: \( \text{CMn}_8\text{O}_6 \). Stoichiometry protonated: \( \text{CH}_1\text{Mn}_8\text{O}_6 \).

The rhodochrosite crystal unit cell of structure \( \text{CMn}_8\text{O}_6 \) where the load distribution by the molecule was verified in the unrestricted Hartree-Fock method, UHF CEP-4G (Effective core potential [ECP] minimal basis), UHF CEP-31G (ECP split valance) and UHF CEP-121G (ECP triple-split basis), through the analysis of APT and Mulliken loads.

5. Conclusion

The absorption peaks are in a Gaussian between the frequencies 1620 cm\(^{-1}\) and 2520 cm\(^{-1}\).

The Mulliken load method presents a better result when compared to the APT, in the studied set basis, for protonated rhodochrosite crystal, with a smaller load variation \( \delta = 2.650 \) u.a for CEP-121G.

The maximum absorbance peaks in the CEP-4G, CEP-31G and CEP-121G set basis are present at the frequencies 2172.23 cm\(^{-1}\) with a normalized intensity of 0.65, 2231.4 cm\(^{-1}\) and 0.454 and 2177.24 cm\(^{-1}\) and 1.0 respectively.

Later studies could check the advantages and disadvantages of rhodochrosite in the treatment of cancer through synchrotron radiation, such as one oscillator crystal.

An in-depth study is necessary to verify the absorption by the tumoral and non-tumoral tissues of rhodochrosite, before and after irradiating of synchrotron radiation using Small–Angle X-Ray Scattering (SAXS), Ultra–Small Angle X–Ray Scattering (USAXS), Fluctuation X–Ray Scattering (FXS), Wide–Angle X–Ray Scattering (WAXS), Grazing–Incidence Small–Angle X–Ray Scattering (GISAXS), Grazing–Incidence Wide–Angle X–Ray Scattering (GIWAXS), Small–Angle Neutron Scattering (SANS), Grazing–Incidence Small–Angle Neutron Scattering (GISANS), X–Ray Diffraction (XRD), Powder X–Ray Diffraction (PXRD), Wide–Angle X–Ray Diffraction (WAXD), Grazing–Incidence X–Ray Diffraction (GIXD) and Energy–Dispersive X–Ray Diffraction (EDXRD).

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