Vibrational properties of Diamantane and Amlodipine using density functional theory

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Abstract

Vibrational properties of Gallium phosphide (GaP) diamantine,Amlodipine and(GaP) diamantine bonded with Amlodipine are investigated using density functional theory at the PBE/6-31(d) level.Physical properties of Amlodipine which is an anti-hypertensive approximately one nanometer molecule is simulated theoretically and compared with experimentally results.Density functional theory is used in this simulation to analysis of vibrational modes in terms of reduced masses, force constants and IR intensity. Vibrational frequencies of GaP diamantane are compared with bulk experiment and GaP diamantane binded with Amlodipine.The result GaP longitudinal optical (LO) vibration frequency at 376.9 cm^{-1}, Amlodipine longitudinal optical (LO) vibration frequency at 194 cm^{-1}and bonded diamantine with amlodipine longitudinal optical (LO) vibration frequency at 65.61cm^{-1}.Although the associated IR peak of GaP with this mode is not high, IR peak in Amlodipineand IR peak in the bonded diamantine with amlodipine peak will increase in height the size.

Keywords: Diamondoids; Amlodipine; IR intensity; Raman; Diamantan

1. Introduction

Amlodipine is a medication used to lower blood pressure and prevent chest pain. It belongs to a group of medications known as long-acting dihydropyridine-type calcium channel blockers as in figure (1) [1]. Like other medications in this group, Amlodipine lowers blood pressure by relaxing the muscles controlling the diameter of blood vessels in the body [2]. Gallium phosphide is a semiconductor with indirect band gapin its zincblende structure [3].It can be reduce GaP particle size to the nanoscale by using diamondiod as shown in figure (2). Recently, a collection of particles with increasing number of atoms and varying size are found to be building blocks of nanomaterials that are called diamondoids [4]. The term diamondoid is used to describe hydrocarbon molecules that are totally or largely superimposable on the diamond lattice. The lower limit of this definition is set at adamantane ($C_{10}H_{16}$) to prevent the inclusion of cyclohexane and other simple alkanes [5].The diamondoid (or diamond hydrocarbon) classification can be further separated into two groups: diamondoids that are only partly superimposable on the diamond lattice and diamondoids which are completely superimposable on the diamond lattice. Molecules in the latter group that can only be formed by the face-fusing of adamantane units (sharing 6 carbon atoms per pair of adamantanes) are known as polymantanes. The polymantanes form a
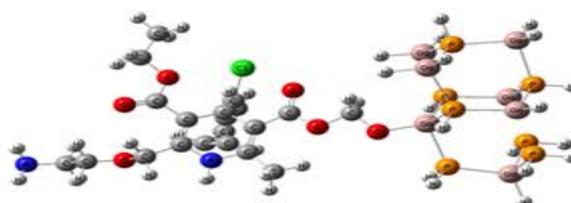
natural series, starting with the smallest molecules (adamantane, diamantane and triamantane), and finishing with an infinite diamond lattice. Between these two points lie micro- and nano-crystal diamond, and the higher diamondoid molecules [6].In the present work we shall use the molecular orbital theory to investigate the physical properties of this medical substance, diamantine and bonded diamantine with Amlodipine are shown in figure (3). These properties include the analysis of vibrational modes in terms of reduced masses, force constants and IR intensity and Raman spectral lines. We use an advanced density functional method that incorporate 6-31G (d) basis set.

Figure 1: Shape of geometrically optimized Amlodipinedrug.

Figure 2: Shape of geometrically optimized GaP-Diamantane

International Journal of Emerging Trends & Technology in Computer Science (IJETTCS)
Web Site: www.ijettcs.org Email: editor@ijettcs.org
**Volume 4, Issue 1, January-February 2015**   **ISSN 2278-6856**

2. Theory

All electron density functional theory (DFT) at the generalized gradient approximation level of Perdew, Burke and Ernzerhof (PBE) is used in the present work.Observing results manifests that PBE/6-31G (d) method and basis are one of the best molecular orbital methods that can be used to simulate large molecules.6-31G (d) basis are available for all the atoms in Amelodipine. Gaussian 09 program is used in the present work to perform this task [7].Investigated molecule atomic coordinates are introduced to the program. These coordinates are optimized so that there are no forces on all the atoms in amlodipine. Figures (1), (2) and (3) shows amlodipine, diamantine and Amlodipine bonded with diamantane molecules that is geometrically optimized using PBE/6-31G method.Nanomaterials are those materials that are at least one of its dimensions (1-100n) and can be used in many molecular characteristics account and can be obtained in two ways namely: bottom-up or top-down methods from molecular or solid state theories respectively. Density functional theory at the Perdew, Burke and Ernzerhof (PBE) level is used in the present work. 6-31G (d) basis that include polarization functions are sophisticated enough to describe amlodipine, diamantane and Amlodipine bonded with diamantane orbitals withreasonable accuracy that match experimental properties. It can calculate reduced mass, IR intensity, force constant and Raman spectra.

