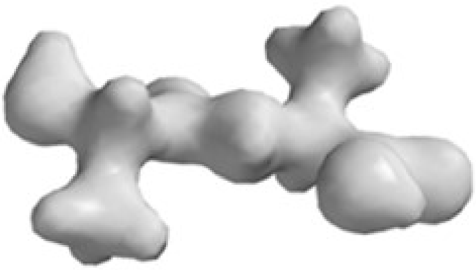
Topic: Molecular Art

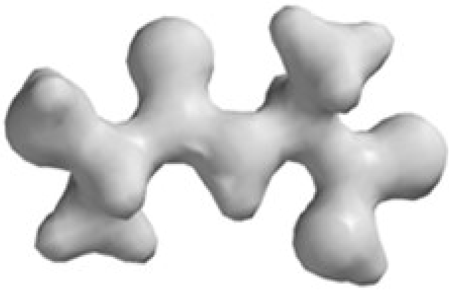
Author:
Paul G. Mezey
Memorial University of Newfoundland
Department of Chemistry
Canada
www.mun.ca/research/chairs/mezey.php

Main References:
[1] Paul G. Mezey, "*Shape in Chemistry: An Introduction to Molecular Shape and Topology*", VCH, New York, 1993,
[2] Paul G. Mezey, "*The Role of Imperfect Symmetry in Nature, Art, Mathematics, and Chemistry: Approximate Symmetry and Symmetry Deficiency Measures* ", J. Internat. Soc. Interdisc. Study Symmetry, 2004, 166-169 (2004).
[3] Paul G. Mezey, "*The Holographic Electron Density Theorem and Quantum Similarity Measures* ", Mol. Phys., 96, 169-178 (1999).
[4] Paul G. Mezey, "*Fuzzy Electron Density Fragments* ", Acc. Chem.Res., 47, 2821-2827 (2014).

Abstract:

Motivated by the early efforts of the mathematical genius of Felix Klein of the Erlangen Program fame, who made interesting efforts to provide some mathematical description of those geometrical shapes which people find beautiful, the study of molecular shapes involves both geometrical and topological approaches [1-4]. The perception of molecular beauty, intricate shapes, as well as an intriguing combination of functionality and shape changes, provide impressions which are leading to the initial scientific associations as the seeds for both novel scientific methods and to a new appreciation of the artisitc richness of the microscopic world of molecules. The two images of the electron density cloud of the alanylalanine dipeptide molecule, shown below, exhibit many of the richness, beauty, and grace of molecular shapes. The mathematical tools of topology used for their characterisation provide the intellectual beauty of logical harmony of human thought processes with the natural world.





Contact:
paul.mezey@gmail.com

Keywords:

Molecular shape, topology, molecular beauty, shape analysis, shape groups, similarity measures, complementarity measures

Topological Beauty and Molecular Shape

Paul G. Mezey, PhD, DSc

Canada Research Chair, Scientific Modelling and Simulation,

Memorial University of Newfoundland, St. John's, NL Canada

email: paul.mezey@gmail.com

Motivated by the early efforts of the mathematical genius of Felix Klein of the Erlangen Program fame, who made interesting efforts to provide some mathematical description of those geometrical shapes which people find beautiful, the study of molecular shapes involves both geometrical and topological approaches [1-4]. The perception of molecular beauty, intricate shapes, as well as an intriguing combination of functionality and shape changes, provide impressions which are leading to the initial scientific associations as the seeds for both novel scientific methods and to a new appreciation of the artisitc richness of the microscopic world of molecules. The two images of the electron density cloud of the alanylalanine dipeptide molecule, shown below, exhibit many of the richness, beauty, and grace of molecular shapes. The mathematical tools of topology used for their characterisation provide the intellectual beauty of logical harmony of human thought processes with the natural world.

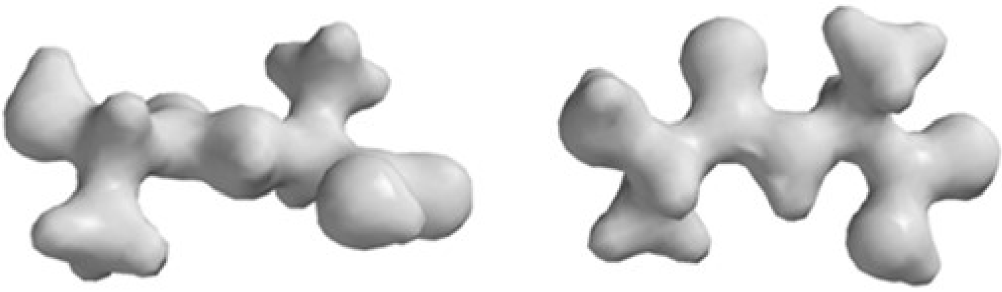


Figure 1. The shape of the electron density cloud of the alanylalanine dipeptide molecule, shown at the relatively high density threshold value of 0.1 atomic units

One of the most fascinating aspects of topology is its special adaptability not only to a great variety of earlier, seemingly very divers mathematical fields, but also to applies fields of science, everyday life, and art. It is mot by accident that he nick-name "rubber geometry" is often used for topology, where not the precise geometrical distances, angles, and coordinate values are important, but the way various entities are connected. Just as my identity is not changed when the distance between my eyebrows become shorter if I think hard, that is, when some geometrical aspects change, the same is true for molecules, which do preserve their identity during minor geometrical changes, for example, in some vibrational processes. However, my topology is still the same if I frown or smile, and the identity of molecules is also preserved during formal geometrical changes in vibrational processes.

