

Calculation by UFF method of frequencies and vibrational temperatures of the unit cell of the rhodochrosite crystal

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Abstract

The electronic oscillator circuit that uses the mechanical resonance of a vibrating crystal of piezoelectric material to create an electrical signal with a precise frequency is a crystal oscillator. Particularly one using a quartz crystal works by distorting the crystal with an electric field, when voltage is applied to an electrode near or on the crystal. Other crystals such as rhodochrosite also have piezoelectric properties. The rhodochrosite as crystal oscillator for being an alternative to those of quartz. The rhodochrosite ($MnCO_3$) shows complete solid solution with siderite ($FeCO_3$), and it may contain substantial amounts of Zn, Mg, Co, and Ca. A molecular dynamic via molecular mechanics using the UFF (Universal Forces Field) provided the vibrational frequencies of the fundamental structure of the crystal molecule. The frequencies and vibrational temperatures of the unit cell of rhodochrosite obtained by UFF were calculated in the range from 0.6059 to 1,731.38 cm^{-1} and 0.87 to 2,491.06 K, respectively.

Keywords: Rhodochrosite; UFF; Synchrotron Radiation; Quartz Crystal; RLC Circuit; Cancer Cells.

1. Introduction

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]

The electronic oscillator circuit that uses the mechanical resonance of a vibrating crystal of piezoelectric material to create an electrical signal with a precise frequency is a crystal oscillator. The most common type of piezoelectric resonator used is the quartz crystal, so oscillator circuits incorporating them became known as crystal oscillators. Particularly one using a quartz crystal works by distorting the crystal with an electric field, when voltage is applied to an electrode near or on the crystal. This property is known as electrostriction or inverse piezoelectricity. [2] When the field is removed, the quartz - which oscillates in a precise frequency - generates an electric field as it returns to its previous shape, and this can generate a voltage. The result is that a quartz crystal behaves like an RLC circuit (resistor (R), inductor (L), and capacitor (C)), but with a much higher Q factor. Quartz crystals are manufactured for frequencies from a few tens of kilohertz to hundreds of megahertz. More than two billion crystals are manufactured annually. Most are used for consumer devices such as wristwatches, clocks, radios, computers, cellphones, signal generators and oscilloscopes. [3 - 5]

But other crystals such as rhodochrosite also have piezoelectric properties. The rhodochrosite as crystal oscillator for being an alternative to those of quartz. The rhodochrosite ($MnCO_3$) shows complete solid solution with siderite ($FeCO_3$), and it may contain substantial amounts of Zn, Mg, Co, and Ca. The Kutnohorite [$CaMn(CO_3)_2$] is a dolomite group mineral intermediary between rhodochrosite and calcite. [3 - 5]



Fig. 1: Rolled Rhodochrosite from Argentina. Ruler in Centimeters [6].

2. Methods

A molecular dynamic via molecular mechanics using the UFF (Universal Forces Field) may provide the vibrational frequencies of the fundamental structure of the crystal molecule in an Bases set Zero Differential Overlap (ZDO) [7-10].

In short the goal of molecular mechanics is to predict the detailed structure and physical properties of molecules. Examples of physical properties that can be calculated include enthalpies of formation, entropies, dipole moments, and strain energies. Molecular mechanics calculates the energy of a molecule and then adjusts the energy through changes in bond lengths and angles to obtain the minimum energy structure. [7-10].

$$E_{se} = E_{str} + E_{bend} + E_{str-bend} + E_{oop} + E_{tor} + E_{vdw} + E_{qq} \quad (1)$$

The steric energy, bond stretching, bending, stretch-bend, out of plane, and torsion interactions are called bonded interactions because the atoms involved must be directly bonded or bonded to a common atom. The van der Waals and electrostatic (qq) interactions are between non-bonded atoms. [7-10]

2.1. Hardware and software

For calculations a computer models was used: Intel® Core™ i3-3220 CPU @ 3.3 GHz x 4 processors [12], Memory DDR3 4 GB, HD SATA WDC WD7500 AZEK-00RKKAA0 750.1 GB and DVD-RAM SATA GH24NS9 ATAPI, Graphics Intel® Ivy Bridge [13].

