PuH_n, PuH^+

2000

F: PuH+
P: 3

134:242949 **Potential energy function and stability of PuHn+ (n = 1, 2, 3).** Li, Quan; Liu, Xiao-ya; Wang, Hong-yan; Zhu, Zheng he; Fu, Yi-bei; Wang, Xiao-lin; Sun, Ying. Inst. Atomic Molecular Physics, Sichuan Univ., Chengdu, Peop. Rep. China. Wuli Xuebao (2000), 49(12), 2347-2351. in Chinese.

The theor. study on PuHn+ (n = 1, 2, 3) using the d. functional method (B3LYP) shows that PuH+ and PuH2+ can be stable and PuH3+ (7Σ-) cannot be stable. Electronic ground states are X7Σ- (PuH+) and X8Σ- (PuH2+), and their force consts. and spectroscopic data have been worked out.

2000

F: PuH2+
P: 3

134:242949 **Potential energy function and stability of PuHn+ (n = 1, 2, 3).** Li, Quan; Liu, Xiao-ya; Wang, Hong-yan; Zhu, Zheng he; Fu, Yi-bei; Wang, Xiao-lin; Sun, Ying. Inst. Atomic Molecular Physics, Sichuan Univ., Chengdu, Peop. Rep. China. Wuli Xuebao (2000), 49(12), 2347-2351. in Chinese.

The theor. study on PuHn+ (n = 1, 2, 3) using the d. functional method (B3LYP) shows that PuH+ and PuH2+ can be stable and PuH3+ (7Σ-) cannot be stable. Electronic ground states are X7Σ- (PuH+) and X8Σ- (PuH2+), and their force consts. and spectroscopic data have been worked out.

2000

F: PuH3+
P: 3

134:242949 **Potential energy function and stability of PuHn+ (n = 1, 2, 3).** Li, Quan; Liu, Xiao-ya; Wang, Hong-yan; Zhu, Zheng he; Fu, Yi-bei; Wang, Xiao-lin; Sun, Ying. Inst. Atomic Molecular Physics, Sichuan Univ., Chengdu, Peop. Rep. China. Wuli Xuebao (2000), 49(12), 2347-2351. in Chinese.

The theor. study on PuHn+ (n = 1, 2, 3) using the d. functional method (B3LYP) shows that PuH+ and PuH2+ can be stable and PuH3+ (7Σ-) cannot be stable. Electronic ground states are X7Σ- (PuH+) and X8Σ- (PuH2+), and their force consts. and spectroscopic data have been worked out.

2000

F: PuH
P: ~~3~~ 2,3
133:49154 Ab initio calculations on the potential energy function and thermodynamic functions for the ground state X8.SIGMA.+of PuH. Gao, Tao; Wang, Hong-yan; Zhu, Zheng-he; Sun, Ying; Wang, Xioa-lin; Fu, Yi-bei(Institute Atomic and Molecular, Sichuan University Chengdu 610065, Peop. Rep. China
Yuanzi Yu Fenzi Wuli Xuebao, 17(1), 46-52 (Chinese) The potential energy function for the ground state X8.SIGMA.+ of PuH has been worked out by the QCISD method, based on the approxn. of a Relativis Effective

7

$X^8\Sigma^+$

C.A 2000, 133 w4.

Core Potential (RECP) for atom Pu and an all-electron 6-311g* basis set for the H atom. The calcn. results for Re, De, Be, α_e, ω_e, $\omega_e x_e$ are -2.28 A, 1.2227 eV, 3.2334, 0.07742, 1146.2632 and 24.7514 cm^{-1} resp. Addnl., the formation thermodn. functions .DELTA.H0, .DELTA.S0 .DELTA.G0 and C.upsilon., of PuH(s) between 298.15-911K are also worked out

ΔH°, ΔS°, ΔG°

C_v

PuH+

2001

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135: 262518b **Structure and potential energy function of PuX+ (X = O, H, N, C).** Li, Quan; Wang, Hong-Yan; Jiang, Gang; Zhu, Zheng-He (Dep. Chem., Sichuan Normal Univ., Chengdu, Peop. Rep. China 610066). *Wuli Huaxue Xuebao* 2001, 17(7), 622–625 (Ch), Beijing Daxue Chubanshe. The theor. study on PuX+ (X = O, H, N, C) using the d. functional method (B3LYP) shows that PuO+, PuH+, PuN+ and PuC+ can be stable. Ground electronic states are $X^6\Sigma^-$(PuO+), $X^7\Sigma^-$(PuH+), $X^5\Sigma^+$(PuN+) and $X^8\Sigma^-$(PuC+). Their potential energy functions are in agreement with the Murrell–Sorbie function. Their force consts. and spectroscopic data have been obtained.

C.A. 2001, 135, N18

2001

F: PuH2
P: 3

135:10217 **Study on analytical potential energy function for PuH2 molecule.** Li, Quan; Liu, Xiao-ya; Jiang, Gang; Zhu, Zheng-he. Inst. Atomic and Mol. Phys., Sichuan Univ., Chengdu, Peop. Rep. China. Yuanzi Yu Fenzi Wuli Xuebao (2001), 18(1), 91-93. in Chinese.

The equil. structure of PuH2 mol. has been obtained and optimized using the B3LYP method in the Gaussian 94 program system. The optimized parameters are: RPuH = 0.21691 nm, RHPu = 0.21691 nm, ∠HPuH = 160.3396°, dissocn. energy De = 3.0045 eV, and harmonic frequencies v1 (A1) = 293.4140 cm-1, v2(B2) = 1209.27 5 cm-1, v3(A1) = 1262.2149 cm-1. An anal. potential energy function for PuH2 mol. was obtained using the many-body expansion method.