HeH

1967

7 (He_2, He_2^+, HeH^+, H_3^+, H_4^{2+}, HeH^-, LiH, BeH^+)

IX 102

Frost A. A.

J. Chem. Phys, 1967, 47, v10, 3714-3716 (англ)

Floating spherical Gaussian orbital model of molecular structure.

II One- and two-electron-pair systems

10 12

РЖХим, 1968, 23Б73

XI-4192

40917.1262 Ph,Ch,TC	30526 HeH^-	02 *	1974 Ч-6275

Chisholm C.D.H., Lodge K.B. An expansion method for calculating molecular properties. IV. Energies of some excited sigma states of one-electron and two-electron molecular systems.

"Mol. Phys.", 1974, 28, N1, 249-271
(англ.)

ВИНИТИ

HeH^-

1982

Paidarova I., Vojtík J.,
Polák R.

расчёт
молекул.,
структ.

Chem. Phys., 1982, 72,
N 1-2, 119-129.

(сл. HeH; III)

$He H^-$

1982

Silver D. M., Wilson S.

потенц. кривые

Proc. Roy. Soc. London, 1982, A383, N 1785, 477–483.

(см. He_2; $\overline{III}$)

H^-He 1983

99: 111020v **Molecular negative ions.** Olson, Ronald E. (Mol. Phys. Lab., SRI Int., Menlo Park, CA 94025 USA). *Energy Storage Redistrib. Mol.* 1983, 185–202 (Eng). Edited by Hinze, Juergen. Plenum: New York, N. Y. In a theor. study of possible mechanisms of electron detachment from neg. at. ions in collisions with neutral atoms, calcns. were done on: (*a*) potential-energy curves [PEC's] for H^- in collisions with He, Ne, Na, and Ca; (*b*) cross sections for H^- in collisions with Na, K, Rb, and Cs; and (*c*) PEC's for Li^- in collisions with Na, K, and Ca.

помечено:
ф-ие

H^-Ne, H^-Na, H^-Ca,
Li^-Na, Li^-K, Li^-Ca

(+6) ☒

C. A. 1983, 99, N 14

HeH⁻

1997

126: 229826s **Is HeH⁻ a stable system?** Bendazzoli, Gian Luigi; Evangelisti, Stefano; Passarini, Fabrizio (Dipartimento di Chimica Fisica e Inorganica, Universita di Bologna, Viale Risorgimento 4, I–40136 Bologna, Italy). *Chem. Phys.* **1997**, 215(2), 217–225 (Eng), Elsevier. We present an ab initio study of the HeH^- system. This hypothetical mol. is isoelectronic with the He_2 dimer, whose existence has been predicted for a long time and recently confirmed by expt. We performed calcns. on this system at several levels of accuracy, with extended basis sets contg. up to 179 at. basis functions. All methods predicted a well in the Born–Oppenheimer energy curve, with a min. located at an internuclear sepn. of about 12 to 13 bohr. Its depth is extremely small: about 4 to 6 K, depending on the method used to compute the electronic wave function and on the at. basis set. By solving numerically the Schroedinger equation for the nuclei, we obtained two vibrational levels, lying at about 0.8 K and 0.1 K below dissocn., resp. While the precise value of their energies is uncertain, we believe that their presence, regardless of the level of approxn. used, strongly support the existence of this so far undetected species.

стабильность теор. расч

С. А. 1997, 126, N 17

HeH⁻

2001

134: 212993m **Ab initio study of the ground-state potential of XH^- anions (X=He,Ne,Ar).** Vallet, V.; Bendazzoli, G. L.; Evangelisti, S. (Laboratoire de Physique Quantique, UMR 5626, Universite Paul Sabatier-118, F-31062 Toulouse, Fr.). *Chem. Phys.* 2001, 263(1), 33-40 (Eng), Elsevier Science B.V. The ground-state energy curves of HeH^-, NeH^- and ArH^- have been computed at coupled-cluster level using large basis sets. These dimers are weakly bound systems, due to the interaction between the neg. ion H^- and the (polarized) rare-gas atom. The Schrodinger equation for the nuclei has been solved, and the energy levels have been computed. The effect of replacing the innermost electrons with pseudopotentials has also been investigated on the heaviest system ArH^-.

ab initio расчет потенциал осн. сост.

(+2) NeH⁻, ArH⁻

C.A. 2001, 134, N15