

B-C-P-H-Hal

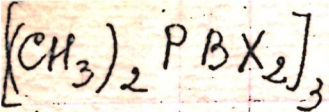


$B_{10}H_{12}P(C_6H_5)_3$ Pace R. F. 1961
et al.

U. R.
chemp

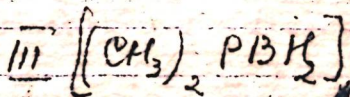
Bep-7048-V

"J. Chem. Soc."
1961, May, 2196-289



1962

Шарпан А. С

X=CH₃, Trans. Far. Soc. 59, 14, 806F,
ClИК-спектры и спектры к. ф.
В некоторых фосфоритовых
соединениях

41017.8408

Ch, Ph, TC

$(CH_3)_2PClBH_3$ ²⁰⁹³²
 $(CH_3)_2PClBD_3$

1974

024-6953

Odom J.D., Reithmiller S., Durig J.R.

Spectra and structure of phosphorus-boron compounds. V. Synthesis and spectroscopic study of dimethylchlorophosphineborane.

"J. Inorg. and Nucl. Chem.", 1974, 36, N 8, 1713-1720

(англ.)

0215 пик

181 183

207

ВИНИТИ

$\text{CH}_3\text{PF}_2\cdot\text{BNH}_3$

ХЗ-13191

1975

11 Д506. Микроволновый спектр и дипольный момент метилдифторфосфинборана. Creswell Robert A., Elzaro R. A., Schwendeman R. H. Microwave spectrum and dipole moment of methyldifluorophosphine—borane. «Inorg. Chem.», 1975, 14, № 9, 2256—2259 (англ.)

Измерены и отождествлены микроволн. спектры четырех изотопич. образцов молекулы $\text{CH}_3\text{PF}_2\cdot\text{BNH}_3$. Из измерения эффекта Штарка найдены значения дипольного момента и его компонентов: $\mu_a=3,52$, $\mu_b=1,76$ и $\mu_{\text{общ.}}=3,94$ ед. Дебая. Определена величина границы барьера внутреннего вращения CH_3 - и BNH_3 -групп, равная 2000 кал/мол. Найдена длина связи $r(\text{P}-\text{B})=1,84\pm 0,02$ Å.

Д.И.И.

ф. 1976 № 11

ВФ-3207-ХУ

CH₃PF₂BH₃

13191

1975

M.B.

CH₃PF₂BH₃

139191v Microwave spectrum and dipole moment of methyldifluorophosphine-borane. Creswell, Robert A.; Elzaro, R. A.; Schwendeman, R. H. (Dep. Chem., Michigan State Univ., East Lansing, Mich.). *Inorg. Chem.* 1975, 14(9), 2256-9 (Eng). The microwave spectra of MePF₂-¹¹BH₃, MePF₂-¹⁰BH₃, MePF₂-¹¹BD₃ and MePF₂-¹⁰BD₃ were assigned. Stark effect measurements gave the following values for the dipole moment and its components: $\mu_a = 3.52(5)$ D, $\mu_b = 1.76(5)$ D, $\mu_c = 0.0$ D, and $\mu = 3.94(5)$ D. The absence of resolvable internal rotation splittings in the ground state yields lower limits of about 2000 cal/mole for the barriers to both Me and BH₃ group internal rotation. By judicious transfer of structural parameters from related mols. $r(P-B)$ was estd. to be 1.84 ± 0.02 Å.

13191-1
B9-3207-X

C.A. 1975 83 N16

$\text{CH}_3\text{OPF} \cdot \text{BN}_3$

1976

18 Б323. Определение конформации аддуктов дифторфосфина методом микроволновой спектроскопии низкого разрешения. Huebner J., Cohn K. Conformation of difluorophosphine adducts by means of low resolution microwave spectroscopy. «J. Cryst. and Mol. Struct.», 1976, 6, № 1, 65—70 (англ.)

