Na - соединения

Na^+-комплексы с H_2O, NH_3, CH_4, C_2H_4, CO, N_2.

1984

Sauer Joachim,
Hobza Pavel.

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65, N 4, 291 – 302.

(см. Li^+-комплексы с
H_2O, NH_3, CH_4, C_2H_4, CO, N_2. III)

1998

F: NaFr
P: 3

130:257571 Calculation of alkali-metal dimers on the basis of a model perturbation theory. Glushkov, A. V.; Efimov, V. A.; Gopchenko, E. D.; Dan'kov, S. V.; Polishchuk, V. N.; Shpinareva, I. M. (Odessa Hydrometeoro Institute, Ukraine). Russ. Phys. J., 41(5), 492-498 (English) 1998 On the basis of pseudopotential theory, within the framework of a formal accurate model perturbation theory of Rayleigh-Schrodinger type with a ze approxn. inoculating potential, the calcn. of some diat. alkali mols. in and heteronuclear variants LiM (M

= Li, Na, K, Rb, Cs, Fr) is considered. local model potential of Gell-Mann type is adopted as the zero-approxn. potential. The calcn. results for the energy parameters - in particular, energy of dissocn. - are given; some of these results are obtained here f first time. The calcn. demonstrates the fundamental role of two basic se order perturbation-theory effects in achieving acceptable accuracy: polarizational interaction of the valence particles through the core; and screening of these particles.

1999

F: NaAu
P: 3
130:259038 Photoionization Spectroscopy of KAu and NaAu Diatomics. Stangassinger, A.; Knight, A. M.; Duncan, M. A. (Department of Chemistry University of Georgia, Athens, GA 30602, USA) . J. Phys. Chem. A, 103(11), 1547-1552 (English) 1999 The new metal diatomics KAu and NaAu are studied using resonant 2-photon ionization (R2PI) electronic spectroscopy. These species are produced by vaporization of a salted Au rod in a pulsed nozzle cluster source. Anal. spectra provides

the vibrational consts. for the excited states and corre to specific at. asymptotes. Energetic cycles provide detns. of the groun dissocn. energies. The values are D0'' = 2.75 .+-. 0.2 eV for KAu and D0 2.64 .+-. 0.2 eV for NaAu. These dissocn. energies for the heteronuclear diatomics are significantly greater than those for the corresponding homo diatomics Na2, K2, or Au2. Partial ionic character in the ground state b is implicated, analogous to that obsd. previously for Ag and Cu-alkali diatomics.

F: NaRb
P: 3

[от. 40259 а"]

2000

133:49159 Theoretical study of the electronic structure of the LiRb and N molecules. Korek, M.; Allouche, A. R.; Kobeissi, M.; Chaalan, A.; Dagher, Fakherddin, K.; Aubert-Frecon, M. Beirut Arab University Beirut, Lebanon Chem. Phys., 256(1), 1-6 (English) 2000 The potential energy has been calcd. over a wide range of internuclear distances for the 28 lowest mol. states of LiRb and NaRb mols., using an initio method based on non-empirical pseudopotentials, parametrized l-dep polarization potentials and full valence CI calcns. Mol. spectroscopic c have been derived for the bound states with a regular shape. A good desc of the exptl. known ground state for NaRb is obtained. Tables providing extensive data of energy values vs. internuclear distances are available following address htt P://lasim.univ-lyon1.fr/allouche/lirbnarb.htm.

C.A. 2000, 133

2000

F: Na6Pb
P: 3

133:325882 Structure and stability of Na6Pb clusters. Han, Young- Kyu; Hirao, Kimihiko Department of Applied Chemistry, Graduate School of Engineering, The University of Tokyo Hongo, Tokyo 113-8656, Japan J. Chem. Phys., 113(16), 6613-6617 (English) 2000. The geometric and electronic structures of the bimetallic cluster, Na6Pb, were calcd. using the d. functional and coupled-cluster approaches, with a relativistic effective core potential and one-electron spin-orbit operators. Six possible isomeric Na6Pb structures (Oh, D3h, D3d, C5v, C3v, and C2v) were examd., and the highly sym. Oh structure was found to be the most stable form. The stabilities of the clusters correlate well with the Pb-Na bond distances and with the charge transfer from the Na6 subsystem to the more electroneg. Pb atom. The binding energies were found to vary according to the structure, with a spread of about 0.1 eV and 0.3 eV for the d. functional and coupled-cluster calcns., resp. These are of the same order, and somewhat smaller, as are found for the Na6Mg clusters (about 0.5 eV), demonstrating that the stabilization of the Na6Pb cluster is not particularly dependent on the geometric structures. At the same time, we found that the Na6Pb cluster is more stable as the symmetry is higher.