P-F

~~14, 12,~~ 13 в. 1968

PX_4, POX_2, PX_1, PX_2, PX_3, POX (Do p-x)

X - галоген. XIII 1917 ~~XI 2655~~

Гаркин О. Ф., Дяткина М. В.

Ж. структ. химии, 1968, 9 (2), 275-278.

СА, 1968, 69, с 18, 69838 w Ю

PF_5, PF_2, PF_3, P_2F_4, P_3F_5, F_6P_4 (Vi) 1969
Solan. D.,
U.S. Clearinghouse Fed. Sci. Tech. XIII 1247
Inform., PB Rep., 1969, PB-184 819, 247pp
(anal.)
Reduction, reactions, and spectra of low-valent highly reactive chemical species - with special emphasis on the phosphorous - fluoride system

LO 11 (B) CA 1970 V72, N18, 96190x

P-F

1972

PF, PF_2; PF_3; PF_4; PF_5; P_2F_4

Companion, A. L.; Hsia, Y. P.

"J. Mol. Struct."

Datan, J, A. кв. мех. расч.

1972, 14, N1, 117-26.

(см N-F, III)

PFx

1974

(Vi)

V 31396k Vibrational spectroscopy of some substituted phosphorus fluorides. Fey, George T. K. (Univ. Massachusetts, Amherst, Mass.). 1973, 218 pp. (Eng). Avail. Univ. Microfilms, Ann Arbor, Mich., Order No. 73-31,083. From *Diss. Abstr. Int. B* 1974, 34(7), 3151-2.

C.A. 1974. 81. N4

$P_2F_{11}^-$ | Ом. 19356 | 1984

Gutsev G. L., Boldyrev A. I.,

теор.
расчет.

Chem. Phys. Lett., 1984,
108, N3, 250-254.

$P_2F_{11}^-$

Оп. 20925

1984

Гущев Г.Л., Болдырев А.И.,

Ж; Журн. структурн. хим., 1984, 25, № 5, 16–20.

1986

PF_n

Berkowitz J., Gibson S. T., et al.

фотоион. масспектр.

Croat. Chem. Acta 1986, 59(3), 573-26.

(см. NH_n; III)

$(PH_4)^+(HF_2)^-$ 1986

Kurnig Ingrid J.,
Szczesniak M. M. et al.

u.n. J. Phys. Chem., 1986,
90, N 18, 4253-4258.

(ссс. $(NH_4)^+(HF_2)^-$; III)

Галогениды P

1986

105: 104961s **Correlation between force constants and geometric parameters for halides of phosphorus, arsenic, and antimony.** Kuznetsov, S. L.; Kharitonov, Yu. Ya. (Inst. Obshch. Neorg. Khim. im. Kurnakova, Moscow, USSR). *Zh. Neorg. Khim.* 1986, 31(7), 1716–22 (Russ). A system of dependence was found between the force consts. and geometric parameters for the halides of P, and the possibility is shown of its application for finding the force consts. and vibrational frequencies of Group VA halides.

Ур, спектр. парам., спектроскоп.

(+2) ☒

Галогениды As

С.А. 1986, 105, N 12

F_5P^+
(PF_5^+)

[om. 30490] 1988

Jacox M.E.,

Ti,
Di;

J. Phys. and chem. Ref. Data, 1988, 17, N2, 505.

$F_4P_2^+$ $(P_2F_4^+)$ | om. 30490 | 1988

Jacox M. E.,

Ti, Di; J. Phys. and Chem. Ref. Data, 1988, 17, N 2, 504.

FP_2^+

1988

Яковсон В.В.,
Зюбина Т.С. и др.

ЖС. теорган. химии.
1988. 33, N 12. С. 2997-
3000.

м.п.

(сеч. FN_2^+; III)

$P_2F_{11}^-$ 1990

Kölmel Ch., Palm G.,

et al.

Chem. Phys. Lett. 1990.

м.п. 173, N2-3. С. 151-156.

(см. PF_5; III)

PF_{K+1}^{-}

1990

Сапожников В.В.,
Сологоник В.Г.