Измерены в области частот от 18 до 40 ГГц МВ-спектры низкого разрешения двух аддуктов дифторфосфина, $\text{CH}_3\text{OPF} \cdot \text{BN}_3$: Р-аддукта (I) и О-аддукта (II). Наблюдаемые МВ-переходы отнесены к двум конформерам из четырех возможных для I и двух возможных для II. В предположении, что группа бора расположена симметрично, а метильная группа имеет тетраэдрич. конфигурацию; определены структурные параметры I и II, соотв.: $r(\text{PF}) = 1,557$ и $1,587$ А, $r(\text{PO}) = 1,54$ и $1,59$ А, $r(\text{CO}) = 1,446$ и $1,466$ А, $\angle \text{FPF} = 96,8$ и $95,2^\circ$, $\angle \text{OPF} = 103,3$ и $101,7^\circ$, $\angle \text{COP} = 123,5$ и 120° , и для I: $r(\text{PB}) = 1,88$ А, $\angle \text{OPB} = 116^\circ$, и для II: $r(\text{OB}) = 1,50$ А, $\angle \text{COB} = 120^\circ$. С. Н. Мурзин

структ.
парам.

2. 1977 № 18

$\text{CH}_3\text{OPF}_2 \cdot \text{BH}_3$

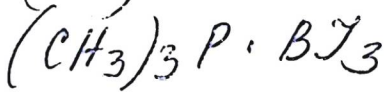
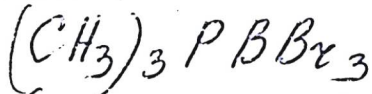
1976

86: 98318h Conformation of difluorophosphine adducts by means of low resolution microwave spectroscopy. Huerner, J.; Cohn, K. (California State Coll., Bakersfield, Calif.). *J. Cryst. Mol. Struct.* 1976, 6(1), 65-70 (Eng). Conformation and structural parameters of $\text{MeOPF}_2\text{BH}_3$ were obtained by using low-resoln. microwave spectroscopy. Two groups of peaks were obsd. in the *K*-band and 3 in the *R*-band. They were centered at 18,380; 23,000; 27,590; 32,170; and 36,790 MHz. These were assocd. with transitions between *J* levels 3-4, 4-5, 5-6, 6-7, and 7-8. The value of $(B + C)$ was calcd. as 4596 ± 5 MHz.

сфукт.
напар.

С.А. 1977. St. 14

1974



87: 108732a Phosphine-borane derivatives. 9. Vibrational spectra of the trimethylphosphine adducts of boron trihalides. Drake, John E.; Hencer, J. Lawrence; Rapp, Bernard (Dep. Chem., Univ. Windsor, Windsor, Ont.). *Inorg. Chem.* 1977, 16(9), 2289-94 (Eng). The IR and Raman spectra of $\text{Me}_3\text{P.BCl}_3$, $\text{Me}_3\text{P.BBr}_3$, and $\text{Me}_3\text{P.BI}_3$ are reported. A normal-coordinate anal., utilizing a modified Urey-Bradley force field, supports the assignments. The values of K_{PB} obtained using this modified force field are consistent with the increase in relative Lewis acidity along the series $\text{BCl}_3 < \text{BBr}_3 < \text{BI}_3$. In all of the adducts, the P-B force const. is larger than in the corresponding $\text{PH}_3.\text{BX}_3$ species.

✓
C.A. 1977.

C.A. 1974. 87 n 14

$(CH_3)_3P \cdot BCl_3$

DM. 8930

1979

8 Б90. Электронографическое исследование строения аддукта $(CH_3)_3P \cdot BCl_3$. Iijima Kinya, Shibata Shuzo. Molecular structure of trimethylphosphine-boron trichloride by gas electron diffraction. «Bull. Chem. Soc. Jap.», 1979, 52, № 11, 3204—3207 (англ.)

