THE DIATOMIC MOLECULAR SPECTROSCOPY DATABASE: DATA-SCIENCE DRIVEN APPLICATIONS

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Spectroscopic constants of molecules characterize the unique fingerprints of molecules and atoms. In particular, for diatomic molecules, spectroscopic constants encapsulate essential information about different applications in atomic, molecular, and optical physics, such as laser cooling or quantum information. To help find molecules well-suited for a given application, we have developed a database linked to an interactive website.[a] The spectroscopic constants and Franck-Condon factors can be retrieved in useful formats from the website or via an application programming interface. New data can also be uploaded upon acceptance by the web managers.

By applying machine-learning approaches to this dataset, we show that the spectroscopic constants, including the equilibrium distance, harmonic vibrational frequency, and binding energy, are correlated and depend solely on the constituent's groups and periods. Based on these relationships, ground-state spectroscopic constants of polar diatomic molecules can be predicted with a relative error of $< 5\%$, whereas the same properties for the A-excited electron state are predicted with an error of $< 11\%$.[b] Anyone can make these predictions with access to our database, and it does not require any quantum chemistry knowledge.

Separately, we construct a database consisting of experimental electric dipole moments of 162 diatomic molecules. We show that the dipole moment of diatomic molecules is related to the constituent atoms' atomic properties, including electron affinity and ionization potential, and molecular properties that describe the force on the electrons at the equilibrium distance.[c]

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[a] X. Liu, S. Truppe, G. Meijer and J. Pérez-Ríos, J. Cheminform. **12**, 31 (2020)

[b] X. Liu, G. Meijer and J. Pérez-Ríos, arXiv:2005.07913 (2020)

[c] X. Liu, G. Meijer and J. Pérez-Ríos, Phys. Chem. Chem. Phys. **22**, 24191 (2020)