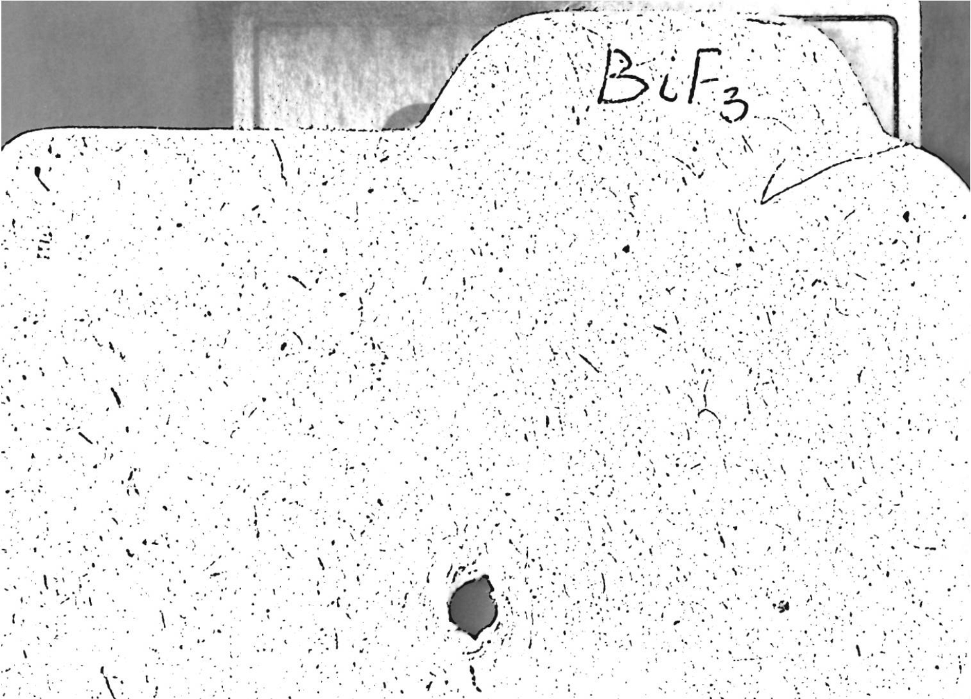
BiF_3

ν_i (YX_3, где Y = N, P, As, Pb, Sb, Bi, РХ 1967
X = H, F, Cl, CH_3, $C{\equiv}CH$)

Suit W. M. A., Maas J. H. van der. Spectrochim. acta, 1967, A23, N8, 2453-55

XIII 936

есть ориг

РХ 1968

10

сил. пост. (BiF_3, SbF_3) 13 1971

XIII 708

Rai S. N., Thakur S. N.,

Indian J. Pure and Appl. Phys, 1971, 9, №1, 61-62 (англ)

Intramolecular force fields in group VB trihalides.

РЖХим, 1971, 17Б68

10 5

PCl_3; PBr_3; PJ_3; AsF_3, $AsCl_3$, $AsBr_3$

J_3; SbF_3, $AsCl_3$; $AsBr_3$, AsJ_3; SbF_3;

Cl_3; $SbBr_3$; SbJ_3; BiF_3, $BiCl_3$

Br_3, BiJ_3 (м.и.) XIII 541

[illegible] Тимошин~~ин~~ В.С.,

Содиев И.Н.

Оптика и спектроск., 1971,

31, №6, 1027-29

Ⓕ

РХ72

20

PF_3; AsF_3; SbF_3; BiF_3; BF_3;
PCl_3; $AsCl_3$; $SbCl_3$; $BiCl_3$; BCl_3;
PBr_3; $AsBr_3$; $SbBr_3$; $BiBr_3$; BBr_3;
PI_3; AsI_3; SbI_3; BiI_3; BI_3

пост.
центро-
бежн.
растяж.

1972

13, 14 в.

XIII 233,

Тимощин В.С., Годнев И.Н.,
Изв. высш. учеб. завед., физ., 1972,
15, N12, 141-3 (русск.)

