Potential Energy Curves of Diatomic Alkali Molecules Datasets

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Abstract

The datasets described in this article contain potential energy curves for several diatomic systems. The data was obtained via high-performance computing using MOLPRO, a system of ab initio programs for advanced molecular electronic structure calculations. The datasets allow to model bond lengths, energy levels, spectra and time-evolution of molecular dimers for which the data are presented.

Keywords: diatomic molecules, dimers, potential energy curves

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Specification table (Data records)

Subject area	Physics, Chemistry
More specific subject area	Atomic and molecular physics
Type of data	Numerical data
How the data was acquired	The data was obtained in calculations using the MOLPRO program package version 2012.1.43
Data format	The tables are in .csv format
Data source location	MOST Wiedzy Open Research Catalog, Gdańsk University of Technology, Gdańsk, Poland
Data accessibility	The datasets are available free of charge under Creative Commons Licenses

Background

Potential energy (hyper)surfaces describe energy of the electronic states of molecular systems and their changes with respect to the changes of the positions of the nuclei, creating the “energy landscape” of molecular geometry. It is an instrumental tool in the analysis of molecular conformations, transition states and chemical reaction dynamics (Thrular et al, 1987). In a diatomic molecule, in which there are only two atoms, the position of the nuclei can be expressed by only one coordinate, hence the potential energy surface reduces to a potential energy curve (PEC). Each curve corresponds to one electronic state of group representation and angular momentum. The ranges of the internuclear distances in the datasets depend on the described system. Our datasets consists of several chosen systems of diatomic molecules, created from pairs of alkali metal atoms. Such dimers are of particular interest in applications concerning ultracold (with an internal temperature in the range of mK) molecular systems, Bose-Einstein condensation, and coherent control of chemical reactions. Possible applications of strongly polar ultracold molecules include using long-range electric dipole-dipole interactions between polar molecules for the design of optical quantum systems. The internal degrees of freedom of polar molecules could be used as a medium for quantum information. The creation, storage as well as control of such molecules in optical lattices, created by a strong laser field, could be used to construct quantum computers (Pazyuk, 2015).

Methods

The potential energy curves were obtained using methods of quantum chemistry using Molpro, a software package developed for accurate ab initio quantum chemistry calculations (Werner et al., 2012; Werner et al., 2020). The potential energy curves were obtained within the Born-Oppenheimer approximation. The core electrons and relativistic effects were treated using the energy-consistent effective core potentials (ECP) from the Stuttgart/Cologne Group with the customised core polarisation potentials (CPP). The valence electrons were described using customised basis sets; the CASSCF and MRCI methods. A detailed discussion of this methodology is described in our previous works (Jasik et al., 2006; Wiatr et al., 2015; Jasik et al., 2018).

Data quality and availability

The quality of the datasets is realised by carefully optimised computational basis sets, and parameters of ECPs, as well as CPPs. The quality analysis of the potential energy curves available in the presented datasets is always based on a comparison with the results of other theoretical and experimental studies. As an example, Fig. 36.1. shows the comparison of the ground state of the NaRb molecule presented in the dataset with other available results. Overall, very good agreement is visible. All of the presented PECs are characterised by common spectroscopic parameters, such as bond length (Re), dissociation energy (De), or vibrational constant (we). Comparison of these features with data provided by other authors is also used for verification of the quality of the dataset. A detailed analysis of the spectroscopic parameters is available in our previous works (Jasik et al., 2006; Wiatr et al., 2015; Jasik et al., 2018).

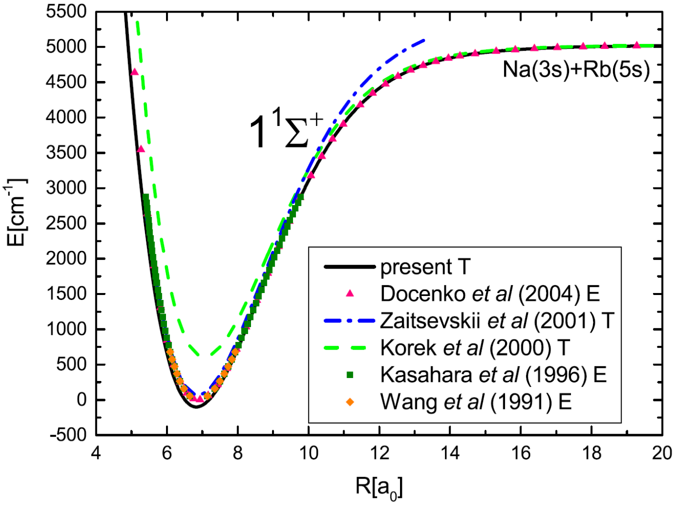

Fig. 36.1. Comparison of the ground 11Σ+ state of the NaRb molecule with experimental data obtained by (Docenko et al., 2004), (Kasahara et al., 1996), and (Wang et al., 1991), as well as with other theoretical results presented by (Zaitsevskii et al., 2001) and (Korek et al., 2000). The capital letter T refers to theoretical results and E denotes experimental data. (Wiatr et al., 2015)

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10.34808/t0yk-w861
10.34808/3kb8-st86
10.34808/bvx6-xs32
10.34808/1200-rr20
10.34808/1td6-pr92
10.34808/mjms-th03
10.34808/fj1r-d796
10.34808/75xd-bk46
10.34808/vpkc-xp73
10.34808/0vde-kw18

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