Accepted Manuscript

Quasirelativistic potential energy curves and transition dipole moments of NaRb

M. Wiatr, P. Jasik, T. Kilich, J.E. Sienkiewicz, H. Stoll

PII:	S0301-0104(17)30602-X
DOI:	https://doi.org/10.1016/j.chemphys.2017.10.005
Reference:	CHEMPH 9857
To appear in:	Chemical Physics

Received Date:26 July 2017Accepted Date:21 October 2017



Please cite this article as: M. Wiatr, P. Jasik, T. Kilich, J.E. Sienkiewicz, H. Stoll, Quasirelativistic potential energy curves and transition dipole moments of NaRb, *Chemical Physics* (2017), doi: https://doi.org/10.1016/j.chemphys. 2017.10.005

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 proof before it is published in its final 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.

ACCEPTED MANUSCRIPT

Quasirelativistic potential energy curves and transition dipole moments of NaRb

M. Wiatr, P. Jasik^{*}, T. Kilich, J.E. Sienkiewicz^{*}

Department of Theoretical Physics and Quantum Information, Faculty of Applied Physics and Mathematics, Gdansk University of Technology, ul. Gabriela Narutowicza 11/12, 80-233 Gdansk, Poland

H. Stoll

Institute for Theoretical Chemistry, University of Stuttgart, Pfaffenwaldring 55, D-70569 Stuttgart, Germany

Abstract

We report on extensive calculations of quasi-relativistic potential energy curves and, for the first time, transition dipole moments including spin-orbit and scalar-relativistic effects of the NaRb molecule. The calculated curves of the 0^+ , 0^- , 1, 2 and 3 molecular states correlate for large internuclear separation with the fourteen lowest atomic energies up to the Na(3s ${}^{2}S_{1/2}$)+Rb(7s ${}^{2}S_{1/2}$) atomic limit. Several new features of the potential energy curves have been found.

Keywords: potential energy curves, spin-orbit effect, MRCI, spectroscopic parameters, transition dipole moment functions

1. Introduction

The interest in laser cooling and trapping of atoms shifts to polar diatomic molecules since, due to their internal degrees of freedom, they may find broader applications in ultracold chemistry, quantum information and quantum simulations. Particularly, the heteronuclear alkali dimers attract considerable atten-

Preprint submitted to Chemical Physics

^{*}Corresponding authors

Email addresses: patjasik@pg.edu.pl (P. Jasik), jes@mif.pg.gda.pl (J.E. Sienkiewicz)

Download English Version:

https://daneshyari.com/en/article/7837410

Download Persian Version:

https://daneshyari.com/article/7837410

Daneshyari.com