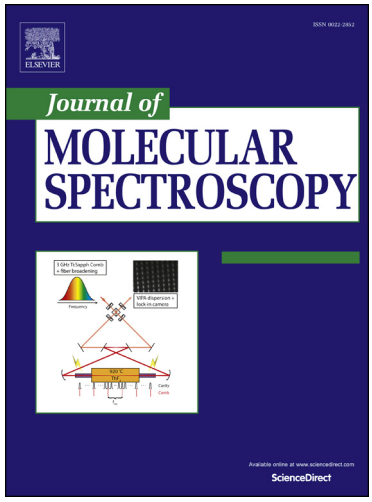

New model for datasets citation and extraction reproducibility in VAMDC

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New model for datasets citation and extraction reproducibility in VAMDC⋆.

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Abstract

In this paper we present a new paradigm for the identification of datasets extracted from the Virtual Atomic and Molecular Data Centre (VAMDC) e-science infrastructure. Such identification includes information on the origin and version of the datasets, references associated to individual data in the datasets, as well as timestamps linked to the extraction procedure. This paradigm is described through the modifications of the language used to exchange data within the VAMDC and through the services that will implement those modifications. This new paradigm should enforce traceability of datasets, favor reproducibility of datasets extraction, and facilitate the systematic citation of the authors having originally measured and/or calculated the extracted atomic and molecular data.

Keywords: database, data citation, atomic data, molecular data

1. Introduction

Atomic and Molecular Data Providers are often at the forefront in defining new paradigms for the dissemination of their data to the scientific community:

Since the second half of 1990s, with the spread of the Internet, some historical databases such as VALD [Piskunov et al. (1995)], HITRAN [Rothman (1983), Rothman et al. (2013)], the Submillimeter, millimeter and microwave spectral line catalog (so-called JPL Catalogue) [Pickett et al. (1998)], CDMS

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