

Abstract Submitted
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Universal relationships of spectroscopic constants for diatomic molecules XIANGYUE LIU, JESUS PEREZ-RIOS, Fritz-Haber Institute of the Max-Planck Society — The systematic study of spectroscopic constants in diatomic molecules has been of interest in the atomic, molecular, and optical physics community since the birth of quantum chemistry. However, such a task has never been undertaken within the paradigm of artificial intelligence. Here, we present a study from a data science perspective, based on machine learning techniques, to elucidate the inherent relationship among the principal spectroscopic constants for diatomic molecules. As a result, it is possible to predict the principal spectroscopic constants of a molecule by looking at the simple atomic properties of the parent atoms.

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