ASSIGNMENT AND EXTRACTION OF VIBRATIONAL DYNAMICS FROM EXPERIMENTALLY AND THEORETICALLY OBTAINED SPECTROSCOPIC HAMILTONIANS IN COMPLEX SPECTRAL REGIONS

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An analysis, requiring only trivial calculation as the computer is only used for graphics, of experimentally and theoretically obtained spectroscopic Hamiltonians is shown to yield a dynamically based assignment of complex molecular spectra. Also revealed is the motional model upon which the levels are quantized. The complexity in these multiresonant regions is shown to be due to the interleaving of ladders with conventional state quantisation each based on different dynamical models. The method is based on qualitative ideas from non-linear dynamics and allows the sorting of states into rather simple spectral ladders of common dynamics, a step which no experimental technique can do. Examples are DCO, CHBrClF, and the ‘unassignable‘ bending spectrum of acetylene.