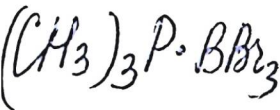
Методом газовой электронографии при 190° исследовано строение аддукта $(CH_3)_3P \cdot BCl_3$ (I). Сделаны

предположения, что группы CH_3 имеют симметрию C_{3v} и находятся в шахматном положении по отношению к связи $P-B$, а I имеет шахматную конформацию симметрии C_{3v} . Получены след. величины межъядерных расстояний (А), амплитуд колебаний (А) и углов (град):
 $r_g(B-Cl) = 1,851(7)$; $r_g(P-B) = 1,941(16)$; $r_g(C-P) = 1,800(4)$; $r_g(C-H) = 1,099(5)$; $r_g(Cl-Cl) = 3,022(5)$; $r_g(C-C) = 2,936(10)$; $l(B-Cl) = 0,067(6)$; $l(C-P) = 0,048(4)$; $l(C-H) = 0,073(5)$; $l(C-Cl) = 0,092(4)$; $l(C-Cl)_{\text{транс}} = 0,106(8)$; $l(C-Cl)_{\text{гош}} = 0,238(10)$; $l(P-H) = 0,113(10)$; $\angle PCN = 113,7(9)$; $\angle ClBCl = 109,5(4)$; $\angle CPC = 109,3(3)$. Посредством сравнения эксперим. и рас-

X. 1980 N 8

четной амплитуд колебаний для пары атомов (C—Cl)_{гош} оценена величина торзионной силовой постоянной $Y(P—B) = 0,12$ (2) мдин·А и рассчитан барьер внутреннего вращения (БВВ) вокруг связи P—B, равный 3,8 (7) ккал/моль. Обсуждаются БВВ в I и сходных молекулах, а также анализируются изменения в молекулах доноров и акцепторов, происходящие при образовании I и (CH₃)₃N·BCl₃. Г. В. Гиричев

1981



3 Б153. Молекулярная структура триметилфосфина-трибромид бора, определенная методом газовой электронографии. Iijima Kinya, Koshimizu Eiichi, Shibata Shuzo. Molecular structure of trimethylphosphine-boron tribromide as determined by gas electron diffraction. «Bull. Chem. Soc. Jap.», 1981, 54, № 8, 2255—2259 (англ.)

геометр.,
структ.

Методом газовой электронографии изучена структура молекулы $(\text{CH}_3)_3\text{P} \cdot \text{BBr}_3$. В структурном анализе использовались ~~данные колебательной спектроскопии~~ для расчета амплитуд колебаний и поправок на эффект сокращения. Найдены след. значения межъядерных расстояний (r_g , Å) и углов: $\text{B}-\text{Br}$ $2,010 \pm 0,009$, $\text{P}-\text{B}$

$1,946 \pm 0,029$, $\text{C}-\text{P}$ $1,804 \pm 0,004$, $\text{C}-\text{H}$ $1,098 \pm 0,010$, $\angle \text{BrBBr}$ $111,7 \pm 0,7^\circ$, $\angle \text{CPC}$ $108 \pm 0,7^\circ$. Приводятся также параметры r_α -структуры. На основе полученных эксперим. данных проведена оценка величины барьера внутреннего вращения вокруг связи $\text{P}-\text{B}$, к-рая оказалась равной 10 ккал/моль.

В. Спиридонов

X. 1982, 19, №3

$(\text{CH}_3)_3\text{P} \cdot \text{B} \cdot \text{I}_3$

1982

5 Б103. Молекулярное строение комплекса триметилфосфина с трийодидом бора по данным газовой электронографии. The molecular structure of trimethylphosphine-boron triiodide as studied by gas-phase electron diffraction. Iijima Kinya, Koshimizu Eiichi, Shibata Shuzo. «Bull. Chem. Soc. Jap.», 1982, 55, № 8, 2551—2554 (англ.)