Молекул. структура.

м.п. Иваново, 1990. с. 38-47.

(Сер. NaF_{K+1}^{-}; III)

P_2F_2

1991

12 Д181. Многократные связи в перфтордифосфене (FPPF) и перфтордифосфинилидене (PPF_2). Multiple bonding in perfluorodiphosphene (FPPF) and perfluorodiphosphinylidene (PPF_2) / Jin S., Colegrove Th., Schaefer (III) H. F. // Inorg. Chem.— 1991.— **30**, № 15.— С. 2969—2977.— Англ.

Неэмпирическим методом ССП и КВ с учетом одно- и двукратных возбуждений в трехэкспонентном базисе с включением двойной поляризации рассчитаны 7 энергетич. минимумов для системы P_2F_2. Проведен анализ природы связей в этих молекулах. Показано, что одна из структур соответствует плоской конфигурации PPF_2 и содержит тройную связь P—P. При этом центральный атом P имеет формальную валентность 5, обусловленную преимущественно ионным характером связей P—F. Показано, что тройная связь состоит в основном из *s*- и *p*-орбиталей P.

М.П.

ф. 1991, N 12

FPPF

PPF_2

1991

115: 79260j Multiple bonding in perfluorodiphosphene (FPPF) and perfluorodiphosphinylidene (PPF_2). Jin, Suqian; Colegrove, Brenda Thies; Schaefer, Henry F., III (Cent. Comput. Quantum Chem., Univ. Georgia, Athens, GA 30602 USA). *Inorg. Chem.* 1991, 30(15), 2969–77 (Eng). Seven energy min. for the P_2F_2 system have been detd. by means of ab initio self-consistent-field (SCF) and single- and double-excitation CI (CISD) analytic gradient methods using basis sets as large as triple ζ-plus double polarization (TZ2P). Detailed analyses of the bonding nature of these structures have been carried out, with an emphasis on the P-P. In particular, authors find one structure corresponding to a planar PPF_2 configuration that contains a P-P triple bond, yielding a central phosphorus atom with a formal valence of 5. Their results indicate that this hypervalence is primarily the result of the ionic character of the P-F bonds, and the triple bond is comprised mainly of phosphorus s and p orbitals.

структура

расчет

C. A. 1991, 115, N8

PF_n — PF_n^- ($n=1-5$)

ОМ 36828 1992

7 7Б1034. Исследование структуры и стабилизации соединений PF_n, $n=1—5$, и их анионов методом функционала плотности /Гуцев Г. Л. //Изв. РАН. Сер. хим. .—1992 .—№ 10 .—С. 2219—2232 .—Рус.

Электронная и геометрич. структура фторидов фосфора PF_n, $n=1—5$, и их однократно заряженных отриц. ионов рассчитана в рамках метода функционала плотности. Рассмотрены как основные, так и низколежащие возбужденные состояния обоих рядов. Впервые получены структурные параметры нейтр. радикалов PF_2, PF_4 и их анионов. Рассчитаны адиабатич. и вертикальное сродство к электрону (СЭ) нейтр. фторидов фосфора и первые потенциалы ионизации анионов. Согласно результатам вычислений все фториды фосфора обладают положит. $СЭ_{ад}$, за исключением PF_3, СЭ к-рого находится вблизи нулевого значения и требует дальнейших исследований. Рассчитаны энергии диссоциации по различным каналам как нейтр., так и отрицательно заряженных фторидов фосфора. Все PF_n и PF_n^-, $n=1—5$, стабильны в газ. фазе. Анионы PF^-, PF_2^-, PF_3^- и PF_5^- обладают возбужденными состояниями, устойчивыми по отношению как к отрыву внеш. электрона, так и к диссоциации. Бил. 70.

М.П.

