Accepted Manuscript

Unusual chemical bonding in the beryllium dimer and its twelve vibrational levels

A.V. Mitin

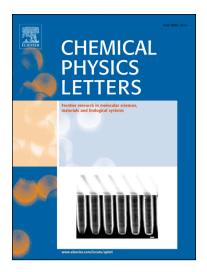
PII: S0009-2614(17)30527-4

DOI: http://dx.doi.org/10.1016/j.cplett.2017.05.071

Reference: CPLETT 34860

To appear in: Chemical Physics Letters

Received Date: 7 February 2017 Accepted Date: 29 May 2017



Please cite this article as: A.V. Mitin, Unusual chemical bonding in the beryllium dimer and its twelve vibrational levels, *Chemical Physics Letters* (2017), doi: http://dx.doi.org/10.1016/j.cplett.2017.05.071

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

Unusual chemical bonding in the beryllium dimer and its twelve vibrational levels

A. V. Mitin*

Chemistry Department, M. V. Lomonosov Moscow State University, 119991 Moscow, Russia

Moscow Institute of Physics and Technology, 9 Institutskiy per., Dolgoprudny, Moscow Region, 141700, Russia

Joint Institute for High Temperatures of RAS, Izhorskaya st. 13 Bd.2, 125412 Moscow, Russia

Abstract

The ab initio calculations have shown that the atoms in the beryllium dimer are covalently bound at the low-lying vibrational energy levels with ν =0-4, while at the higher levels with ν =5-11 the atoms are bonded by the van der Waals forces near the right turning points. The developed ab initio modified EMO potential function, in distinction with the original EMO function, which was used for a description of the experimental vibrational levels, not only has the correct dissociation energy, but also describes all twelve vibrational energy levels with a smaller RMS error of less than 0.4 cm⁻¹.

Keywords: covalent bonding, van der Waals bonding, vibrational energy levels, beryllium dimer

1. Introduction

The latest spectral experiment reported in [1] has caused a new wave of research in the beryllium dimer, because it has become the first many-electrons molecule for which almost all vibrational energy levels are experimentally detected. Thus, theoreticians got an excellent example for testing the many-

^{*}Corresponding author Email address: mitin@phys.chem.msu.ru (A. V. Mitin)

Download English Version:

https://daneshyari.com/en/article/5377649

Download Persian Version:

https://daneshyari.com/article/5377649

Daneshyari.com