Electric-field gradient sorts molecules according to their shape

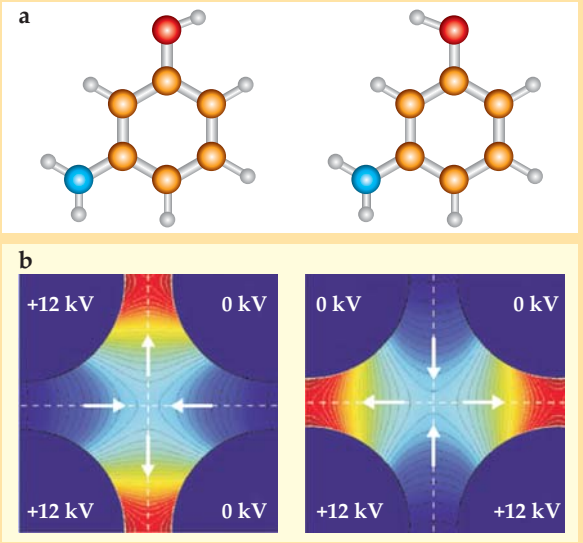
Physically distinct but chemically identical molecules can have different electric dipole moments and therefore can respond differently to an inhomogeneous electric field.

Stereoisomers are molecules that have all the same atoms connected in the same way but arranged differently in space. Conformational isomers, or conformers, are stereoisomers that can readily interconvert at room temperature and are typically considered versions of the same molecule. An understanding of conformers is particularly important in the study of biological systems, since a biomolecule's function is so often related to its physical shape. Protein folding, for example, involves the interconversion of conformers. But it's difficult to study conformers individually because any room-temperature sample necessarily contains a mix of them, and they respond identically to the usual separation techniques, such as mass spectrometry.

Now, Jochen Küpper, his student Frank Filsinger, and colleagues at the Fritz Haber Institute in Berlin, Germany, have developed a way to spatially separate conformers in a molecular beam.[1] They looked at the *cis* and *trans* conformers of the molecule 3-aminophenol, shown in the figure on page 18. As with many biomolecules, the 3AP conformers have very different electric dipole moments, mostly because of the position of the lone pairs of electrons on the oxygen atom. Küpper and colleagues put 3AP into a molecular beam, which cools the internal motions of the molecule enough to suppress the interconversion. They then separated the two conformers using the Stark effect, the shifting of the molecular energies in response to an external electric field.

Encountering an inhomogeneous electric field, both conformers are drawn to the high-field regions. But *cis*-3AP, which has a much larger dipole moment than *trans*-3AP, is pulled more strongly. Küpper and colleagues created their inhomogeneous field using four long, parallel, cylindrical rods, to which they applied voltages that switched between the configurations shown in the figure. The configuration on the left focuses the molecules horizontally and defocuses them vertically, and the configuration on the right does just the opposite. The researchers controlled which molecules were transmitted by adjusting the switching frequency. For a given frequency, molecules of one particular dipole moment are optimally focused, those with lower dipole moments are not focused, and those with higher dipole moments are defocused so much that they escape. For *cis*-3AP, the optimal switching frequency is around 3 kHz; for *trans*-3AP, it is around 1.5 kHz.

The selection technique not only sorts the molecules by shape but also facilitates their alignment in space. A molecular beam containing oriented molecules of a single conformer could



(a) The conformers of 3-aminophenol: *trans*-3AP (left) and *cis*-3AP (right). Carbon atoms are shown in yellow, nitrogen in blue, oxygen in red, and hydrogen in white. Only the position of the uppermost H atom differs between the two structures, but that variation is enough to give them different electric dipole moments. **(b)** The electric-field configurations used to separate the 3AP conformers. Regions of high electric field are shown in red, and regions of low electric field are shown in blue. The white arrows indicate the directions of the focusing and defocusing forces on the molecules. The frequency of switching between the two configurations determines which conformer is transmitted. (Adapted from ref. 1.)

be useful for studying molecular structure using x-ray or electron diffraction. The use of x rays to determine the shape of a single structure has been demonstrated (see PHYSICS TODAY, January 2007, page 19). As Küpper explains, the benefit of a constantly renewed beam of identical molecules is that "you can irradiate the samples with intense x-ray pulses and sum up the images for as long as you want—in principle, every image will look the same, because each fresh sample looks the same, even in real space."