3. Results and discussion

Figures (4-6) are related to vibrational spectroscopy of Amlodipine, GaP diamantine and amlodipine bonded with diamantane. In Figure (4-a) the reduced masses of molecular vibrations are shown. The dashed line represents the bulk experimental GaP longitudinal optical (LO) vibration frequency at 376.9 cm^{-1} [8]. The highest reduce mass mode (HRMM) in Figure (4-b), Amlodipine longitudinal optical (LO) vibration frequency at 194 cm^{-1}and figure (4-c) related diamantine with amlodipine longitudinal optical (LO) vibration frequency at 65.61cm^{-1}. And the highest force constant mode (HFCM) [9] in Figure (5).
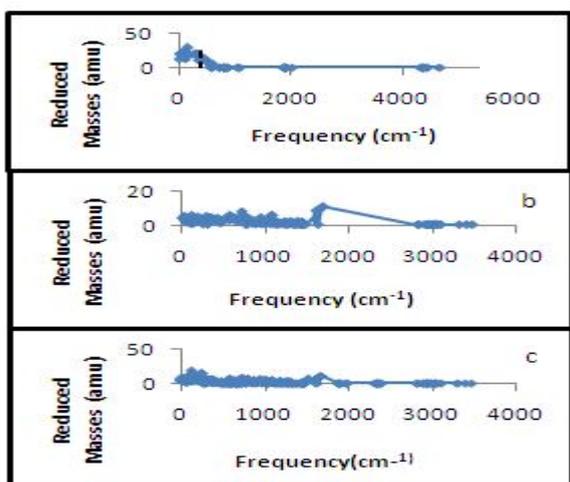
Although the associated IR peak in Fig (6) with this mode is not high the reduced mass. The reduced mass of two particles of masses m_a and m_b is given by:
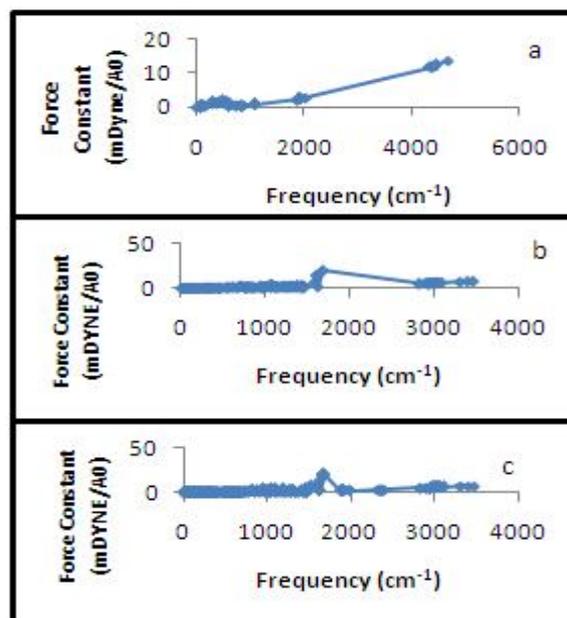
$$\mu = \frac{m_a * m_b}{m_a + m_b} \qquad (1).$$

The reduced masses in Fig (5-a) reach 12 amu which is nearly the reduced mass between two P atoms. This shows that some vibrations might include one kind of atoms and exclude the other.
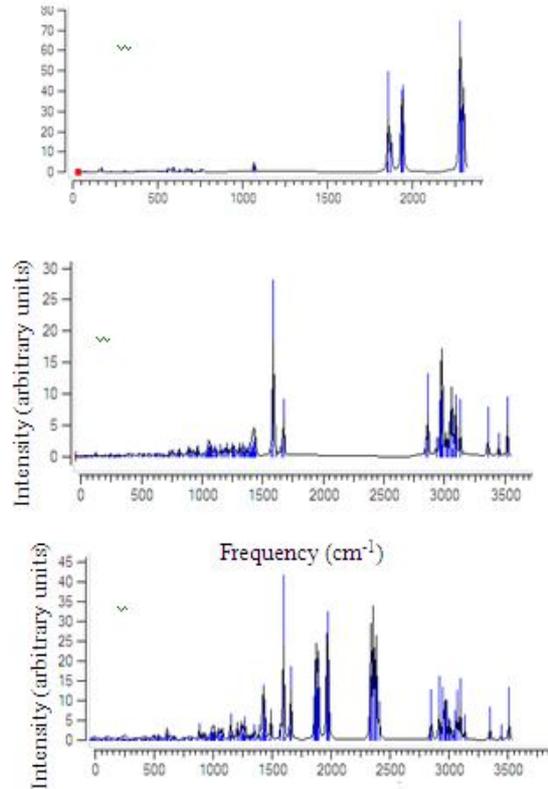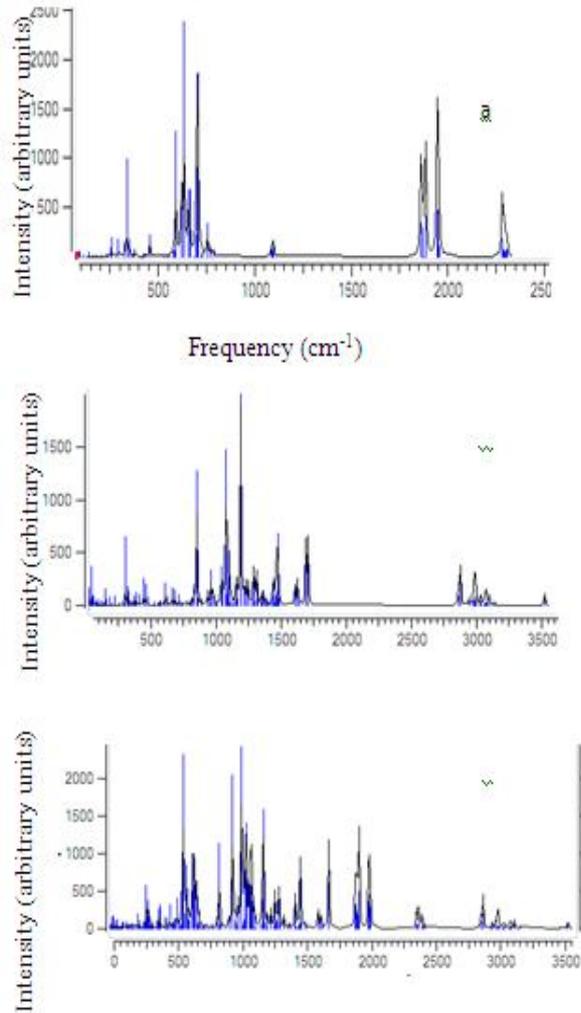
The reduced masses of Amlodipine in figure (5-b) reach (7amu) which is nearly the reduced mass between two atoms Cl-C and figure (5-c) reduced masses of bonded diamantine with Amlodipine near (8amu) which is nearly the reduced mass between two atoms C-Ga. The vibrations after (471 cm^{-1}) are all hydrogen of Ga-P Diamantane related vibrations since they all have the approximate reduced mass one. Although the reduced masses after 471 cm^{-1} are all nearly equal to one the force constants keep in increasing because the frequency of vibration is proportional to the square root of force constant:

