Hg-M

HgH_2 оп. 29619 1988

109: 135331y The mercury–molecular hydrogen system: potential energy surfaces of the low-lying states, reactivity of the 6s6p states of mercury on molecular hydrogen, classical dynamic study of $Hg(^3P_1) + H_2$ half collision. Bernier, A.; Millie, P. (Dep. Phys. Chim., CEN/SACLAY, 91191 Gif-sur-Yvette, Fr.). *J. Chem. Phys.* 1988, 88(8), 4843–54 (Eng). Potential energy surfaces for HgH_2 have been calcd. using a nonempirical relativistic effective core potential incorporating CI by means of the CIPSI algorithm (CI by perturbation with multiconfigurational zeroth-o 'er wave function selected by iterative process). Core-valence polarization and correlation energy are included via a perturbative treatment. Spin-orbit coupling is introduced through an effective Hamiltonian. These theor. results are used to discuss the exptl. ones for the $Hg(^3P_1) + H_2 \rightarrow HgH(X^2\Sigma^+) + H$ reaction. The different behaviors of the two van der Waals complexes are explained. Dynamical studies and classical trajectories calcns. confirm that the dominant pathway is a direct dissocn. on the first excited surface and is responsible for a highly peaked rotational distribution of the HgH product, in agreement with expt.

поверхность (потенц.)

C. A. 1988, 109, N 16.

$(HgH_2)_2$ 1994

Kaupp Martin, von Schnering Hans Georg.

Li.n. Inorg. Chem. 1994. 33, N 12. C. 2555-2564.

(see. $(HgF_2)_2$; III)

Mg12

1994

Kaupp M., von Schnering H.G.,

ΔH гене- Inorg. Chem., 1994, 33, N21,
рация, 4718 - 4722.
теор. рас-
чет

(см. ZnF2; III)

Mg_2H_2
Mg_2H_2

Om 38205

1995

Legay - Jomaire M, Legay F,

J Phys Chem., 1995, 99,
(20) 16945 - 16952.

FTIR Study of the Photoche-
mistry of Mg and H_2 in a Matri-

gen Matrix. Formation and Dissociation of HgH_2 and $H\,Hg\,Hg\,H$.

$(HgH_2)_2$

2000

ab initio paper

133: 140578j **Ab initio studies of the dimers $(HgH_2)_2$ and $(HgMe_2)_2$. Metallophilic attraction and the van der Waals radii of mercury.** Pyykko, Pekka; Straka, Michal (Department of Chemistry, University of Helsinki, Helsinki, Finland). *Phys. Chem. Chem. Phys.* 2000, 2(11), 2489–2493 (Eng), Royal Society of Chemistry. The title compds. are used to det., for the first time, the energy of the 'metallophilic' attraction between two Hg(II) compds. The dispersion and electrostatic multipole components to this attraction are analyzed. The present purely theor. mol. data suggest a mercury(II) van der Waals radius of 175(7) pm.

(H)

C. A. 2000, 133, N10.

$[Hg(CH_3)_2]_2$