Х.1993, №7

PF_n

Ом 36828

1992

$n = 1 \div 5$

118: 154988v Investigation of the structure and stability of phosphorus fluorides (PF_n) compounds, n = 1-5, and their anions by density functional methods. Gritsev, G. L. (Inst. Chem. Phys., Chernogolovka, Russia 142432). *Izv. Akad. Nauk, Ser. Khim.* 1992, (10), 2219-32 (Russ). The electronic and geometrical structures of the PF_n, n = 1-5, and their singly charged anions have been calcd. by d. functional methods. Both the ground and low-lying excited states are considered. The structural parameters of the neutral radicals PF_2, PF_4 and their anions are obtained. The vertical and adiabatic electron affinities (EA) of the neutrals as well as the first ionization potentials of the anions are detd. According to the results of the calcns. all the phosphorus fluorides considered possess the pos. EA_{ad} except PF_3 which has EA_{ad} about zero and requires further investigations. Dissocn. energies through different channels are calcd. for both series. All PF_n and PF_n^-, n = 1-5, are stable in the gas phase. The anions PF^-, PF_2^-, PF_3^-, and PF_5^- possess the excited states which are stable both to dissocn. and the loss of an extra electron.

теорет. расчет структуры и стабильн.

C.A. 1993, 118, N 16

ОМ 36 828 1992

PF_n

$n=1-5$

3 Д96. Исследование структуры и стабильности соединений PF_n, $n=1—5$, и их анионов методом функционала плотности / Гуцев Г. Л. // Изв. РАН. Сер. хим. .— 1992 , № 10 .— С. 2219—2232

Электронная и геометрическая структура фторидов фосфора PF_n, $n=1—5$, и их однократно заряженных отрицательных ионов рассчитана в рамках метода функционала плотности. Рассмотрены как основные, так и низколежащие возбужденные состояния обоих рядов. Получены структурные параметры нейтральных радикалов PF_2, PF и их анионов. Рассчитаны адиабатическое и вертикальное средство к электрону (СЭ) нейтральных фторидов фосфора и первые потенциалы ионизации анионов. Согласно результатам вычислений все фториды фосфора обладают положительным $СЭ^{ад}$, за исключением PF_3, СЭ которого находится вблизи нулевого значения. Рассчитаны энергии диссоциации по различным каналам как нейтральных, так и отрицательно заряженных фторидов фосфора. Все PF_n и PF_n^-, $n=1\div5$, стабильны в газовой фазе. Анионы PF^-, PF^{2-}, PF_3^- и PF_5^- обладают возбужденными состояниями, устойчивыми по отношению как к отрыву внешнего электрона, так и к диссоциации.

структура; спектроскопия

Ф 1993, №3

Фторидн Р

1993

22 Б1052. **Строгая интерпретация электронных волновых функций. 2. Электронная структура некоторых фторидов и оксидов фосфора, серы и хлора.** Rigorous interpretation of electronic wave functions .2. .Electronic structures of selected phosphorus, sulfur, and chlorine fluorides and oxides /Cioslowski Jerzy, Mixon Stacey T. //Inorg. Chem. .—1993 .—32 ,№ 15 .—С. 3209—3216 .—Англ.

М.Л.

Х.1994, N22

PF_n

PF_n^-

1993

19 Б1041. Теоретическое изучение структуры и стабильности рядов молекул PF_n и PF_n^- (n=1—6). A theoretical study on the structure and stability of the PF_n and PF_n^- series n=1—6 / Gutsev G. L. // J. Chem. Phys. .—1993 .—98 ,№ 1 .—С. 444—452 .—Англ.

М.Л.

Х. 1994, №19.

PF_n, PF_n^-

$n = 1 \div 6$

1993

118: 110102x **A theoretical study on the structure and stability of phosphorus fluorides and their mononegative ions (PF_n and PF_n^- n = 1-6).** Gutsev, G. L. (Inst. Chem. Phys., Chernogolovka, Russia 142432). *J. Chem. Phys.* **1993**, 98(1), 444-52 (Eng). The electronic and geometrical structures were studied of the title compds. by a d. functional method. The ground and some low-lying excited states of both series were considered. The results were used for an estn. of the adiabatic electronic affinity (E.A.$_{ad}$) of the neutrals and fragmentation energies through different decay channels of both series. All the neutral species possess a pos. E.A.$_{ad}$, except for PF_3 whose E.A.$_{ad}$ is near zero from the neg. energy side; all the members of both series are stable towards dissocn. Some excited states which are stable towards the loss of an extra electron and dissocn. are found for all the anions except for PF_3^-.

