# Low-lying quasibound states of $H_2^{16}O$

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Quasibound (also called resonance) states of a system are metastable states which have sufficient energy to brake up the system into its subsystems. They can be associated with outgoing eigenfunctions of the Hamiltonian, diverging exponentially at infinity. Due to the outgoing boundary condition, the eigenvalues corresponding to resonance states are complex.

Techniques of non-Hermitian quantum chemistry merged with efficient nuclear motion computational algorithms allow the determination of quasibound rovibrational states of strongly-bound triatomic molecules.

The molecule chosen to present the methods is $H_2^{16}O$, for which an accurate global potential energy surface [1], previous computation of resonance states [2], and some Feshbach ($J = 0$, where $J$ is the quantum number characterizing overall rotations of the molecule) and shape ($J \neq 0$) resonances measured via a state-selective, triple-resonance technique [3] are available.

Characterization of the computed resonance states is performed via probability density plots (see Fig. 1.) based on rovibrational wavefunctions obtained as the eigenfunctions of non-Hermitian Hamiltonians. Just like for bound states, such plots provide useful details about the nature of the resonance states, such as dissociative behavior, effect of rotational excitation on resonance state lifetimes, etc.

Interested readers can find more in depth information in a recently published paper [4], which covers a substantial part of the presented results.

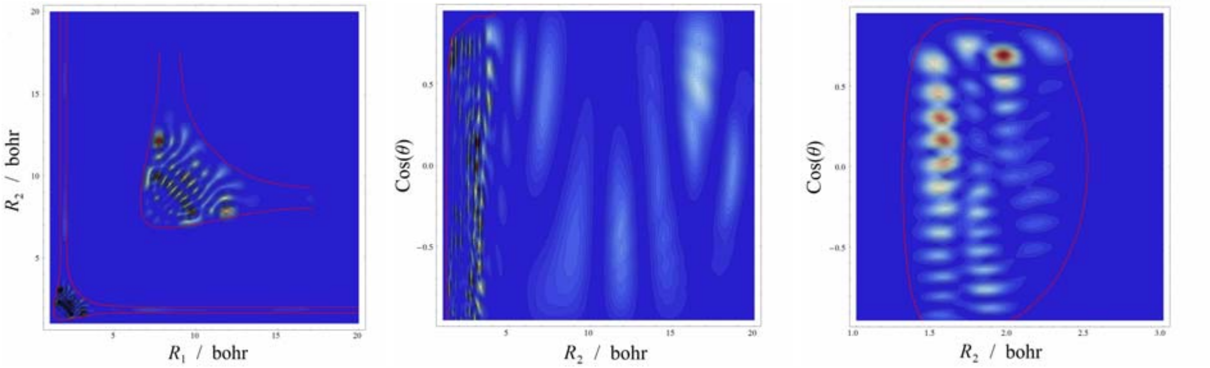

Figure 1. Two-dimensional sections of probability densitiy plots obtained from eigenfunctions of non-Hermitian rovibrational Hamiltonians , where $R_1$ and $R_2$ are the two OH bond lengths and $\theta$ is the HOH bond angle. The area near the equilibrium structure is also shown enlarged in the leftmost picture.

[1] A. G. Császár, E. Mátyus, T. Szidarovszky, L. Lodi, N. F. Zobov, S. V. Shirin, O. L. Polyansky and J. Tennyson, *J. Quant. Spectr. Rad. Transfer*, (**2010**), 111, 1043
[2] N. F. Zobov, S. V. Shirin, L. Lodi, B. C. Silva, J. Tennyson, A. G. Császár and O. L. Polyansky, *Chem. Phys. Lett.*, (**2011**), 507, 48
[3] M. Grechko, P. Maksyutenko, T. R. Rizzo and O. V. Boyarkin, *J. Chem. Phys.*, (**2010**), 133, 081103
[4] T. Szidarovszky, A. G. Császár, *Mol. Phys.*, (**2013**), doi: 10.1080/00268976.2013.793831