

Hg-M

HgH₂

OM. 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 $\text{Hg}(^3\text{P}_1) + \text{H}_2$ 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-order 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 $\text{Hg}(^3\text{P}_1) + \text{H}_2 \rightarrow \text{HgH}(X^2\Sigma^+) + \text{H}$ reaction. The different behaviors of the two van der Waals complexes are explained. Dynamical studies and classical trajectories calcs. confirm that the dominant pathway is a direct disson. on the first excited surface and is responsible for a highly peaked rotational distribution of the HgH product, in agreement with expt.

нотенз.
(потеряности)

C. A. 1988, 109, N 16.

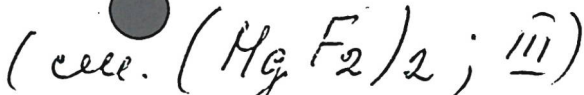


1994

Kaupp Martin, von Schne-
ring Hans Georg.

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Inorg. Chem. 1994. 33,
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HgH₂

1994

Kaupp M., von Schnerig H. F.,

ΔH geme-
myasun,
meop. pac-
tem.

Inorg. Chem., 1994, 33, N21,
4718 - 4722.

(all. ZnF₂; III)

HgH₂
Hg₂H₂

[Am 38 205]

1995

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(20) J Phys Chem., 1995, 99,
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FTIR study of the photoche-
mistry of Hg and H₂ in a Nitro-

gen Matrix: Formation and
Dissociation of HgH_2 and
 H Hg Hg H .

2000

 $(\text{HgH}_2)_2$ ab initio
panen

133: 140578j Ab initio studies of the dimers $(\text{HgH}_2)_2$ and $(\text{HgMe}_2)_2$. 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, No.

 $[\text{Hg}(\text{CH}_3)_2]_2$