теор. расчет структ. и сродств.

C.A. 1993, 118, N 12

P_2F_{11}
$P_2F_{11}^-$

1993

Beetsev B.L.,

Zh. Fiz. Khim. 1993,
67(4), 681-5.

сродство,
Ae, теор-
расчет

(соед. PF_6, PF_6^-; III)

1996

F: P-F

P: 3

17Б1282. Микроволновые спектры, неэмпирические расчеты и структура фторфосфана и хлорфосфана. Millimeter-wave spectra, ab initio calculations, and structures of fluorophosphane and chlorophosphane / Drean P., Paplewski M., Demaison J., Breidung J., Thiel W., Beckers H., Burger H. // Inorg. Chem. - 1996. - 35, 26. - С. 7671-7678. - Англ.

Место хранения ГПНТБ России

F: PF(n)
P: 3
18Б147. Структура, термохимия и сродство к электрону PF[n] и PF[n]{-}, n=1-6. [Исследование методом функционала плотности с использованием различных функционалов]. Structures, thermochemistry, and electron affinities of the PF[n] and PF[n]{-} series, n=1-6 / Tschumper Gregory S., Fermann Justin T., Schaefer Henry F. (III) // J. Chem. Phys. - 104, 10. - С. 3676-3683. - Англ.

F: PF(n)-
P: 3
18Б147. Структура, термохимия и сродство к электрону PF[n] и PF[n]{-}, n=1-6. [Исследование методом функционала плотности с использованием различных функционалов]. Structures, thermochemistry, and electron affinities of the PF[n] and PF[n]{-} series, n=1-6 / Tschumper Gregory S., Fermann Justin T., Schaefer Henry F. (III) // J. Chem. Phys. - 104, 10. - С. 3676-3683. - Англ.

PF_n, PF_n^-

$n = 1 \div 6$

1996

124: 186140c **Structures, thermochemistry, and electron affinities of the PF_n and PF_n^- series, n = 1–6.** Tschumper, Gregory S.; Fermann, Justin T.; Schaefer, Henry F., III (Cent. Computational Chem., Univ. Georgia, Athens, GA 30602 USA). *J. Chem. Phys.* **1996**, 104(10), 3676–83 (Eng). A quantum mech. study of the phosphorus fluorides and their singly charged anions was carried out. A range of d. functional methods was used. Optimized geometries, adiabatic electron affinities, vertical electron affinities, vertical detachment energies, and stabilities toward the loss of a single fluorine atom or fluorine ion are reported. These properties were evaluated exhaustively using four exchange–correlation functionals: Becke's 1988 exchange functional with the correlation functional of Lee, Yang, and Parr, Becke's 1988 exchange functional with the 1986 correlation functional of Perdew, Becke's three parameter Hartree–Fock/d. functional hybrid exchange functional with the correlation functional of Lee, Yang, and Parr and Becke's half–and–half Hartree–Fock/d. functional hybrid exchange functional with the correlation functional of Lee, Yang, and Parr (BHLYP). These exchange–correlation functionals were used in conjunction with a double–ζ plus polarization basis and a double–ζ plus polarization basis set which was augmented with an even tempered set of s and p diffuse functions. Less complete examns. of the local spin d. approxn., Becke's 1988 exchange

структура, термохим., Ае, теор. расчет

С. А. 1996, 124, N 14

functional with the 1991 correlation functional of Perdew and Wang are also reported. Results were compared to the limited exptl. data to see which combination of functional and basis set, if any, reproduced known results and could be expected to make accurate predictions where exptl. data is absent. This comparison shows that the BHLYP exchange–correlation functional reproduces the known exptl. geometrical parameters quite well. From work on related systems, the BHLYP method appears to predict the most reliable mol. electron affinities. With the double–ζ plus polarization basis set augmented with s and p diffuse functions, the predicted BHLYP adiabatic electron affinities are 0.71 eV (PF), 0.75 eV (PF_2), 0 (PF_3), 3.17 eV (PF_4), and 1.25 eV (PF_5). These theor. electron affinities are expected to lie somewhat above the true values. The PF_6 mol. is predicted to be dissociative with respect to PF_5 and F, but PF_6^- is significantly bound with respect to either PF_5+F^- or PF_5^-+F.

