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A Comparative Study of Conformational Behavior of Isotretinoin (13–*Cis* Retinoic Acid) and Tretinoin (All–*Trans* Retinoic Acid (ATRA)) Nano Particles as Anti–Cancer Nano Drugs under Synchrotron Radiations Using Hartree–Fock (HF) and Density Functional Theory (DFT) Methods

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In order to know about the conformational behavior of isotretinoin (13–*cis* retinoic acid) and tretinoin (all–*trans* retinoic acid (ATRA)) Nano particles under synchrotron radiations in which the accelerating particle beam travels around a fixed closed–loop path **(Figure 1a and 1b)**, we have calculated the optimized molecular geometries of isotretinoin (13–*cis* retinoic acid) and tretinoin (all–*trans* retinoic acid (ATRA)) Nanoparticles. Calculations are carried out on the structures of these Nano compounds using Hartree–Fock (HF) calculations and also Density Functional Theory (DFT) methods by performing HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP levels of theory using the standard 31G, 6–31G*, 6–31+G*, 6–31G(3df, 3pd), 6–311G, 6–311G* and 6–311+G* basis sets of the Gaussian 09 [1–24]. The equilibrium structures and comparative heats of formation have been calculated and analyzed for these Nano compounds. A comparative study of shows that the HF optimized molecular structures of the isotretinoin (13–*cis* retinoic acid) and tretinoin (all–*trans* retinoic acid (ATRA)) Nano particles are in good arrangement with those of the HF/6–31G(3df, 3pd) method **(Figure 2)**.

On the other hand, isotretinoin (13–*cis* retinoic acid) and tretinoin (all–*trans* retinoic acid (ATRA)) Nano particles under synchrotron radiations in which the accelerating particle beam travels around a fixed closed–loop path are spread throughout nature which motivates their use as oral pharmaceutical Nano drugs primarily used to treat severe nodular acne which motivates their use as reaction substrates [25–55]. Rarely, they are also used to prevent certain skin cancers (squamous–cell carcinoma) and also in the

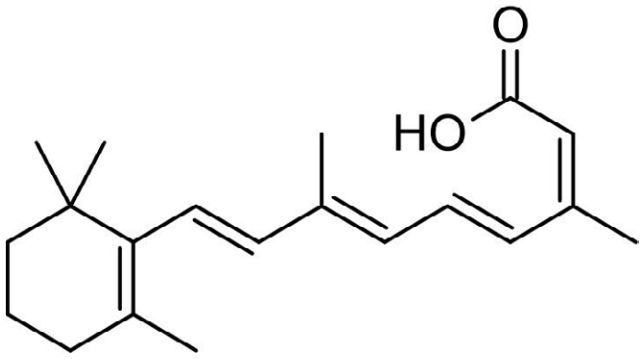

Figure 1a Molecular structure of isotretinoin (13–*cis* retinoic acid) Nano particles[1-14].

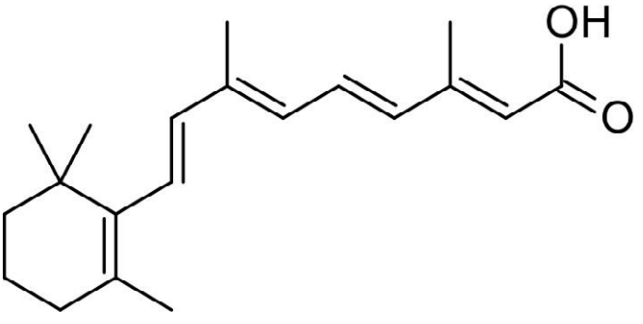

Figure 1b Molecular structure of tretinoin (all– *trans* retinoic acid (ATRA)) Nano particles [1–14].

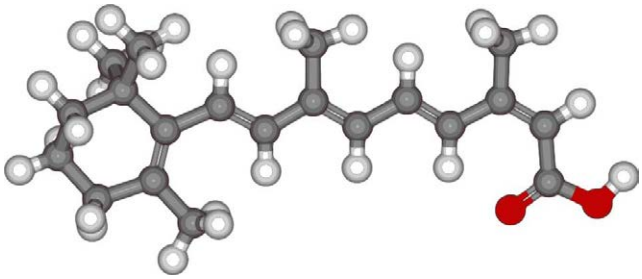

Figure 2 Optimized molecular structure of isotretinoin (13–*cis* retinoic acid) Nano particles in the HF/6–31G (3df, 3pd) method [1–14].

treatment of other cancers under synchrotron radiations in which the accelerating particle beam travels around a fixed closed–loop path [25–55]. Moreover, they are used to treat harlequin–type ichthyosis, a usually lethal skin disease, and lamellar ichthyosis under synchrotron radiations in which the accelerating particle beam travels around a fixed closed–loop path [25–55]. It should be noted that they are retinoid, meaning they are related to vitamin A (beta–carotene), and are found in small quantities naturally in the body under synchrotron radiations in which the accelerating particle beam travels around a fixed closed–loop path [25–55]. Isotretinoin (13–*cis* retinoic acid) isomer, tretinoin (all–*trans* retinoic acid (ATRA)), is also an acne drug under synchrotron radiations in which the accelerating particle beam travels around a fixed closed–loop path [25–55]. A high number of their oxygenated derivatives are used as flavours and fragrances in the food and perfume industries under synchrotron radiations in which the accelerating particle beam travels around a fixed closed–loop path [25–55].

In the course of our editorial, we have investigated the isotretinoin (13–*cis* retinoic acid) and tretinoin (all–*trans* retinoic acid (ATRA)) Nano particles as anti–cancer Nano drugs under synchrotron radiations in which the accelerating particle beam travels around a fixed closed–loop path. Also, in the present editorial, we have calculated the optimized molecular geometries of isotretinoin (13–*cis* retinoic acid) Nano particles **(Figure 2)**. This anti–cancer Nano drug is used to manufacture a number of products for the pharmaceutical, biochemical, medical and medicinal industries under synchrotron radiations in which the accelerating particle beam travels around a fixed closed–loop path. This anti–cancer Nano drug is also the precursor for creation of many pharmaceutical, biochemical, medical and medicinal Nano compounds under synchrotron radiations in which the accelerating particle beam travels around a fixed closed–loop path. Therefore, it can be concluded that in order to know more about the conformational behavior of this Nano compound, we have investigated conformational analysis of it under synchrotron radiations in which the accelerating particle beam travels around a fixed closed–loop path.

The high level Density Functional Theory (DFT) method with 6–31G(3df, 3pd) basis set is used to obtain the optimum structures of isotretinoin (13–*cis* retinoic acid) Nano particles. The HF– optimized molecular structures were used as the initial geometry in these Density Functional Theory (DFT) calculations. In addition, a comparative study shows that the HF optimized molecular structures of the isotretinoin (13–*cis* retinoic acid) Nano particles are in good arrangement with those of the HF/6–31G (3df, 3pd) method. Furthermore, similar to the HF method, HF/6–31G (3df, 3pd) heats of formation is the largest for isotretinoin (13–*cis* retinoic acid) Nano particles and the least for tretinoin (all–*trans* retinoic acid (ATRA)) Nano particles. Therefore, it can be concluded that HF method can approximate the optimized molecular structures of isotretinoin (13–*cis* retinoic acid) and tretinoin (all–*trans* retinoic acid (ATRA)) Nano particles within an acceptable and reasonable accuracy and precision in much shorter times.

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