Se-F

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– 1682 (англ.)

Vibrational spectra and force
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A.P.

(see. F^-; III)

GeH_x; GeF_x; $GeCl_x$; $Ge(HCl)_x$; $Ge(CH_3)_x$ (Ze
I
$Ge(CN)_x$; $Ge(NO)_x$; AsH_x; AsF_x; $AsCl_x$;
$As(CH_3)_x$; $As(CN)_xF$; $As(NO)_x$; SeH_x; SeF_x;
$SeCl_x$; $Se(CH_3)_x$; $Se(CN)_x$; $Se(NO)_x$;
HBr; BrF; $BrCl$; $BrCN$; $BrCH_3$; $BrNO$
Li m.g. Hase H. L.; Schweig A.;
Theor Chim. Acta; 1973;
31; N3, 215-220

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Lo (9)

Ca74/2

SeF_n Thynne J.C.J. 1973

(to)

„Int. J. Mass. Spectrom. Ion. Phys."
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● (cer. WF_4 ; III)

Se F_x

1948

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Ber. Bunsenges Phys. Chem.
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u.k. смотр
в дальнейшем

см. SF_2 — III

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Simons B.dl.

электрон. структура, расчет

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Cell. AlF_5^{2-}-III

$2Se_2X_2 = SeX_2 + Se_3X_2$

$3Se_2X_2 = SeX_2 + Se_4X_2$

(где X = Cl или Br)

Кр

1989

14 Б1190. Диспропорционирование дихлорида дисеплена Se_2Cl_2 и дибромида диселена Se_2Br_2. The disproportionation of diselenium dichloride, Se_2Cl_2, and diselenium dibromide, Se_2Br_2 / Lamoureux M., Milne J. // Can. J. Chem.— 1989.— 67, № 11.— С. 1936—1941.— Англ.; рез. фр.

Изучены спектры КР (λ 647,1 нм) р-ров Se и $SeCl_4$ в Se_2Cl_2 (I), а также Se в Se_2Br_2 (II). Анализ спектров указывает на то, что в р-рах происходит диспропорционирование типа $2Se_2X_2 = SeX_2 + Se_3X_2$ и $3Se_2X_2 = SeX_2 + Se_4X_2$ (где X = Cl или Br). Оценены константы равновесия для соотв-щих р-ций диспропорционирования. Отмечено, что в смесях I с II образуется Se_2ClBr. Полученные данные подтверждаются результатами исследования спектров ЯМР (^{77}Se). А. В. Бобров

Х. 1990, № 14

Sel 5 — | ОП-36283 | 1991

Электрон. строение, теор. расчет

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1995

F: SeF5
P: 3
9Б1180. Прямая оценка равновесных геометрий молекул с использованием газовой электронографии в реальном времени. 2. Гексафторид селена Direct evaluation of equilibrium molecular geometries using real-time gas electron diffraction. 2. Selenium hexafluoride / Maggard Paul, Lobastov Vladimir A., Schafer Lothar, Ewbank John D., Ischenko Anatoli A. // J. Phys Chem. - 1995. - 99, N 35. - C. 13115-13117. - Англ. Место хранения ГПТБ
Методом газовой электронографии (т-ра 298-573К) исследована структура молекулы SeF[6]. При анализе, учитывающем температурную зависимость распределения интенсивности в экспериментальной электронограмме рассмотрено влияние: кумулянтов более высокого порядка многократного рассеяния, использованной модели ангармонических колебаний морзевского типа. Величина R[e](Se-F)=1,6784 А.

Р. ЖХ. N9, 1996

F: SeFn
P: 3
131:356313 The Electron Affinities of the Selenium Fluorides SeFn (n = 1-

Li, Qian-shu; Xu, Wen-guo; Xie, Yaoming; Schaefer, Henry F., III School of Chemical Engineering and Materials Science, Institute of Bejing Techno Beijing 100081, Peop. Rep. China

J. Phys. Chem. A, 103(37), 7496-7505 (English) 1999 The mol. structures, electron affinities, and dissocn. energies of the SeFn/SeFn- (n = 1-7) species were examd. using hybrid Hartree-Fock/d. fun theory (DFT). The three different types of electron affinities reported work are the adiabatic electron affinity (EAad), the vertical electron af (EAvert), and the vertical detachment energy (VDE). The first Se-F disso energies of the SeFn and SeFn- species were also been reported. The basi used in this work is of double-.zeta. plus polarization quality with addn and p-type diffuse functions, and is denoted

as DZP++. Four different d. functionals (BHLYP, B3LYP, BP86, and BLYP) were used in this work. Among the best for predicting mol. structures and energies was found to be BHLY whereas other methods generally overestimated bond lengths. Neutral SeF7 found to have no structures that were significantly bound with respect to dissocn. SeF7- structures with D5h, C4v, and C3v symmetry were found to very close in energy. The most reliable adiabatic electron affinities, o at the DZP++ BHLYP level of theory, are 1.99 eV (Se), 2.37 eV (SeF), 2.21 (SeF2), 3.39 eV (SeF3), 2.50 eV (SeF4), 5.23 eV (SeF5), and 3.13 eV (SeF6 BHLYP adiabatic electron affinities of the Se atom, SeF5, and SeF6 mols. predicted by this work are in good agreement with the exptl. results, but predicted electron affinities for SeF4 are much larger than the exptl. va (1.7 .+-. 0.1 eV) obtained by the electron impact appearance energy (EIAE method, which usually gives lower EAad values. The other mol. electron affinities (SeFn, n = 1, 2, 3, 7) are unknown exptl. The predicted verti detachment energy for SeF7- is very large, 8.01 eV. The neutral bond dis energies De(Fn-1Se-F) are largely unknown exptl. For SeF5, the DFT metho predict De(F4Se-F) = 0.88-1.67 eV, which is lower than the exptl. estd. v 2.8 eV. The DZP++ BLYP bond dissocn. energy value, De(F5Se-F) = 3.15 eV, slightly lower than the dissocn. energies predicted by the other methods BHLYP, 3.34 eV; DZP++ B3LYP, 3.31 eV; DZP++ BP86, 3.44 eV). Except for t DZP++ BP86 result, theory matches the exptl. est. 3.15 .+-. 0.2 eV based thermochem. data. Excluding the DZP++ BHLYP results, the dissocn. energy diat. SeF ranges from 3.4 to 3.80 eV among which the DZP++ B3LYP result (eV) is in best agreement with the exptl. value (3.5 eV). For the bond di value of the anion De(SeF5- -F) the DZP++ BHLYP method gives De(SeF5- -F) eV, whereas the DZP++ B3LYP, DZP++ BP86, and DZP++ BLYP methods predict d energies (B3LYP, 1.83 eV; BP86, 2.26 eV; BLYP, 2.13 eV) that are larger t expt. (1.09 .+-. 0.1 eV). It is concluded that the d. functional methods although very useful in establishing trends, must be used very carefully. Moreover, addnl. (SeFn-SeFn-) expts. are required to precisely establish reliability of the different d. functional methods.