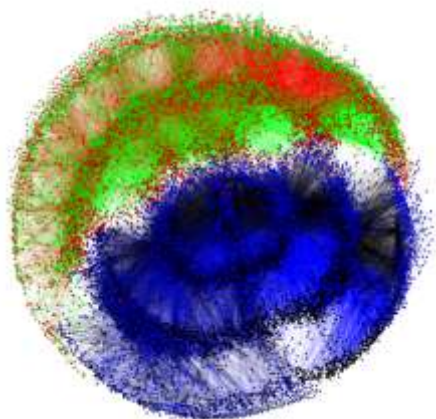# Simple molecules as complex systems

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For individual molecules quantum mechanics (QM) offers a simple, natural and elegant way to build large-scale complex networks: quantized energy levels are the nodes, allowed transitions among the levels are the links, and transition intensities supply the weights. QM networks are intrinsic properties of molecules and they are characterized experimentally via spectroscopy; thus, realizations of QM networks are called spectroscopic networks (SN) [1]. As demonstrated for the rovibrational states of $H_2^{16}O$, the molecule governing the greenhouse effect on earth through millions of its spectroscopic transitions (links), both the measured and first-principles computed one-photon absorption SNs containing experimentally accessible transitions appear to have heavy-tailed degree distributions. The proposed novel view of high-resolution spectroscopy and the observed degree distributions have important implications: appearance of a core of highly interconnected hubs among the nodes, a generally disassortative connection preference, considerable robustness and error tolerance, and an "ultra-small-world" property. The network-theoretical view of spectroscopy offers a data reduction facility via a minimum-weight spanning tree approach, which can assist high-resolution spectroscopists to improve the efficiency of the assignment of their measured spectra[2].

The MARVEL algorithm [3] and code we developed is based on the theory of spectroscopic networks and combines it with a weighted linear least-squares protocol for data inversion. MARVEL, standing for Measured Active Rotational-Vibrational Energy Levels, can be employed to determine experimental energy levels and their uncertainties from a database of experimentally measured and assigned transitions coming from high-resolution spectroscopy. Algorithmic improvements characterizing the second generation of the MARVEL code [4] make it possible to invert the information contained in hundreds of thousands of transitions and obtain the underlying energy levels. The most important application of MARVEL has been the determination of all the known "experimental" energy levels of all the major isotopologues of the water molecule(for example,[5]).We also applied successfully the MARVEL code for the H_3^+, H_2D^+, and D_2H^+ molecules [6,7].

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