NEWS & VIEWS

CHEMICAL PHYSICS

# Molecular conformations fielded

Albert Stolow

**Studies of molecular dynamics can be foiled by the presence of stereoisomers — molecules that have the same bond sequence arranged in different geometries. This problem has now been deflected.**

In the ancient Indian tale of six blind men encountering an elephant, each man approaches the creature from a different direction. One finds the trunk, another a leg, the third the tail, and so on, whereupon they naturally disagree with each other as to the true appearance of the elephant (Fig. 1). And so it is with molecules — molecular properties and dynamics seem to depend on the direction from which you view them. To make matters worse, some molecules can exist as different stereoisomers — molecules that have identical atoms and sequences of bonds, but which have bonds that point in different directions. If elephants came in two versions, one in which the legs point towards the ground and another in which they point towards the sky, these two versions would be stereoisomers. Such a situation would clearly further complicate the deliberations of the six blind men.

Similarly, the presence of stereoisomers within a sample of molecules can lead to confusion in studies of molecular dynamics, because any measurements taken are generally averages of the properties of all of the stereoisomers. Because the dynamics of stereoisomers can vary greatly (as would the relative locomotive abilities of our elephantine stereoisomers), the average result may not pertain to any molecule at all. Reporting in *Angewandte Chemie*, Filsinger *et al.*[1] describe an approach for spatially separating stereoisomers of neutral molecules using electric fields. This avoids the detrimental averaging of results, opening up a way to study molecular dynamics that could fully benefit from emerging ultrafast measurement techniques.

**Figure 1 | The blind men and the elephant.** Each man experiences something different depending on his angle of approach, in the same way that measurements of molecular properties seem to depend on the direction from which the molecules are viewed.

As is often the case, the most powerful techniques rely on a simple premise. Filsinger and colleagues' method relies on a phenomenon discovered by Otto Stern and Walter Gerlach in 1922. In a classic experiment[2], Stern and Gerlach demonstrated that a beam of silver atoms was deflected in a magnetic field, a finding that hastened the birth of quantum mechanics. In a subsequent paper[3], Stern suggested that electric fields could be used to spatially separate quantum states of neutral molecules. His proposal was based on an electric property of molecules known as the dipole moment. The basic idea is that molecules 'feel' electric fields differently, depending on the value of their dipole moment. The stronger the electric interaction of the dipole moment with the field, the larger the possible deflection of a beam of molecules from its otherwise straight-line path.

The fact that some molecular bonds in stereoisomers point in different directions can lead to different dipole moments for each isomer. Filsinger *et al.*[1] recognized that this is the key to spatially separating stereoisomers using Stern's electric-deflection technique. For demonstration purposes, Filsinger *et al.* studied 3-aminophenol, which comes in only two stereoisomers (designated as *cis*- and *trans*-isomers) that differ in the orientation of an oxygen–hydrogen bond (Fig. 2, overleaf). Each stereoisomer has a different dipole moment. The authors show convincingly that the *cis*- and *trans*-isomers in a molecular beam are deflected by different amounts in electric fields, and that this effect can be used to physically separate the isomers. The simplicity of this approach speaks volumes.

Until now, stereoisomers in mixtures could be selectively detected using highly resolved spectroscopic methods, but this did not allow stereoisomers to be spatially separated for practical use. Filsinger and colleagues' technique is therefore immensely valuable, although it does have limitations: it requires the stereoisomers to have sufficiently different dipole moments, and works best when the molecules are extremely cold, which can be difficult to achieve. Another method for separating stereoisomers in molecular beams using electric fields has previously been reported[4], but the fields concerned were relatively complex. The advantage of the present deflection technique[1] is that it is simple enough to be readily used by researchers working in a range of other fields — and therein lies its importance.

There is a worldwide effort to develop new approaches for studying ultrafast molecular dynamics, with good reason. In the twentieth century, much of the progress in understanding the molecular underpinnings of our world focused on the basic structures of molecules, and the relationship of structure to function. Molecules, however, are seldom static. They often undergo dynamic processes, such as chemical reactions, and so a purely structural view is unlikely to be sufficient. The next step must therefore be to understand the dynamics of molecular processes.

Unfortunately, dynamics–function relationships do not yet exist. Many new ultrafast techniques are thus being proposed by which to study the 'structural dynamics' of molecular processes — the changes in position of atoms in molecules measured as a function of time. Methods such as time-resolved X-ray[5] or electron diffraction[6,7] and X-ray absorption[8] can directly map out atomic motions. Other time-resolved techniques are able to observe both atomic motions and electronic rearrangements, and even their coupling as bonds rearrange in concert with atomic motions — for example, photoelectron spectroscopy[9,10] (which studies the distribution of electrons emitted from molecules when they are irradiated with ultraviolet or soft X-ray light) and high harmonic generation[11,12] (which studies the burst of ultraviolet or soft X-ray light emitted from molecules when they are irradiated with intense, near-infrared laser pulses).