Электронографически определена структура $(\text{CH}_3)_3\text{P} \cdot \text{B} \cdot \text{I}_3$ в газовой фазе. Амплитуды колебаний и поправки на эффект сокращения рассчитаны по силовому полю, взятому из лит-ры, но с внесением изменений. Получены след. геометрич. параметры ($r_g, \angle_\alpha$): B—I 2,233(3) А, P—B 1,947(11), C—P 1,809(3), C—H 1,094(8), $\angle \text{I—B—I}$ 111,6(0,3)°, $\angle \text{C—P—C}$ 106,0(0,5). Относительно связей P—C и P—B осуществляются шахматные конформации. При переходе из газообразного состояния в крист. в изучаемом комплексе длина донорно-акцепторной связи P—B сокращается до 1,918(15) А.

В. Мاستрюков

структура

Х. 1983, 19, № 5

P_2BCl_{13}

1986

19 Б1265. Ионная изомеризация с участием моногалогид-иона; спектр комбинационного рассеяния новых тетрахлорфосфониевых частиц. Single halide ionic isomerism; the Raman spectrum of a novel tetrachlorophosphonium species. Finch A., Gates P. N., Muir A. S. «J. Chem. Res. Synop.», 1986, № 2, 68—69 (англ.)

Измерен спектр КР P_2BCl_{13} (I), имеющего ионное строение $[PCl_4^+]_2[BCl_4^-][Cl^-]$, аналогичного метастабильной форме пятихлористого фосфора $[PCl_4^+]_2[PCl_6^-][Cl^-]$ и родственного соединению $[PCl_4^+][BCl_4^-]$ (II). Проведено отнесение частот колебаний в спектрах I и II. Спектры I и II различаются в обл. частот симм. и антисимм. вал. кол. иона PCl_4^- . В спектре I имеется интенсивная линия решеточного колебания при 58 см^{-1} , к-рая отсутствует в спектре II. Различие в спектрах I и II связано с присутствием в I моногалогид-иона Cl^- . При нагревании I обратимо переходит в II по схеме: $2([PCl_4^+]_2[BCl_4^-][Cl^-]) \rightleftharpoons [PCl_4^+][PCl_6^-] + 2([PCl_4^+][BCl_4^-])$. И. А. Гарбузова

спектр КР

X. 1986, 19, N19

C₂H₄F₂P-BH₃

1987

(CKP)

106: 185167h Spectra and structure of phosphorus-boron compounds. Part XXIV. Infrared and Raman spectra, conformational analysis, vibrational assignment and normal coordinate analysis of ethyldifluorophosphine-borane. Durig, J. R.; Rizzolo, J. J.; Sullivan, J. F.; Cheng, Mei Shio; Hizer, T. J.; Odom, J. D. (Dep. Chem., Univ. South Carolina, Columbia, SC 29208 USA). *J. Mol. Struct.* 1987, 156(3-4), 267-91 (Eng). The Raman spectra (10-3200 cm⁻¹) of EtF₂P-BH₃ and -BD₃ were recorded for the solid and fluid phases, and depolarization data were recorded for the liquied phase. The IR spectra (50-3200 cm⁻¹) were recorded for the solid and gaseous phases. These data allow the complete assignment, except for the BH₃ and CH₃ internal torsions, of the fundamental vibrations based on band contours, depolarization values, isotopic shift factors, and group frequencies. The asym. torsion was assigned to a weak broad band obsd. at 78 and 76 cm⁻¹ in the -d₀ and -d₃ compds., resp. A variable temp. study of the Raman spectrum of the liq. shows that EtF₂P-BH₃ exists in the trans and gauche conformers with an enthalpy difference of 157 ± 35 cm⁻¹ (450 ± 100 cal mol⁻¹) with the trans conformer being more stable in this phase, and the only form present in the cryst. solid. A normal coordinate calcn. is carried out utilizing a modified valence force field

C.A. 1987, 106, N 22

$\text{CH}_3\text{CH}_2\text{PF}_2\text{BH}_3$ | Om. 26032 |

1987

Durig J.A., Rizzolo J.J.,
et al.,

cramp,
cnpypypa J. Mol. Struct., 1987,
156, N3-4, 267-291.

$\text{CH}_3\text{PF}_2\text{BH}_3$ | Dm. 26 031 |

1987

$\text{CH}_3\text{PF}_2\text{BD}_3$

Odom J.D., Stanley H.E.
et al.,

Раман и J. Raman Spectrosc., 1987,
ИК спектр,
структура 18, N 1, 25-35.

