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High-Resolution Spectroscopy of Hexamethylenetetramine (HMT) C₆N₄H₁₂

new abstract

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Electronic Structure of NaHe Including Spin-orbit Coupling and Dipole Moments

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Theoretical Investigation of the Shift of the Degenerate Vibrations in the FSO₃ Radical

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J43 **Evangelisti L., Maris A., Melandri S., Caminati W.**

Internal Dynamics in Phenylacetate

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J44 **Kirkpatrick R., Masiello T., Martin M., Nibler J.W., Maki A., Weber A., Blake T.A.**

High Resolution Infrared Studies of the ν_{10} , ν_{11} , ν_{14} , and ν_{18} Levels of [1.1.1]propellane

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J30 **Mondelain D., Kassi S., Campargue A., Barbe A., De Backer M.-R., Starikova E., Tyuterev V.**

The CW-CRDS Spectra of the ¹⁶O¹⁸O¹⁶O Ozone Isotopologue Near 6200 cm⁻¹: Experiment and Analysis of Three New Bands

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J40 **Hezma A., Abdelghany A., Allam M., AbdelRazek E., El-Bahy G.**

Physical Studies of Nano-Hydroxapatite-Polyacrylic Acid with Cellulose Acetate

Electronic structure of NaHe including spin-orbit coupling and dipole moments

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Alkali metals constitute an optical opacity source to condense out dust grains in cool substellar atmospheres. Their resonance lines can form in deep regions in atmospheres of methane brown dwarfs leading then to a pseudo-continuum that shapes the emitted spectrum from the UV to the Near-Infrared spectral range¹. A description of the alkali-helium interactions is needed to describe the far wings of alkali resonance lines in the presence of high densities of Helium perturber involved in model atmospheres and spectra predictions²⁻³. In this case, the accuracy of calculated spectral line profiles is strongly dependent of the quality of molecular potential energy curves and dipole moments.

With recent experiments on the spectroscopy of alkali dimers through Helium nanodroplets⁴⁻⁵, accurate calculations on the electronic structure of the alkali-Helium molecules are now required including spin-orbit coupling and a determination of transition dipole moments. In the past, few theoretical investigations have been achieved on these molecules⁶⁻⁸ for the lowest excited states while they remain practically unknown experimentally⁹. Large discrepancies have been observed between calculations leading to the necessity to provide new theoretical data on these molecules. So, in the framework of a model potential type method, we have determined potential energy curves and dipole moments for 34 $^2\Lambda^{(+/-)}$ states dissociating adiabatically up to Na(7s)+He (*i.e.* 15 asymptotes) in a range of 02-50a₀. A synthesis of the main results will be presented and discussed.

References

- [1] A Burrows, M.S. Marley, C.M. Sharp, *ApJ* **531**, 438, 2000
- [2] N.F. Allard, F.Allard, P.H. Hauschildt, J.F. Kielkopf, L. Machin, *A&A* **411**, L473, 2003
- [3] N.F. Allard, F.Allard, J.F. Kielkopf, *A&A* **440**, 1195, 2005
- [4] F.R. Brühl, R.A. Miron, W.E. Ernst, *J. Chem. Phys.* **115**, 10275, 2001
- [5] W.E. Ernst, R. Huber, S. Jiang, R. Beuc, M. Movre, G. Pichler, *J. Chem. Phys.* **124**, 024313, 2006
- [6] J. Pascale, *Phys. Rev. A* **28**, 632, 1983
- [7] G. Theodorakopoulos, I. D. Ptesalakis, *J. Phys. B: At. Mol. Opt. Phys.* **26**, 4367, 1993
- [8] A.R. Allouche, K. Alioua, M. Bouledroua, M. Aubert-Frécon, *Chem. Phys.* **355**, 85, 2009
- [9] M.D. Havey, S.E. Frolking, J.J. Wright, *Phys. Rev. Lett.* **45**, 1783, 1980