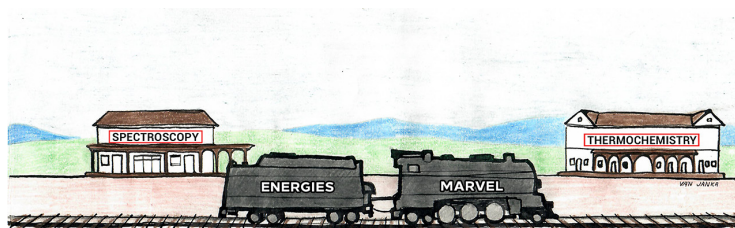


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Improved high-resolution spectroscopic data for molecular oxygen

Raima Larter

The MARVEL algorithm is used to validate experimental rovibronic transitions for $^{16}\text{O}_2$, allowing the calculation of accurate thermochemical data.



Accurate characterization of rovibronic (rotational-vibrational-electronic) transitions of important atmospheric species is needed for a number of scientific and engineering applications, including the calculation of equations of state. In this paper by Furtenbacher et al., information about a large number of rovibronic transitions involving the seven lowest electronic states is collected for the main isotopic form of molecular oxygen, $^{16}\text{O}_2$.

O_2 is the second-most abundant molecular species in earth's atmosphere, and as such a large number of spectroscopic studies have been carried out to characterize its rovibronic transitions. The authors evaluated all relevant literature values and collected more than 24,000 observed transitions. These were combined with more than 6,000 artificial transitions to create a hybrid spectroscopic database.

The technique used to validate the experimental transitions and determine the associated energy levels involves an algorithm known as the Measured Active Rotational-Vibrational Energy Levels, or MARVEL, which was developed by two of the authors in previous studies. MARVEL relies on the construction of a spectroscopic network, where the vertices are measured energy levels and the edges are the connecting transitions.

After the hybrid database was constructed, the authors calculated the temperature-dependent internal partition function $Q_{\text{int}}(T)$ for $^{16}\text{O}_2$. From $Q_{\text{int}}(T)$ the authors were able to calculate additional thermodynamic quantities, including the heat capacity, entropy and enthalpy over a wide temperature range. These data will be used in place of less accurate data for the development of a new equation of state for the ideal gas form of molecular oxygen.

It is noteworthy that most of the data collection and analysis was carried out by five 16- and 17-year-old high school students in Hungary. All of these young scientists are coauthors on the current report.

Source: "MARVEL analysis of the measured high-resolution rovibronic spectra and definitive ideal-gas thermochemistry of the $^{16}\text{O}_2$ molecule," by Tibor Furtenbacher, Mátyás Norváth, Dávid Koller, Panna Sólyom, Anna Balogh, István Balogh, and Attila G. Császár, *Journal of Physical and Chemical Reference Data* (2019). The article can be accessed at <https://doi.org/10.1063/1.5083135>.

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