$\text{CH}_3\text{PF}_2\text{BH}_3$

1987

106; 164857t. Spectra and structure of phosphorus-boron compounds. XXIII - Raman and infrared spectra, vibrational assignment and normal coordinate analysis of methyldifluorophosphineborane. Odom, J. D.; Stanley, A. E.; Cheng, Mei Shio; Durig, J. R. (Dep. Chem., Univ. South Carolina, Columbia, SC 29208 USA). *J. Raman Spectrosc.* 1987, 18(1), 25-35 (Eng). The Raman (10-3500 cm^{-1}) and IR (20-3500 cm^{-1}) spectra of MePF_2BH_3 and MePF_2BD_3 were recorded for the gaseous and solid states. The Raman spectrum of the liq. was recorded, and qual. depolarization values were measured. All the fundamental modes except the 2 internal rotations were assigned using band contours, depolarization values, isotopic shifts, and group frequencies. A normal coordinate calcn. was carried out using a modified valence force field to calc. the frequencies and the potential energy distributions. The observation of 5 Raman lines in the spectrum of the solid, and the observation of the doubling of several of the intramol. fundamentals, indicate that there are ≥ 2 mols. per primitive cell. These results are compared with similar quantities in some corresponding mols.

(UK u CKP)

C. A. 1987, 106, N 20.

$\text{CH}_3\text{CH}_2\text{P}(\text{BH}_3)\text{Cl}_2$

1988

(CKP, UK)

109: 179347n Spectra and structure of phosphorus-boron compounds-XXVI. Infrared and Raman spectra, conformational stability and normal coordinate analysis of ethyldichlorophosphine-borane. Odom, J. D.; Hizer, T. J.; Stanley, A. E.; Tonker, T. L.; Durig, J. R. (Dep. Chem., Univ. South Carolina, Columbia, SC 29208 USA). *Spectrochim. Acta, Part A* 1988, 44A(7), 631-4. (Eng). The Raman (10-3500 cm^{-1}) and IR (50-3500 cm^{-1}) spectra of solid ethyldichlorophosphine-borane, $\text{CH}_3\text{CH}_2\text{P}(\text{BH}_3)\text{Cl}_2$ and its deuterated analog, $\text{CH}_3\text{CH}_2\text{P}(\text{BD}_3)\text{Cl}_2$ were recorded. Addnl., the IR spectra of the gases and the Raman spectra of the liqs. were recorded and qual. depolarization ratios were obtained. Based on the fact that several distinct Raman lines disappear on going from the liq. to the solid state, it is concluded that the mol. exists as a mixt. of the gauche and trans conformers, with the trans conformer being more stable in the liq. phase, and the only one present in the solid phase. From a temp. study of the Raman spectrum of the liq., the enthalpy difference between the gauche and trans conformers was nearly zero. Based on Raman depolarization data, group frequencies, isotopic shift factors and IR band contours, a complete vibrational assignment has been proposed for the trans conformer. The assignment is

C.A. 1988, 109, N20

supported by a normal coordinate calcn. which was carried out utilizing a modified valence force field to obtain the frequencies of the normal modes and the potential energy distribution. The BH₃ torsion was obsd. at 188 cm⁻¹, while the BD₃ torsion was not obsd. The Me torsions in the spectra of the solids were obsd. 209 and 202 cm⁻¹ for the normal and deuterated species, resp. From the torsional data, barriers to internal rotation were calcd. The asym. torsional mode was obsd. for the trans conformer in the IR spectra of the gas phase at 108 and 104 cm⁻¹ for the BH₃ and BD₃ species, resp. These results are compared with similar quantities for some corresponding organophosphine-borane compds.

