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D_0 207-I-ТКВ

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Реакцией фтора с йодом в р-ре CCl_3F при —45° получен порошкообразный монофторид йода (**I**), разлагающийся при —14° на JF_5 и J_2 и гидролизующийся щел. р-ром с образованием J^-, JO_3^- и F^-. 1 *л* CCl_3F при —60° р-ряет ~0,6 **I**, синие р-ры **I** в 20%-ном олеуме поглощают при 15 750, 20 000 и 24 500 *см*⁻¹. **I** дает 1 : 1-аддукты с Py, Dipy и хинолином; **I**·Py разлагается при 110°, в ИК-спектре его содержится полоса **I** при 420 *см*⁻¹. В р-ре CH_3CN при —40° **I** реагирует с CsF: $3\ \mathbf{I}+3CsF=Cs_3JF_6+F_2$, и с CsCl: $4\ \mathbf{I}+2CsCl=CsJF_4+CsJCl_2+J_2$.

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135:24954 **Theoretical Calculation of Bond Dissociation Energies and Enthalpies of Formation for Halogenated Molecules.** Lazarou, Yannis G.; Prosmitis, Alexandros V.; Papadimitriou, Vassileios C.; Papagiannakopoulos, Panos. Institute of Physical Chemistry, National Center for Scientific Research Demokritos, Aghia Paraskevi, Greece. J. Phys. Chem. A (2001), 105(27), 6729-6742. in English.

The bond dissocn. energies and the enthalpies of formation of halogenated mols. were theor. calcd., and the results were compared with the corresponding exptl. values in order to examine the reliability of a large no. of levels of theory in thermochem. calcns. D. functional theory using a multitude of exchange and correlation functionals, Moller-Plesset perturbation theory, and QCISD(T) and CCSD(T) methods were employed, with all-electron and effective-core potential basis sets of varying complexity. A small set of 19 mols. was selected, consisting of X2, HX, and CH3X (X = F, Cl, Br, and I), the mixed-halogen mols. ClF, BrF, BrCl, IF, and ICl, and H2 and CH4. The calcd.

bond dissocn. energies were cor. for basis set superposition errors and the first-order spin-orbit coupling in the 2P state of halogen atoms. In addn., the enthalpies of formation of all mols. in the set as well as those of Me (CH3) and halomethyl radicals (CH2X) were also calcd. by using the corresponding atomization reactions, cor. for the spin-orbit coupling in the 3P state of carbon atom and the 2P state of halogen atoms. Levels of theory employing the B3P86 functional with moderately large basis sets, augmented with diffusion and polarization functions, were found to be sufficiently reliable in the calcn. of bond dissocn. energies of closed-shell halogenated mols. In particular, the B3P86/6-311++G(2df,p) level of theory was found to be the most accurate, with an RMS deviation of 6 kJ·mol-1 for 23 bond dissocn. energies, with a negligible dependence of the accuracy on the level of theory chosen for the geometry optimization. In addn., the B3P86 functional in combination with small basis sets was found to be superior to B3LYP and MP2 in the calcn. of mol. structures. Regarding the calcd. enthalpies of formation, G2 theory was the most accurate, with an RMS deviation of 9 kJ·mol-1, followed by several combinations of the B3PW91 and B3LYP functionals with mostly large basis sets. However, the B3P86 functional tends to overbind open-shell species, resulting in an underestimation of the enthalpies of formation for polyat. mols. Extension of the bond dissocn. energy calcns. at levels of theory employing the B3P86 functional to a larger set of 60 bonds in 41 halogen-contg. mols. revealed systematic errors dependent on the mol. size. Therefore, the calcd. bond dissocn. energies at the B3P86/6-311++G(2df,p) level of theory were empirically improved by increasing the abs. energies of the radicals by the quantity 9 × 10-5·Ne Hartrees (Ne = total no. of electrons of the radical), with a subsequent lowering of the RMS deviation in the larger set to 8.0 kJ·mol-1.