Chemistry

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Pulling polymers into line

One way to line up the tangled strands of a polymer is to stretch the material. This alignment often strongly influences the polymer's properties. Now some researchers have found a way to use magnetic fields to align polymer molecules quickly and efficiently. "Using a magnetic field adds a new dimension to the processing of materials," says polymer scientist Samuel I. Stupp of the University of Illinois at Urbana-Champaign.

Stupp and his colleagues start with a liquid crystal polymer, such as an aromatic polyester. Like any polymer, this type of material consists of a large number of repeating units arranged in a long molecular chain. Unlike many other polymers, however, these special polymer molecules, when in the liquid state, tend to organize themselves into a loose pattern characteristic of liquid crystals.

To make the liquid crystal polymers more responsive to magnetic fields, small units of organometallic compounds such as copper complexes are added. These additives, which are paramagnetic and interact strongly with an external magnetic field, find places within the polymer chain or attach themselves loosely to the polymer's backbone. Thus, when the liquid polymer is under the field's influence, the polymer molecules are pulled into line. When the material solidifies, the induced pattern is frozen into place.

The insertion of paramagnetic segments greatly speeds the alignment process so that it takes only minutes. Without such units dispersed along the polymer chains, magnetic alignment could take hours or days. The new method also overcomes some of the problems associated with using electric fields to achieve the same goal.

Stupp has discovered that magnetic alignment can significantly change a polymer's properties, particularly in certain directions. In one experiment, alignment increased a material's electrical conductivity in one direction by about 100 times. This process also alters a polymer's optical and mechanical properties.

Aligning polymer molecules in certain directions may turn out to be useful for strengthening thin plastic films often used as coatings. Normally, the molecules in a thin film line up so that they stand upright like a brush's bristles, stretching from the lower to the upper surface of the film. A magnetic field could pull these molecules so that they lie flat, parallel to the film's surfaces.

Computing a molecular shortcut

Chemists at the University of Houston at University Park have developed a computational method for theoretically predicting how strongly two particular molecules would bind together in the presence of a solvent. In the past, such predictions have been difficult to make because of the complexity of the interactions among the two binding molecules and the many solvent molecules. The Houston group, led by J. Andrew McCammon, has found a way to circumvent the problem by using a kind of "computational alchemy."

First, the researchers compute the step-by-step behavior within a solvent of, say, a drug molecule already captured by a receptor molecule. Then the initial drug molecule is mathematically transformed into a new molecule with a slightly different structure. Again, the step-by-step behavior of this new receptor-drug combination is computed. When these data are combined with simulations of how the two drugs interact with the solvent when the receptor isn't present, the researchers can deduce whether the modified drug binds with a particular receptor more or less strongly than the original drug molecule. In this way they can determine how useful the new drug would be without having to compute exactly how this molecule binds with the receptor.

The danger of polyester-cotton blends

A chemist at the University of California at Davis reports that some polyester-cotton-blend clothing can burn "up to 25 percent faster" than clothing made either from pure synthetics such as polyester or from pure "cellulosic" fibers such as cotton or rayon. "Lightweight polyester-cotton blends, in certain apparel uses, are very dangerous," says researcher Howard L. Needles. Moreover, he notes that while a pure synthetic will melt and fall away from the body as it burns – tending to self-extinguish – the blends hold together, giving flames and heat a greater chance of causing body burns. As a result, he feels that lightweight blends – those weighing less than 4 ounces per square yard – are inappropriate for some clothing, particularly for children or the elderly. As a substitute, he recommends pure polyester.

Despite previous research suggesting that polyester-cotton blends should be less flammable than pure cotton, these blends have been involved in a disproportionate number of clothing fires, he notes. The primary reason, his research now suggests, is that when textile makers move from producing pure cottons to making a blend, they tend to reduce the weight of the fabric. And his studies show that fabric weight per square yard is the largest factor affecting flammability.

However, Needles and his co-worker, Cynthia Walker, were able to show differences even between fabrics of the same weight. For example, they found that pure cellulosic fabrics are somewhat less flammable than polyester-cellulosic blends of the same weight. One reason, they say, may be that as the polyester melts, "it wicks and spreads" burning temperatures quickly over the cotton, enhancing the flame front's spread. Even among cellulosic fabrics they found flammability differences. Pure rayon burns faster than an equal weight of pure cotton, and polyester-rayon blends burn faster than polyester-cotton blends of the same weight.

Needles criticizes the way fabrics are tested for flammability in the United States. "If the test fabric doesn't ignite after being exposed to a flame for one second, it passes," he says. "That really only excludes 'torch' fabrics, those that practically explode when they're lit." Even tissue paper passes that test, he notes. At least as important as ignition time, he believes, is how fast a fabric burns in the vertical position – a factor not now considered in these tests.

Another major factor affecting flammability is apparel design. "You don't hear about a tight-fitting dress shirt engulfing someone in flames," Needles says. "It's always . . . something that's loose and gives a good air-fabric mix that spreads flames around the body," he says.

Beefing up the flavor arsenal

Flavor chemists have been stymied in their search for the compounds that give beef its characteristic taste. "Most flavors are in the volatile or aromatic components of foods," notes Chi-Tang Ho at Rutgers University in New Brunswick, N.J. His work has shown that 130 volatiles – readily vaporizable chemicals – contribute to the "fried chicken" flavor. However, he could not find a combination of volatiles that generates a beefy taste. Now, together with Stephen Chang and Tzou-Chi Huang, Ho has identified a single pair of nonvolatile peptides (compounds derived from two or more amino acids) that imparts a beef flavor.

These compounds may make possible the meatless creation of beef-flavored gravy or soups. They also hold promise as an alternative to monosodium glutamate (MSG) as a new "flavor enhancer." Says Ho, "Our hope is that the compounds we have discovered, since they are routinely eaten in beef, will prove to have the good effects of MSG without its bad effects" – those "Chinese-restaurant-syndrome" headaches and aftertaste.