1967

PH_2X
$X = F, Cl, Br, I$

Burger, Hans; et al.,

св-ва,
ab initio
расчет

Adv. Ser. Phys. Chem.,
1967, 3, 56–115.

(см. FCCA ●, III)

Фторид Р 1998

Gillespie, R.J., et al.,

(Re, 4) Adv. Mol. Struct.
Res. 1998, 4, 1-41.

(см. фторид Be; III)

1999

F: PFn
P: 3
131:262905 Atomization Energies, Formation Enthalpies, Bond Dissociation Energies, and Adiabatic Electron Affinities of the PFn/PFn- Series, n = 1 Gu, Jiande; Leszczynski, Jerzy
Computational Center for Molecular Structure and Interactions Department of Chemistry, Jackson State Univers Jackson, MS 39217, USA J. Phys. Chem. A, 103(39), 7856-7860 (English) 1999 The Gaussian-2 theory (G2) and its modified versions (G2MP2, G2M(CC5), a G2M(CC6)) were applied to predict properties of the PFn/PFn- series. The atomization energies, enthalpies of formation, bond dissocn. energies, an adiabatic electron affinities of the PFn/PFn- series calcd. according to theory and its

modified versions are congruous with the available exptl. Among the four tested G2 versions, the G2M(CC5) method is the most reliab all of the calcd. properties. It underestimates the .DELTA.fH.degree. of and PF5 by about 4 kcal/mol and the EA of P and PF by 0.19 and 0.05 eV. G2M(CC5) method has less error accumulation than the G2 theory; fewer computational demands makes the G2M(CC5) theory more suitable for larger than the G2 method. All bond dissocn. energies of PFn-1-F- predicted by BHLYP/DZP++ approach are quite close to those predicted by the G2 theory modifications with a difference of approx. 2 kcal/mol. However, the BHLY method seriously underestimates the PFn-1-F and PFn-1--F bond dissocn. en (by 10-20 kcal/mol).

1999

F: PFn
P: 3
131:262905 Atomization Energies, Formation Enthalpies, Bond Dissociation Energies, and Adiabatic Electron Affinities of the PFn/PFn- Series, n = 1 Gu, Jiande; Leszczynski, Jerzy Computational Center for Molecular Structure and Interactions Department of Chemistry, Jackson State Univers Jackson, MS 39217, USA J. Phys. Chem. A, 103(39), 7856-7860 (English) 1999 The Gaussian-2 theory (G2) and its modified versions (G2MP2, G2M(CC5), a G2M(CC6)) were applied to predict properties of the PFn/PFn- series. The atomization energies, enthalpies of formation, bond dissocn. energies, an adiabatic electron affinities of the PFn/PFn- series calcd. according to theory and its

modified versions are congruous with the available exptl. Among the four tested G2 versions, the G2M(CC5) method is the most reliab all of the calcd. properties. It underestimates the .DELTA.fH.degree. of and PF5 by about 4 kcal/mol and the EA of P and PF by 0.19 and 0.05 eV. G2M(CC5) method has less error accumulation than the G2 theory; fewer computational demands makes the G2M(CC5) theory more suitable for larger than the G2 method. All bond dissocn. energies of PFn-1-F- predicted by BHLYP/DZP++ approach are quite close to those predicted by the G2 theory modifications with a difference of approx. 2 kcal/mol. However, the BHLY method seriously underestimates the PFn-1-F and PFn-1--F bond dissocn. en (by 10-20 kcal/mol).