EFFICIENT COMPRESSION OF MOLECULAR LINE LISTS: APPLICATION OF 'SUPER-ENERGIES' TO THE EXOMOL DATABASE

XUDONG KE LIN, SAMUEL WRIGHT, ALEC OWENS, JONATHAN TENNYSON, SERGEI N. YURCHENKO, *Department of Physics and Astronomy, University College London, London, UK*.

A new compression algorithm for the efficient storage of molecular line lists has been recently presented[a]. The algorithm is based on the effective 'super-energies' developed to produce a compact HITEMP line list for methane. This method assumes a set of artificial lower state (super-)energies and corresponding reference intensities for an approximate description of the temperature dependent molecular absorption (absorption coefficient) on a grid of wavenumbers. The super-energies compression is applied only to the majority ($> 99\%$) of the lines representing the weaker, continuum part of the molecular absorption, while the strongest lines ($< 1\%$) are preserved in the original form to maintain the accuracy of the line list.

Here we adopt and develop the HITEMP compression algorithm to be applicable to the ExoMol data format and generate new compressed line lists for SiO_2,[b] H_2O,[c] KOH and NaOH.[d] We find that using artificial Einstein A coefficients instead of reference intensities provides a more accurate description of the temperature dependence. A typical compression of a line list consisting of, e.g., 40 billions SiO_2 lines is to about 40 million data points. Advantages and limitations of the 'super-energies' approach will be discussed. The compressed molecular line lists will be included in the ExoMol database (WWW.EXOMOL.COM) and their use should greatly facilitate atmospheric retrievals in exoplanets and other hot astronomical bodies.

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