$\text{Cl}_3\text{P} \cdot \text{B} \text{Cl}_2$

2001

ab initio
program
составлен,
 ΔH , кДж/моль
(16)

135: 247452g On the bonding, structure and thermodynamics of phosphorus halide boron halide complexes $\text{X}_3\text{P} \cdot \text{BY}_3$ ($\text{X}, \text{Y} = \text{Cl}, \text{Br}, \text{I}$): Aubauer, C.; Klapotke, T. M.; Schulz, A. (Department of Chemistry, Ludwig-Maximilians University Munchen, D-81377 Munich, Germany). *THEOCHEM* 2001, 543, 285-297 (Eng), Elsevier Science B.V. Donor-acceptor complexes $\text{X}_3\text{P} \cdot \text{BY}_3$ ($\text{X}, \text{Y} = \text{Cl}, \text{Br}, \text{I}$) and their fragments were studied using d. functional (B3LYP) and ab initio methods (MP2, CCSD(T)) with effective core potentials. The bonding, charge transfer and structure of all $\text{X}_3\text{P} \cdot \text{BY}_3$ is discussed on the basis of natural bond orbital (NBO) anal. The estd. free mol. enthalpies of dissociation indicate that all $\text{X}_3\text{P} \cdot \text{BY}_3$ represent thermodynamically labile species which are stabilized by the lattice energies in the solid state. The total distortion energy increases in accordance with the decreasing complex dissociation enthalpy. With regard to halogen exchange between the PX_3 and BY_3 moiety in $\text{X}_3\text{P} \cdot \text{BY}_3$ (g) adducts, only the complexes where $\text{Y} = \text{X}$ and where X represents a heavier halogen than Y are thermodynamically stable.

C.A. 2001, 135, 174

2001

Cl_3PBrI_2
 I_3PBrCl_2

ab initio
 program
 calculation,
 ΔH , cmp - pa
 (16)

135: 247452g On the bonding, structure and thermodynamics of phosphorus halide boron halide complexes $X_3P \cdot BY_3$ ($X, Y = Cl, Br, I$): Aubauer, C.; Klapotke, T. M.; Schulz, A. (Department of Chemistry, Ludwig-Maximilians University Munchen, D-81377 Munich, Germany). *THEOCHEM* 2001, 543, 285-297 (Eng), Elsevier Science B.V. Donor-acceptor complexes $X_3P \cdot BY_3$ ($X, Y = Cl, Br, I$) and their fragments were studied using d. functional (B3LYP) and ab initio methods (MP2, CCSD(T)) with effective core potentials. The bonding, charge transfer and structure of all $X_3P \cdot BY_3$ is discussed on the basis of natural bond orbital (NBO) anal. The estd. free mol. enthalpies of disocn. indicate that all $X_3P \cdot BY_3$ represent thermodynamically labile species which are stabilized by the lattice energies in the solid state. The total distortion energy increases in accordance with the decreasing complex disocn. enthalpy. With regard to halogen exchange between the PX_3 and BY_3 moiety in $X_3P \cdot BY_3$ (g). adducts, only the complexes where $Y=X$ and where X represents a heavier halogen than Y are thermodynamically stable.

C.A. 2001, 135, N77

B₃P. BBr₂

2001

135: 247452g On the bonding, structure and thermodynamics of phosphorus halide boron halide complexes X₃P·BY₃ (X, Y = Cl, Br, I): Aubauer, C.; Klapotke, T. M.; Schulz, A. (Department of Chemistry, Ludwig-Maximilians University Munchen, D-81377 Munich, Germany). *THEOCHEM* 2001, 543, 285-297 (Eng), Elsevier Science B.V. Donor-acceptor complexes X₃P·BY₃ (X, Y = Cl, Br, I) and their fragments were studied using d. functional (B3LYP) and ab initio methods (MP2, CCSD(T)) with effective core potentials. The bonding, charge transfer and structure of all X₃P·BY₃ is discussed on the basis of natural bond orbital (NBO) anal. The estd. free mol. enthalpies of disocn. indicate that all X₃P·BY₃ represent thermodynamically labile species which are stabilized by the lattice energies in the solid state. The total distortion energy increases in accordance with the decreasing complex disocn. enthalpy. With regard to halogen exchange between the PX₃ and BY₃ moiety in X₃P·BY₃ (g) adducts, only the complexes where Y=X and where X represents a heavier halogen than Y are thermodynamically stable.

