Alkanes in Motion

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Abstract

The motion of gas molecules is very complicated owing to the combination of translation, rotation, and vibration. Such motion is difficult to depict using static media, such as the printed page. Also, simple animations tend to focus on only one aspect of molecular motion (*1*). So, to improve students' understanding of molecular motion, Alkanes in Motion, a collection of clip animations generated from molecular dynamics calculations, was produced. It depicts the molecular motion of hydrocarbons in the gas phase. Four animations from the collection are presented here. These four animations consist of two animations each of propane and octadecane, one animation calculated to show translational motion, and one to show vibrational motion.

The molecular motion of alkane molecules was calculated using the molecular dynamics simulation (*2, 3*) in HyperChem (*4*). The simulations were used to obtain the position of each atom of each molecule at each time step. Each simulated molecular system includes 18 carbons (i.e., six propane molecules (Figure 1) and one octadecane (Figure 2)) at a temperature of 600 K and is done using the MM+ method, based on the MM2 functional form, authored by Allinger (*5*).

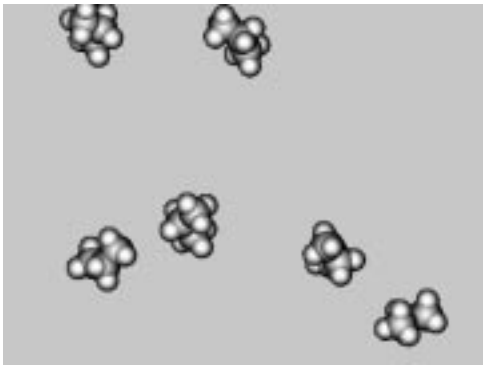

Figure 1. A frame from the Propane in Motion animation.

The time increment of each molecular dynamics calculation was one femtosecond. The graphical display of the results of these calculations was then captured at periodic intervals. To accurately depict vibrational motion, animations were done capturing a frame each femtosecond. To show translational motion, a second animation captured at 25-femtosecond intervals was done. The individual frames were then compiled into a QuickTime animation.

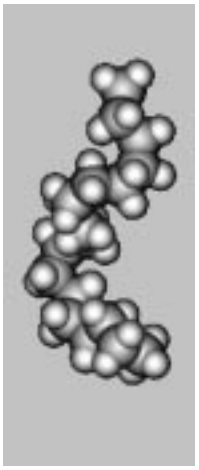

Figure 2. A Frame from the Octadecane in Motion animation.

Each animation contains 900 frames. The molecules are rendered using a CPK-model; the color of carbon is cyan and the color of hydrogen, white. A time stamp was added to show the relative time of molecular motion. The total real time of the one-femtosecond interval animation is 0.9 picoseconds; at the 25-femtosecond capture rate the animation is 22.5 picoseconds in duration.

These animations of hydrocarbon systems clearly and accurately show the motion of molecules in the gas phase. In the one-femtosecond interval animations, the vibration and rotation of C–H and alkyl groups can be

clearly seen. The 25-femtosecond interval animations show translation in addition to vibration and rotation. In some cases they show the detailed motion of atoms in molecules after a collision between two molecules. Previously, only rough and approximate movement of atoms vibrating, rotating, and translating could be shown. These animations depict the movement of molecules more realistically.

Instructor Notes

Incorporating Animations into your own Presentation

Since they are QuickTime files, the animations in Alkanes in Motion are readily incorporated into documents created by applications that are aware of QuickTime. Such applications include word processors (e.g., Word, Word Perfect), presentation software (e.g., PowerPoint), and authoring systems (e.g., HyperCard, Macromind Director).

Please note the *JCE Software* license agreement found inside the front cover of this manual. The Alkanes in Motion animations are licensed for use on up to five computers at one time unless additional copies of the issue are purchased. As the owner you are permitted to make derivative works as described above for your personal use. You many not copy, broadcast, or distribute the animation or derivative works without written permission from *JCE Software*. *JCE Software* welcomes and encourages the submission of works such as classroom exercises, software tutorials, and multimedia presentations that include animations we have published.

For directions on how to incorporate QuickTime files into your documents, consult the documentation that came with your application software.

Acknowledgments

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Citations

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