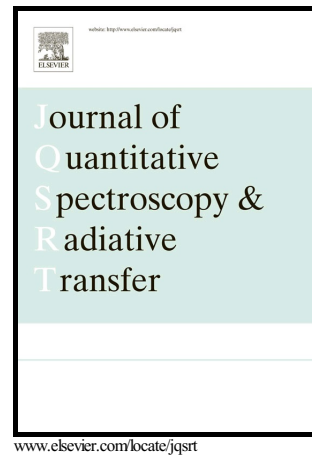


Author's Accepted Manuscript

Cycle bases to the rescue

Roland Tóbiás, Tibor Furtenbacher, Attila G. Császár



PII: S0022-4073(17)30004-3
DOI: <http://dx.doi.org/10.1016/j.jqsrt.2017.03.031>
Reference: JQSRT5641

To appear in: *Journal of Quantitative Spectroscopy and Radiative Transfer*

Received date: 3 January 2017
Revised date: 20 March 2017
Accepted date: 21 March 2017

Cite this article as: Roland Tóbiás, Tibor Furtenbacher and Attila G. Császár
Cycle bases to the rescue, *Journal of Quantitative Spectroscopy and Radiative Transfer*, <http://dx.doi.org/10.1016/j.jqsrt.2017.03.031>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain

Cycle bases to the rescue

Roland Tóbiás^a, Tibor Furtenbacher^a, Attila G. Császár^{*,a}^a MTA-ELTE Complex Chemical Systems Research Group, H-1117 Budapest, Pázmány Péter sétány 1/A, Hungary

Abstract

Cycle bases of graph theory are introduced for the analysis of transition data deposited in line-by-line rovibronic spectroscopic databases. The principal advantage of using cycle bases is that outlier transitions –almost always present in spectroscopic databases built from experimental data originating from many different sources– can be detected and identified straightforwardly and automatically. The data available for six water isotopologues, H_2^{16}O , H_2^{17}O , H_2^{18}O , HD^{16}O , HD^{17}O , and HD^{18}O , in the HITRAN2012 and GEISA2015 databases are used to demonstrate the utility of cycle-basis-based outlier-detection approaches. The spectroscopic databases appear to be sufficiently complete so that the great majority of the entries of the minimum cycle basis have the minimum possible length of four. More than 2000 transition conflicts have been identified for the isotopologue H_2^{16}O in the HITRAN2012 database, the seven common conflict types are discussed. It is recommended to employ cycle bases, and especially a minimum cycle basis, for the analysis of transitions deposited in high-resolution spectroscopic databases.

Keywords: cycle basis, information system, rovibronic transitions, energy levels, MARVEL, database

Download English Version:

<https://daneshyari.com/en/article/7846549>

Download Persian Version:

<https://daneshyari.com/article/7846549>

[Daneshyari.com](https://daneshyari.com)