All of these technical developments, however, suffer from the same problem — averaging over stereoisomers and molecular orientations, leading to a blurring and potential loss of information. An analogy can be made with X-ray diffraction in crystals: the random orientation of crystallites in powder diffraction obscures the detailed information that is obtainable from single-crystal diffraction. Unless this averaging problem is seriously addressed, the new ultrafast techniques for studying molecular dynamics may not live up to their promise. Filsinger and colleagues' spatial selection of stereoisomers is therefore a step towards the full implementation of techniques that aim to illuminate the molecular processes that transform the worlds within and around us. ■

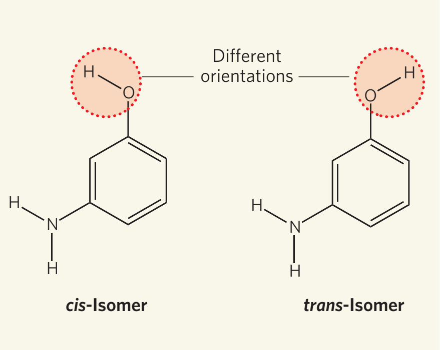

**Figure 2 | The same, but different.** 3-Aminophenol exists as two stereoisomers — *cis-* and *trans-*isomers — which differ only in the orientation of the oxygen–hydrogen bond (highlighted). The isomers are difficult to separate, but Filsinger *et al.*[1] have done so by deflecting a molecular beam of 3-aminophenol in an electric field.

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SOLAR SYSTEM

# Saturn's colossal ring

Matthew S. Tiscareno and Matthew M. Hedman

**A hitherto undetected disk of debris around Saturn is the largest ever found to be orbiting a planet. This ring may hold the key to one of the most enigmatic landscapes in the Solar System.**

On page 1098 of this issue, Verbiscer and colleagues[1] report the discovery of an enormous ring around Saturn. The authors found this most tenuous of Saturn's known rings, which covers some 10,000 times as much area as the planet's photogenic main rings, by using the Spitzer Space Telescope to detect the ring's faint glow in the thermal infrared region of the electromagnetic spectrum. The ring is composed of dust, probably derived primarily from Saturn's distant moon Phoebe. Its discovery lends support to an earlier theory that dusty material from Phoebe is responsible for colouring the two-toned moon Iapetus.

This 'Phoebe ring' of Saturn (Fig. 1) is similar to previously known tenuous rings in the outer Solar System, such as Jupiter's gossamer rings or Saturn's E ring, in that it is composed mainly of small particles (less than 100 micrometres across) that must be constantly replenished from larger source bodies such as moons, because such tiny grains are eroded away or ejected from their host planet's orbit on very short timescales (less than 1,000 years). The Phoebe ring, like Jupiter's gossamer rings, probably consists of the dust ejected from moon surfaces by impacts[2]; by contrast, Saturn's E ring is supplied by geysers emanating from the interior of the planet's moon Enceladus.

But the Phoebe ring is vastly different in scale from other dusty rings. It has a core radius (the distance from Saturn at which the ring's density reaches its peak value) that is about 200 times the radius of Saturn and 50 times that of the E ring, the previous record holder for the Solar System's largest planetary ring. Thanks to its huge dimensions, the Phoebe ring is at least ten times more massive than the E ring, despite having a particle number density (20 particles per cubic kilometre) that is tens of millions of times lower[1].

The destiny of all that mass may be the most interesting aspect of the Phoebe ring's discovery. Just as the icy dust in the E ring spreads out from Enceladus and seems to brightly coat the surfaces of Saturn's inner moons[3], so the dust in the Phoebe ring is expected to spiral inward towards Saturn, where much of it would be swept up by Iapetus, the outermost of Saturn's large moons, whose surface patterns are a 300-year-old mystery.

Because Iapetus keeps one face always towards its parent planet, like most moons in the Solar System, it also keeps one face (the 'leading hemisphere') directed towards its direction of motion. Iapetus' leading hemisphere is among the darkest surfaces in the Solar System (its albedo — the fraction of sunlight that is reflected back into space — is about 4%), whereas the opposite ('trailing') hemisphere and the poles are quite bright. Surfaces of intermediate brightness, however, are almost entirely absent[4]. It has long been considered plausible that dust from Phoebe is the most likely cause of Iapetus' curious coloration[5,6], but broad agreement has been elusive. The spectral match between the two is not exact, and it is unclear whether the differences can be explained by dust deposition at hyper-velocity and subsequent mixing with the native Iapetan surface.

Furthermore, the lack of dark material at Iapetus' poles is unexpected under a simple model of infalling pollution, although this might be explained by a model that includes infall plus subsequent thermal processing. On the other hand, the leading alternative theory — that the dark material somehow comes from within Iapetus — has a difficult time explaining the close alignment of the dark terrain with the leading hemisphere. Verbiscer and colleagues' discovery[1] of a disk of material surrounding Saturn, corresponding to Phoebe's orbit, is strong evidence for an external source for the dark material on Iapetus. However, much work remains to be done to determine the origin and fate of the observed dust.

As it spirals inward, some fraction of the Phoebe ring's dust makes it past Iapetus and continues on towards the next likely targets, the moons Hyperion and Titan. But the chaotic rotation of Hyperion[7] would cause it to become evenly coated with the ring's dust, not asymmetrically as for Iapetus, and for Titan the infall would be just one more component of its already complex surface chemistry[8].

Further observations of this enormous ring would be highly desirable to better determine its structure and spectral properties. In particular, complementary photometry (measurement of an object's brightness) in visible light would constrain the size distribution and albedos of its component particles — are they really as dark as their presumed source (Phoebe) and destination (Iapetus' leading hemisphere)? Furthermore, such observations could clarify whether other moons besides Phoebe are supplying this ring with dust. Phoebe is by far the largest of Saturn's distant moons, but this does not necessarily make it the best source of dust. Although bigger moons present larger targets for dust-generating impacts, their increased surface gravity correspondingly holds on to