ab initio
prae
maßstab H,
ΔH, emp - pa
(46)

C.A. 2001, 135, N17

2001

 $\text{Br}_3\text{P} \cdot \text{BBr}_2$
 $\text{I}_3\text{P} \cdot \text{BI}_2$

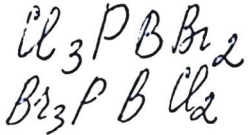
 ab initio
 program
 calculation,
 ΔH , cm⁻¹-pa

(16)

135: 247452g On the bonding, structure and thermodynamics of phosphorus halide boron halide complexes $\text{X}_3\text{P} \cdot \text{BY}_3$ (X, Y = Cl, Br, I): Aubauer, C.; Klapotke, T. M.; Schulz, A. (Department of Chemistry, Ludwig-Maximilians University Munchen, D-81377 Munich, Germany). *THEOCHEM* 2001, 543, 285-297 (Eng), Elsevier Science B.V. Donor-acceptor complexes $\text{X}_3\text{P} \cdot \text{BY}_3$ (X, Y = Cl, Br, I) and their fragments were studied using d. functional (B3LYP) and ab initio methods (MP2, CCSD(T)) with effective core potentials. The bonding, charge transfer and structure of all $\text{X}_3\text{P} \cdot \text{BY}_3$ is discussed on the basis of natural bond orbital (NBO) anal. The estd. free mol. enthalpies of disocn. indicate that all $\text{X}_3\text{P} \cdot \text{BY}_3$ represent thermodynamically labile species which are stabilized by the lattice energies in the solid state. The total distortion energy increases in accordance with the decreasing complex disocn. enthalpy. With regard to halogen exchange between the PX_3 and BY_3 moiety in $\text{X}_3\text{P} \cdot \text{BY}_3$ (g) adducts, only the complexes where Y=X and where X represents a heavier halogen than Y are thermodynamically stable.

C.A. 2001, 135, N74

2001



ab initio
 therm
 calculation,
 ΔH , comp - pa
 (46)

135: 247452g On the bonding, structure and thermodynamics of phosphorus halide boron halide complexes $\text{X}_3\text{P} \cdot \text{BY}_3$ (X, Y = Cl, Br, I). Aubauer, C.; Klapotke, T. M.; Schulz, A. (Department of Chemistry, Ludwig-Maximilians University Munchen, D-81377 Munich, Germany). *THEOCHEM* 2001, 543, 285-297 (Eng), Elsevier Science B.V. Donor-acceptor complexes $\text{X}_3\text{P} \cdot \text{BY}_3$ (X, Y = Cl, Br, I) and their fragments were studied using d. functional (B3LYP) and ab initio methods (MP2, CCSD(T)) with effective core potentials. The bonding, charge transfer and structure of all $\text{X}_3\text{P} \cdot \text{BY}_3$ is discussed on the basis of natural bond orbital (NBO) anal. The estd. free mol. enthalpies of disocn. indicate that all $\text{X}_3\text{P} \cdot \text{BY}_3$ represent thermodynamically labile species which are stabilized by the lattice energies in the solid state. The total distortion energy increases in accordance with the decreasing complex disocn. enthalpy. With regard to halogen exchange between the PX_3 and BY_3 moiety in $\text{X}_3\text{P} \cdot \text{BY}_3$ (g) adducts, only the complexes where $\text{Y}=\text{X}$ and where X represents a heavier halogen than Y are thermodynamically stable.

C.A. 2001, 135, N17

$\text{Cl}_3\text{P} \cdot \text{BCl}_2$

2001

Aubauer C., et al.,

THEOCHEM 2001, 543,
285-297.

at initio
niveau,
смабунт.,
SH, cnp-pr

(Cm.  $\text{Cl}_3\text{P} \cdot \text{BCl}_2$, III,