Постоянные центробежного растяжения молекул типа XY_3
D_{3h} и C_{3v} симметрии.
CA, 1973, 78, N16, 102228h

10 (Ф)

1974

Bi F_3 Структура трифторидов иттрия и висмута по данным дифракции нейтронов.

структура Cheetham A.K.

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(см YF_3; T)

Х.1974.№9

Зак. 247

Оттиск 16637 1983

BiF_3

Novak I., Potts A.W.,

J. Chem. Soc. Dalton Trans., 1983, 4, 635-638.

УФ фото-
электрон-
спектр,
потенц.
ионизации
энергии связи

BiF_3

1989

111: 242939r Laser Raman, infrared spectra of bismuth fluoride and its vibrational analysis. Mohan, S.; Kuttiappan, P. (Raman Sch. Phys., Pondicherry Univ., Pondicherry, 605 006 India). *Indian J. Phys., B* 1989, 63B(3), 386-90 (Eng). The IR and polarized Raman spectra of BiF_3 were studied at 0-200 cm^{-1} and vibrational assignments were made along with a normal coordinate anal. using a general quadratic function. Force consts., vibrational amplitudes at 298.16 K, Coriolis coupling consts., centrifugal distortion consts. and potential energy distributions are reported.

спектр,
Di

C.A.1989, 111, N 26

BiF_3

от 36909

1992

Breidung J., Thiel W.,

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<u>13</u>, N 2, 165-176

геометр.,
колебат.
частоты,
ИК интенс.,
сил. пол.,
ab initio
расчет

BiF_3

BiF_2

BiF

1992

14 Б1072. Три закона в применении к D_0(BiF). Three laws fer D_0(BiF) /Yoo R. K., Ruscic B., Berkowitz J. //Chem. Phys .— 1992 .— **166** ,№ 1—2 .— С. 215—227 .— Англ.

С помощью МС с фотоионизацией и УФ-диапазоне определены кривые выхода фотоионов BiF и BiF_2, образующихся при испарении смеси Bi—BiF_3. Найдено, что адиабатич. ПТ ионизации равны 8,658 ± 0,012 эВ для BiF и 8,05 ± 0,05 эВ для BiF_2. Порог образования Bi^+ из BiF равен 11,12 ± 0,05 эВ; отсюда следует, что энергия диссоциации D_0(BiF) $\leqslant$ 3,84 ± 0,05 эВ. Применение второго и третьего законов термодинамики к равновесной р-ции $2Bi(г) + BiF_3(г) \rightarrow 2BiF(г)$ привело к значению D_0(BiF) = 3,76 ± 0,13 эВ. Аналогично изучение р-ции $Bi(г) + BiF_2(г) \rightarrow 2BiF(г)$ дало след. результаты: D_0(FBi—F) = 3,50 ± 0,15 эВ; D_0(F_2Bi—F) = 4,5 ± 0,2 эВ. Обсуждены причины расхождений между полученными в настоящей работе данными и ранее опубликованными результатами. Библ. 47. А. А. Кирюшкин

D_0

Х. 1993, N 14

1994

BiF_3 и др.

ν_i, структ., V_0.

[illegible]

Swerdtfeger P., Boyd P.D.W., Fisher J.,
Hund P., Liddell M.
JACS, 1994, 116, N21, 9620-33
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1994

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Judit Molnár, Mária Kolonits et al.,

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413-414, 441-446, ●

Мол.
структ.
колебат.
частот.
амплитуд.
электроногр.

F: BiF3
P: 3

1999

132:16588 Symmetry-broken inversion structures for Group 15 EX3 halides. Schwerdtfeger, Peter; Hunt, Patricia Department of Chemistry, The University of Auckland Auckland, N. Z. Adv. Mol. Struct. Res., 5, 223-262 (English) 1999 A review with 79 refs. The inversion process of EX3 Group 15 hydrides and halides is reviewed. All Group 15 hydrides EH3 and N halides NX3 inv through the classical D3h trigonal planar transition state. For the heav halides, however, the a2 HOMO can interchange with the a1 LUMO as pointed in 1980 by Marynick. Consequently, a low lying 1E' excited state can cou with the 1A1' ground state to undergo an e' 2nd-order Jahn-Teller (SOJT) distortion to a lower lying C2v inversion transition state. Hence, for t heavier Group 15 halides the Dixon-Arduengo

