Structure and shape of the molecule determine its reaction rate

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Most molecules occur in several shapes, which may behave very differently. Understanding the shapes of molecules is an important first step in being able to discuss and predict chemical properties. The shapes of molecules are determined by the repulsion between electron pairs in the outer shell of the central atom. Both bond pairs (electron pairs shared by two atoms) and lone pairs (those located on a central atom but not shared) must be considered. The three dimensional shape or configuration of a molecule is an important characteristic. This shape is dependent on the preferred spatial orientation of covalent bonds to atoms having two or more bonding partners. A German-Swiss research team for the first time directly measures the various reaction rates of different forms of the same compound. Many chemical compounds have numerous conformers i.e. different forms of a molecule in which some building blocks are spatially rearranged (rotated). Even tiny changes in structure can greatly affect the properties of a compound and even lead to different reaction products. To investigate these differences, the researchers have built a sorting machine for molecules, which can be used to selectively pick a conformer and feed it into a chemical reaction. The device exploits the fact that generally a change in structure also modifies the dipole moment of a molecule. The dipole moment describes how a molecule interacts with an electric field. The sorting machine generates a non-uniform electric field between an electrically charged rod and a trough. When the researchers send several conformers at once through the narrow slit between the rod and the trough, the field deflects the various conformers to different degrees. The device thus provides sorted beams of different conformers, which can be spatially separated and directed individually into a reaction chamber. The selected conformers differed only in the direction in which a single hydrogen atom is attached to an oxygen atom. As a result, one conformer has a three times larger dipole moment than the other. A tiny change in structure thus leads to big differences in chemical reactivity. In this way, the method allows insights into fundamental reaction mechanisms that can lead to more effective syntheses of new molecules, such as active pharmaceutical ingredients.

REFERENCE