Küpper and colleagues' method achieves only a partial separation because molecules in high rotational states don't feel the focusing and defocusing forces as strongly as those in low rotational states. That problem can be lessened, but not entirely eliminated, by decreasing the rotational temperature of the beam. And biomolecules of interest—such as the amino acid phenylalanine, which has at least six conformers with well-separated dipole moments—are not easy to coax into a molecular beam. Says David Pratt of the University of Pittsburgh, "As usual, the devil is in the details. But I am optimistic that the technique will be broadly applicable."

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Reference

1. F. Filsinger, U. Erlekam, G. von Helden, J. Küpper, G. Meijer, *Phys. Rev. Lett.* **100**, 133003 (2008).

Collider data show evidence for a meson made of four quarks

It's not obvious from quantum chromodynamics what sorts of unusual mesons and baryons experimenters should expect.

In the six decades since the discovery of the pion, more than a hundred other meson species have been found. Most decay by the strong nuclear interactions and therefore live less than 10^{-22} s. So one sees them only as resonant peaks in scattering cross sections or energy distributions. But until now they all had one thing in common: Every known meson was characterized by a combination of quantum numbers—charge, spin, parity, strangeness, charm, and the like—that could be accounted for simply by a quark–antiquark ($q\bar{q}$) pair.

Now the Belle collaboration at the KEKB electron–positron collider in Tsukuba, Japan, has reported impressive evidence for the first manifestly exotic meson—a meson that clearly requires more quarks than just a $q\bar{q}$ pair.[1] Dubbed $Z^{\pm}(4430)$, the new charged meson has a mass of 4.43 GeV, about four and a half times that of the proton. Particle physicists welcome such exceptions as clues to elusive ramifications of quantum chromodynamics, the accepted theory of the strong interactions of quarks and the hadrons (baryons and mesons) they make up.

The giveaway was the new meson's observed decay mode. From among the debris of a billion e^+e^- collisions recorded by Belle since 1999, group members Soo-Kyung Choi and Stephen Olsen have unearthed a resonant peak of some 170 events indicating the strong-interaction decay of a 4.43-GeV meson to a $\pi^{\pm}$ and a ψ' (see the figure on page 19). With a mass of 3.69 GeV, the electrically neutral ψ' is a well-established "charmonium" meson. That is, it's a bound state of the heavy charmed quark (c) and its antiquark ($\bar{c}$). Almost twice as heavy as the proton, the c quark was discovered in the mid-1970s.

Because quarks cannot change character (called flavor) in strong-interaction decays, it's clear that the parent $Z^{\pm}$ already contained a $c\bar{c}$ pair. But c and $\bar{c}$ have equal and opposite charges ($\pm 2e/3$). So they alone can't account for the charge of the $Z^{\pm}$ manifested by its charged-pion decay product. Therefore, in addition to the $c\bar{c}$ pair, the new meson must also harbor two of the light quarks that make up more familiar particles like protons and pions. For the Z^+, it's an up quark (u) with charge $+2e/3$ and an antidown quark ($\bar{d}$) with charge $+e/3$.

The figure shows a distribution of invariant mass—the total energy of the two putative decay products in the reference frame of their center of mass. In the absence of lifetime broadening and experimental error, the histogram would exhibit a zero-width spike at the mass of the parent particle. Taking account of measurement uncertainties, the fit to the invariant-mass peak yields an intrinsic width of about 45 MeV. That's unusually narrow for so heavy a meson in the absence of a selection rule that inhibits strong-interaction decay. The narrowness, by itself, is suggestive of an exotic state.

KEKB, like the similar PEPII collider that recently ceased operation at SLAC,