C. A. 2000, 132

edge inversion process throug T-shaped transition state is preferred. The potential energy surface (PE for these compds. is analyzed. For PF3, AsF3, SbF3, and BiF3 at the Hart Fock level the symmetry breaking occurs immediately upon distortion from C3v min. towards the D3h point of the PES. Different topologies around t sym. D3h point are possible in the planar EX3 arrangement, which connect T- and Y-shaped C2v structures. If e'-SOJT symmetry breaking occurs, the topologies can be derived from either a Mexican hat or a monkey saddle. the high-energy D3h point often cannot be described in a satisfactorily w by single-ref. methods. CASSCF calcns. show significant mixts. between 2 configurations of 1A1' symmetry, 1 which is described by a22a1'0 and deno as D3h(a2) and the 2nd configuration by a20a1'2 and denoted as D3h(a1'). Electron correlation effects are therefore important for the accurate det of the inversion barrier. For mols. with large configuration mixing (PCl PBr3, and PI3) a definite decision on the symmetry of the inversion struc cannot be made without higher level calcns. For the Bi halides the e'-SO distortion is small despite the energetically more favored D3h(a1') configuration. For these mols. the PES connecting the planar structures very shallow and a definite decision on the symmetry of the inversion transition state cannot be made. The question whether or not a mol. deco before it inverts is addressed. Common models for the inversion mechanis and bonding for the EX3 compds. are critically analyzed. Structures, vibrational

F: BiF3
P: 3

134:372013 **Density Functional Studies on the Lone Pair Effect of the Trivalent Group (V) Elements: I. Electronic Structure, Vibronic Coupling, and Chemical Criteria for the Occurrence of Lone Pair Distortions in AX3 Molecules (A=N to Bi; X=H, and F to I).** Atanasov, M.; Reinen, D. Fachbereich Chemie, Philipps-Universitaet und Zentrum fuer Materialwissenschaften, Marburg, Germany. J. Phys. Chem. A (2001), 105(22), 5450-5467. in English.

2001

The energetic, steric, and bonding properties of mols. AX_3 (A = N to Bi; X = H, F to I) are analyzed using d. functional theory. It is found that the "lone pair" in the initial D_{3h} geometry is of central atom p_z character for the NX_3 and AH_3 mols., whereas it possesses s symmetry in all other cases - here generally with a strong delocalization toward the ligands. The stabilization of the distorted C_{3v} geometry is due mainly to covalency effects, whereas steric interaction forces according to the Gillespie-Nyholm model do not seem to play a significant role. The application of the conventional vibronic pseudo Jahn-Teller coupling approach (PJT), here for the D3h→C3v transition [A1'⊗(α2" + α1')⊗A2" interaction], is an appropriate means for inorg. chemists to predict trends for the extent of distortion and for the corresponding energy gain. The vibronic coupling consts. and the vibronic stabilization energies, which mainly det. the total D3h→C3v energy gain, vary according to the sequences F > H > Cl > Br > I (A: N to Bi), and N > P > As > Sb > Bi (X: H,F), the dependence on A being only small or not present (X:Cl to I). Thus, the hardest mols. are the most susceptible to vibronic coupling, the latter energy being approx. imaged by the hardness difference η(C3v) - η(D3h). A roughly inverse trend is obsd. if the extent of the angular distortion τα from D3h to C3v symmetry is considered; here, the softest mols. such as Sb(Bi)Br3 exhibit the largest and NH3 the smallest deviations from D3h geometry. The different sequences for τα are due to the strong influence of the force const., which represents the C3v→D3h restoring energy. It is remarkable that the vibronic coupling energy is strongly correlated with the chem. hardness η (an observable quantity), while the stabilization energy for the D3h→C3v transition is not directly reflected by η, in contrast to what is generally called the "principle of max. hardness".