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} \qquad (2)$$

The vibrations after 471 cm^{-1} are all hydrogen of Ga-P Diamantane related vibrations since they all have the approximate reduced mass one.at the end of Figs (4-6). But Amlodipine to the symmetric and asymmetric C-H start 2989 and 3031 cm^{-1} of join diamantine with amlodipine symmetric and asymmetric Ga-H and P-H at 1918, 2412 and C-H 3092 and 3024 .The highest force constant for the Ga-P vibrations (2.1 mDyne/Å). The highest force constant for the Amlodipine vibrations (21mDyne/Å) and the highest force constant for the bonded diamantine with Amlodipine vibrations (22mDyne/Å).

International Journal of Emerging Trends & Technology in Computer Science (IJETTCS)
Web Site: www.ijettcs.org Email: editor@ijettcs.org
Volume 4, Issue 1, January-February 2015   **ISSN 2278-6856**

Although the associated IR peak of Ga-P in Figure (6-a) can be noted the high peak at red shift and lower peak at blue shift while at figure (6-b) IR peak in Amlodipine most high peak at red shift but very lower peak at blue and figure (6-c) IR peak in the related diamantine with amlodipine peak will increase in height as the size.There is a continuous distribution of the intensities of the red to the blue region.

Figure (7) Note there is a difference between the peaks IR and Raman due to the presence of the selection rules for the operator IR and operator Raman, which is different when you find a transition matrix which results in a difference between the two cases. At figure (7-a) Note from this figure that the highest intensity is located at blue shift, in which the vibrational modes are different, which includesymmetric, asymmetric, wagging, scissor, rocking and twistingmodes and lower intensity is located red shift, which are vibrational modes such as symmetric and asymmetric between Ga-2H and P-2H respectively.Note in Figure (7-b) there are peaks and low intensities in the red region to reach the intensity of about (28) and then go down to zero and then increases in the blue region.Note in Figure (7-c) red region where short peaks are then start upward toward the blue region.

4 Conclusions

GaP diamondoids vibrational properties as close as possible to bulk structures.GaP longitudinal optical (LO) vibration frequency at 376.9 cm^{-1}, Amlodipine longitudinal optical (LO) vibration frequency at 194 cm^{-1} and bonded diamantine with Amlodipinelongitudinal optical (LO) vibration frequency at 65.61cm^{-1}. The reduced masses in Ga-P reach 12 amu which is nearly the reduced mass between two P atoms. This shows that some vibrations might include one kind of atoms and exclude the other. The reduced masses of Amlodipine reach (7) amu and reduced masses of bonded diamantine with Amlodipine near (8) amu. The vibrations after 471 cm^{-1} are all hydrogen of Ga-P Diamantane related vibrations since they all have the approximate reduced mass as 1. Although Note there is a differencebetween the peaks IRand Raman due the presence of the selection rules for the operator IR and operator Raman, which is different when you find a transition matrix which results in a difference between the two cases. And IR peak in the bonded diamantine with Amlodipine peak will increase in height the size.

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