The beauty of a dancing ballerina is enhanced in the harmonious movements which all preserve something essential: they preserve the topology that is common for all the smoothly changing geometries realised during the dance moves. The beauty of the dance is not in the detailed description of the precise geometry and in a listing of all the actual coordinates of each and every cell of the ballerina, but in the harmonious way of preserving the topology, common for all the never-ever captured, incessantly changing geometries of her body. The same is true for the fascinating shapes of incessantly vibrating, moving, an rotating molecules. The shape analysis, shape recognition, and complementarily recognition of molecules, all involve topological concepts, whether this is recognized or not.

Topology can also be regarded as the mathematics of the essential: for solutions of real problems which can be precisely phrased, whether on the scientific level, or in everyday life, or in art, the minor geometrical variations are typically less important than the more essential topological features.

There is another aspect strongly suggesting that topology and beauty are a great match when one has the desire to try to obtain some more formal understanding of what appears esthetically pleasing. Typically, natural objects and live creatures, such as a flower or a galloping horse, or even lifeless utilities, such as an elegant spoon, often appear beautiful for us if they are well-functioning - we seem to have an experience of pleasant feeling if we have a chance to realize that something functions well, it does well what it is supposed to do, so that part of the world works the way it is good for us. Yes, this can be a pleasant, reassuring feeling, that we may, sometimes, associate functionality even with the feeling of beauty. Let us recall, that topology is often referred to as "rubber geometry", so there is a special role for topology in the context of well-functioning, accommodating, and pleasing objects, since by contrast, the rigid, geometrically precisely defined entities, unyielding, stiff objects are often generate negative feelings, in fact, we might find them ugly too. This is another way of recognizing that topology in our mind is connected to the assessment of beauty. Even without realizing this, we often look at the world and the objects, creatures, and even concepts through an innate topological assessment.

In the case of molecules, the intricate shapes of their electron density clouds naturally lend themselves to a topological analysis. This electron density cloud is the very fuzzy object that is the formal "body" of molecules, the body that is sensed by the body of any neighboring molecule and the one that may trigger a stronger interaction leading to some chemical reaction.

There are several factors which have greatly improved our chances to take more and more artistic excursions to the fascinating world of the beauty of molecules. Traditionally, objects which have been easily available to the human senses, observation, and perception, for example, to vision, have been dominating the artists choices as subjects of artistic representation, for example, a colorful tree in the autumn sunshine, or a smiling face. In earlier times, it has been impossible for an artist to be motivated by seeing a molecule, because, simply, molecules are so small that even the best of optical microscopes are useless, if some detail is to be studied. It is a relatively recent development that computer-based molecular modelling approaches are capable of showing in great detail the shapes of electron density clouds, not only in their static arrangements, but in full, three-dimensional motion.

It is also a relevant consideration that the laws of nature on that microscopic level of molecules often lead to phenomena we are not well equipped to follow in detail. Even our concepts are not well suited for that size-range of the universe. On that microscopic level, nature shows a very high degree of variety, there are many millions of already recognized, different molecules. Yet, their study and analysis involves many branches of science, and understanding their behaviour is far from complete. One such consideration is the fuzzy nature of the electron density cloud, manifested on two levels. On the more fundamental level: the Heisenberg Uncertainty relation, one of the most fundamental laws of physics, renders the concept of a "molecular surface" ill-defined, since due to the particle-wave duality of electrons, and the requirement that the uncertainty of the position of an electron, multiplied by the uncertainty of the momentum (velocity times mass) of the electron cannot be smaller than some positive value. This restriction is entirely "alien" to our everyday concepts, where we cannot perceive that nature has such a limitation. Simply, evolution has not provided us with any sensory experience that could ever require to experience such a limitation, so, naturally, our everyday concepts do not include any hint of such a restriction, as a limit to observations.

Another, somewhat less surprising consideration is the fact that molecular electron density clouds are fuzzy, they have no boundaries, they gradually fade by distance, and in a strict sense, a molecular electron density, decreasing exponentially with distance, does not become exactly zero even at very large distances from the atomic nuclei of the molecule. This fact may complicate somewhat the visualization approaches when representing electron density clouds, but by choosing some molecular isodensity contours, MIDCOs, such as those of the alanylalanine dipeptide molecule, shown in the Figure, one can still obtain some pictorial representation.

These images, generated by computer, using false colours, provide often stunningly beautiful, intricate shapes. Yes, even though for their generation one needs a computer, these are still natural shapes just as the shape of a droplet of rain on a leaf, or the bud of a flower.

Molecular electron density clouds are beautiful. Smooth but intricate forms, with abstract, but often thought-provoking forms, they are providing very enjoyable, even addictive visual experiences

I hope that the intellectual beauty of the mathematics of the topological analysis of such electron density shapes, and the actual visual experience of their beauty, as images, or as even changing images during some chemical processes, will provide many with the sense of beauty.

[1] Paul G. Mezey, “*Shape in Chemistry: An Introduction to Molecular Shape and Topology*”, VCH, New York, 1993,

[2] Paul G. Mezey, “*The Role of Imperfect Symmetry in Nature, Art, Mathematics, and Chemistry: Approximate Symmetry and Symmetry Deficiency Measures* ”, J. Internat. Soc. Interdisc. Study Symmetry, 2004, 166-169 (2004).

[3] Paul G. Mezey, “*The Holographic Electron Density Theorem and Quantum Similarity Measures* ”, Mol. Phys., 96, 169-178 (1999).

[4] Paul G. Mezey, “*Fuzzy Electron Density Fragments* ”, Acc. Chem.Res., 47, 2821-2827 (2014).