Casting for molecules

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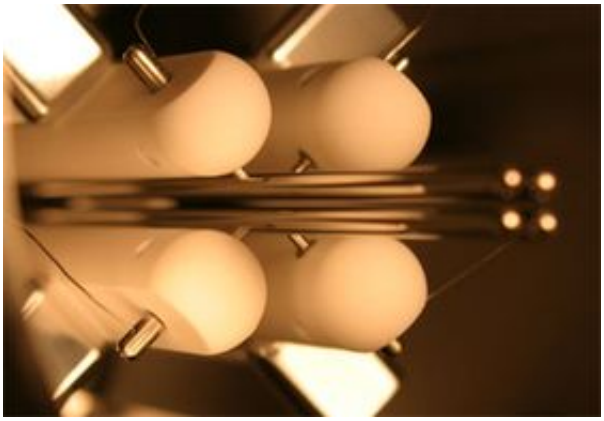

The orientation of the molecules decides whether they will reach the end of this open tube. The electric field between the four metal rods changes constantly so that only conformers with the correct mass-to-dipole-moment ratio can pass through the open tube. Image: Fritz Haber Institute of the Max Planck Society

Many of the larger molecules have something in common with dolls - movable limbs. Physicists at the Fritz Haber Institute of the Max Planck Society in Berlin can now sort molecules according to the direction in which their "arms" and "legs" point. Normally, it is almost impossible to distinguish between these conformers - molecules with different orientation - and, in any event, molecule limbs usually flap about wildly. Nevertheless, orientation is important for biomolecules: they can only do their job when they point their limbs in the right direction.

Taking snapshots of biomolecules is tricky. It is made slightly easier for the biochemists if they can grow crystals from the compounds.

Alternatively, they might be able in future to create gas beams of these molecules and send them through their measuring instruments. However, normally the images of the different conformers overlap and the researchers only get a blurred image of the particles.

"We have now found a way to isolate the conformers, although chemically and physically, it is hardly possible to keep them apart," says Jochen Küpper, who heads the group of scientists at the Fritz Haber Institute. There is only one difference that occurs more often: the conformers have, in many cases, dipoles of different strengths - that is, the positive and negative charges are distributed differently in the molecules. Therefore, they register the strength of an electrical field differently. And the researchers exploit this factor.

"Our filter for conformers works like a quadrupole mass filter," explains Frank Filsinger, who, as a doctoral student, carried out most of the work. Quadrupole mass filters are used in many laboratories to separate molecules by their mass-to-charge ratio. The apparatus used by the researchers in Berlin sorts the particles in a very similar way, with the difference that they isolate them on the basis of their mass and their dipole moment. Dipole moment is a measure of the strength of a dipole.

The scientists tested their new method on an aminophenol - on two conformers in which the hydroxide group of the molecule is oriented differently. This group consists of an oxygen and a hydrogen atom, and is characteristic of alcohols. Their different orientations in the aminophenol are called cis and trans positions. In the cis version, the hydroxide group points to one side of the molecule, in the trans variant it points precisely to the other side. For this reason, the dipole moment of the cis-aminophenol is approximately three times greater than that of its trans counterpart.

In order to isolate the two conformers with the hydroxide "arm" in

different positions, the researchers vaporized a small quantity of the substance and bundled it into a molecular beam. The beam travels exactly one metre in the Berlin researchers' equipment. In order that the cis and trans versions separate over this distance, Küpper and his colleagues apply electrical fields that exert forces on the molecules: they group four electrodes - live metal rods that form a sort of tube - around the molecular beam. The beam moves through this tube. Alternating voltage runs through two electrodes, causing the positive and negative poles to repeatedly jump backwards and forwards. The direction in which the force of the electrical field acts on the molecules changes accordingly.

The frequency of the alternating field is decisive; that is, the speed at which the poles change places. Different dipoles vary in their response to the alternating field. Finally, at a certain frequency of the alternating field only molecules with a certain dipole moment, or more precisely, only those with a certain mass-to-dipole-moment ratio, reach the end of the apparatus. All the others gradually drift out of the trajectory of the beam.

The researchers working with Frank Filsinger in Berlin not only isolated only one specific conformer in this way. They can even sort the conformers by the amount they rotate. Molecules rotate constantly, but not always at the same speed. There is a measure of the speed of rotation - the rotation quantum number, which increases with the rotational speed of the molecule. However, the dipole of the particle becomes thereby increasingly weaker and the electric field has a weaker effect on it. "We also filter out the molecules in the lowest rotation quantum states," says Küpper. This allows the molecules to be oriented in space particularly well. The researchers hope that, in future, they will be able to get all the particles with arms facing in the right direction moving.

"Our method complements other new experiments, such as the X-ray

laser that is currently being developed in Hamburg." This X-ray laser will emit particularly bright light, making it a very sensitive instrument. Many scientists are hoping, therefore, to make images of single biomolecules with it, obviously in the form of a single conformer. The representations of different molecular positions would not blur into a shadowy image in the shots taken with the new large-scale machine. "We are taking the reverse route, however" explains Küpper. "As we can isolate the different conformers and therefore all the molecules in the trial look the same, we are not forced to examine individual molecules," he says, "but might be able to significantly strengthen the signal by observing many molecules with a similar appearance."

Up to now, he and his colleagues have only been able to isolate relatively small particles with the molecular filter. Sorting conformers of larger molecules is not a problem in principle, but in practice. "The separation would work," says Küpper, "but it has not yet been possible to bundle very large, uncharged molecules into a gaseous beam." Many scientists throughout the world are working on this problem - including those at the Fritz Haber Institute.

Citation: Frank Filsinger, Undine Erlekam, Gert von Helden, Jochen Küpper, and Gerard Meijer, Selector for structural isomers of neutral molecules, *Physical Review Letters* 100, 133003 (2008)

Source: Max Planck Society