For calculations of computational dynamics, the Ubuntu Linux version 16.10 system was used [14] and the software used for the molecular dynamics was GAMESS [15-16],

3. Results

Calculations using Molecular Mechanics and methods ab initio in this direction, based on the unit molecular structure of the rhodochrosite crystal, Figure (2), and experimental measurements could provide data from the pros and against the use of a crystal rhodochrosite oscillator, in an RLC circuit, replacing a crystal quartz oscillator.

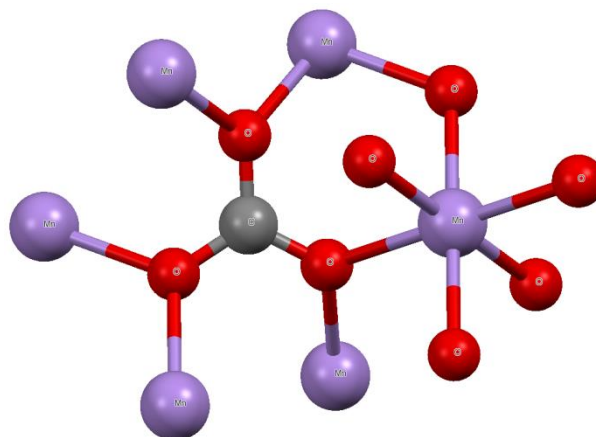


Fig. 2: Cell Structure of A Rhodochrosite Crystal. Represented in Red Color, Oxygen; in the Dark Gray Color, the Carbon and in the Purple Color, The Manganese. [74-78].

Table 1: Rhodochrosite Crystal Vibrational Energy

E (Thermal)	E (Thermal) (KCal/Mol)	CV (Cal/Mol-Kelvin)	S (Cal/Mol-Kelvin)
Electronic	0	0	0
Translational	0.889	2.981	44.328
Rotational	0.889	2.981	35.975
Vibrational	28.592	69.641	254.549
Total	30.369	75.602	334.852

Table (1) shows the vibrational, rotational and translational energies for rhodochrosite crystal, obtained by UFF.

Table 2: Vibrational Temperatures (Kelvin) of Rhodochrosite Crystal

0.87	3.71	5.08	5.64	6.82
7.87	8.73	9.77	9.91	11.31
12.73	12.92	14.57	16.34	17.54
17.89	19.18	20.57	20.88	25.23
28.44	29.85	32.62	34.25	35.06
38.6	40.11	41.18	45.99	47.52
51.25	58.92	62.25	271.71	996.22
996.4	1287.09	2491.01	2491.06	

Table (2) shows the temperatures in Kelvin the crystal of rhodochrosite, obtained by UFF.

Table 3: Vibrational Frequencies (Cm⁻¹) of Rhodochrosite Crystal

0.6059	2.5772	3.5287	3.9185	4.7399	5.4673	6.069
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6.7922	6.8885	7.8622	8.8445	8.9819	10.1271	11.3539
12.193	12.4363	13.3317	14.2963	14.51	17.5325	19.7635
20.7445	22.6701	23.8052	24.3696	26.83	27.8756	28.6216
31.9667	33.0292	35.622	40.949	43.268	188.85	692.41
692.534	894.574	1731.34	1731.38	-	-	-

Table (3) shows the vibrational frequencies in Kelvin the crystal of rhodochrosite, obtained by UFF.

4. Conclusion

The total thermal energy of the rhodochrosite crystal is 30.369 (KCal/Mol), its specific heat is 75.602 (Cal /Mol-Kelvin) and its entropy is 334.852 (Cal/Mol-Kelvin).

The frequencies and vibrational temperatures of the unit cell of rhodochrosite obtained by UFF were calculated in the range from 0.6059 to 1,731.38 cm^{-1} and 0.87 to 2,491.06 K, respectively.

Later studies could check the advantages and disadvantages of rhodochrosite versus quartz crystal, such as crystal oscillator.

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