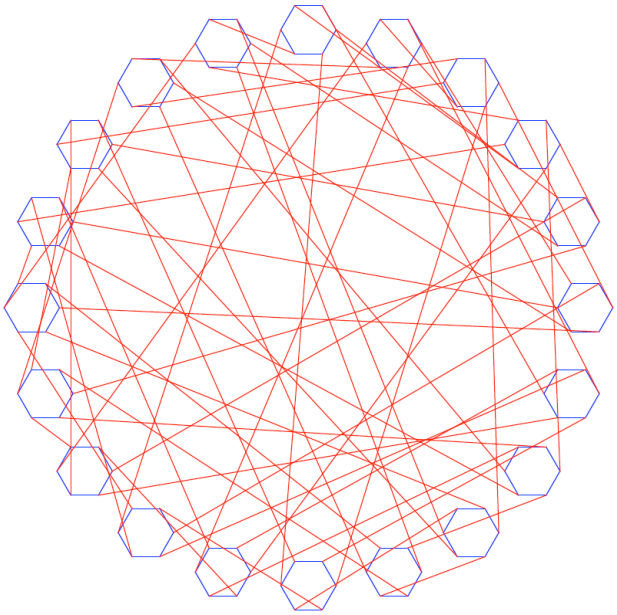
Application of quantum-graph theory to the quantum mechanics of extremely floppy molecules

Csaba Fábri[a,b]

[a] Laboratory of Molecular Structure and Dynamics, Institute of Chemistry, Eötvös Loránd University, Pázmány Péter sétány 1/A, H-1117 Budapest, Hungary
[b] MTA-ELTE Research Group on Complex Chemical Systems, P.O. Box 32, H-1518 Budapest 112, Hungary
E-mail: ficsaba@caesar.elte.hu

A quantum graph is a metric graph equipped with a differential operator.[1,2] Quantum graphs arise naturally in various fields such as physics, chemistry, and engineering. We report the first application of quantum-graph theory to describe the quantum-mechanical motion of extremely floppy molecules defying widely-accepted qualitative models used by chemists and physicists.[3] The new theoretical approach is applied to protonated methane (CH_5^+), an enigmatic system of molecular physics, challenging our traditional understanding of chemical structure and molecular motion. The vertices of the quantum graph correspond to the distinct structures of the molecule (the five hydrogen atoms can be arranged in 5!=120 different ways around the central carbon atom for CH_5^+), while the edges represent different collective nuclear motions transforming the distinct structures into one or another. The quantum-graph model is able to explain the very peculiar behaviour of CH_5^+ in a natural and intuitive way.



[1] G. Berkolaiko and P. Kuchment, Introduction to Quantum Graphs, American Mathematical Society, 2013, vol. 186.
[2] G. Berkolaiko, An elementary introduction to quantum graphs, https://arxiv.org/abs/1603.07356.
[3] C. Fábri, A. G. Császár, *Phys. Chem. Chem. Phys.* **2018**, *20*, 16913.