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Molecular Models of Polymers Used in Sports Equipment

October Featured Molecules

In keeping with the 2008 National Chemistry Week theme of “Having a Ball with Chemistry”, the Featured Molecules this month are a number of monomers and their associated polymers taken from a paper by Sandy VanNatta and John P. Williams on polymers used in making equipment for a variety of high-impact sports *(1)*. The molecules provide students with an introduction to an important area of applied chemistry and also enable them to examine complex structures using the models they have seen applied to small molecules.

It is certainly instructive for students to build small polymer fragments using molecular model kits. Holding a model of *n*-decane, for example, and twisting it in various ways, provides real insight into the multiplicity of conformations available to supermolecules of polyethylene. Computer-based 3-dimensional structure drawing and visualization programs make it possible to construct large oligomers of known polymers and to begin to explore structural properties of new systems. Two such programs, free for academic use, are DSVisualizer and ArgusLab *(2)*. DSVisualizer includes a useful set of tools for building and viewing structures and a “clean geometry” option that applies a Dreiding-like force field. ArgusLab adds the ability to perform both molecular mechanics and semi-empirical geometry optimization and to display various molecular surfaces. Using ArgusLab, or a similar program, students can explore the relative energies of various conformations of the substances they have built electronically. Students who are being introduced to molecular modeling and the use of more sophisticated software can easily explore the effects of the modeling and convergence parameters on the stable structures that are found, and can begin to explore the difference between global and local minima on a molecular potential energy surface. Using the conformational search program in HyperChem 7.5 on a tetramer of vinyl chloride (terminated with H; of SRRS stereochemistry; only CCCC torsions varied), approximately half of the 500 structures examined fell within 6 kcal/mol of the lowest energy structure *(3)*. This number would increase significantly if other torsion angles were included.

The use of computational software allows us to introduce students in introductory chemistry to the idea of multiple conformations, which is so important in biochemistry and much of organic chemistry. In teaching ideas behind conformational stability care should be taken when attributing conformational stability solely to non-bonded repulsions between peripheral atoms on adjacent carbon atoms. Weinhold and co-workers have recently presented strong evidence that the stability of the staggered conformer of ethane relative to the eclipsed form arises from more favorable interactions of C–H sigma bonding orbitals on adjacent carbons *(4)*. The multiplicity of such interactions could well be responsible for conformational stability in more complex systems. Any discussion of conformational stability should also introduce students to the ultimate conformational problem—the folding of proteins—and to the Folding@home project *(5)*.

Literature Cited

1. VanNatta, Sandy; Williams, John P. Impact of Polymers in Impact Sports. *J. Chem. Educ.* **2008,** *85,* 1326–1329.
2. DSVisualizer is available from Accelrys at *http://accelrys.com/products/discovery-studio/visualization/discovery-studio-visualizer.html*, and ArgusLab is available at *http://www.arguslab.com/* (both sites accessed Aug 2008).
3. HyperChem, Professional 7.52, Hypercube, Inc., 1115 NW 4th Street, Gainesville, FL 32601; *http://www.hyper.com/* (accessed Aug 2008).
4. See, for example, Weinhold, F. *Nature* **2001,** *411,* 539.
5. Folding@home. *http://folding.stanford.edu/* (accessed Aug 2008).

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Supplement

Find “Molecular Models of Polymers Used in Sports Equipment” in the *JCE* Digital Library at *http://www.JCE.DivCHED.org/JCEWWW/Features/MonthlyMolecules/2008/Oct/*.

The molecules added to the collection this month are low-density polyethylene (LDPE); polyethylene (PE) polypropylene (PP); poly(methyl methacrylate) (Plexiglas); acrylonitrile butadiene styrene (ABS); polystyrene (PS); polyurethane (PU); polyvinyl chloride (PVC); nylon.