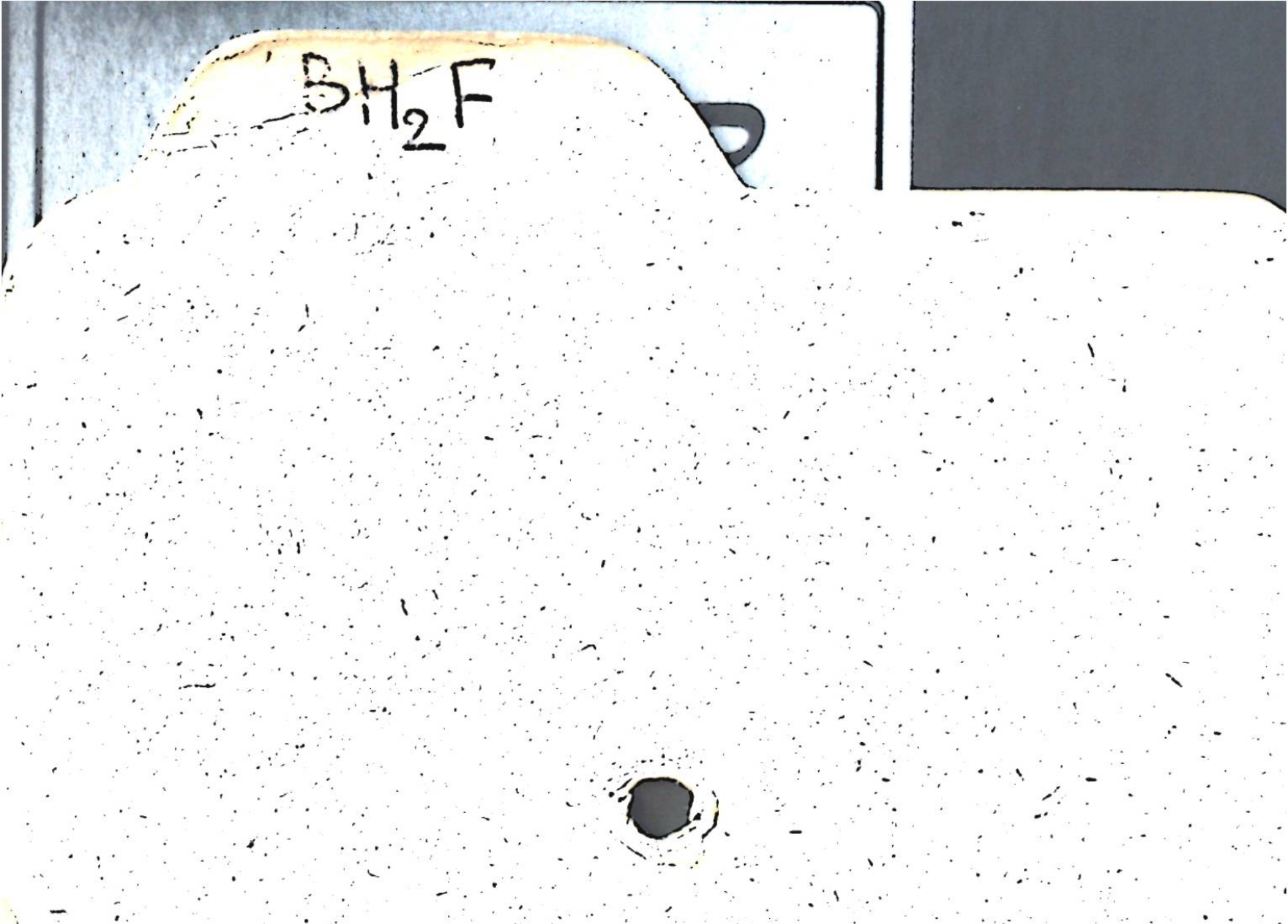
BH_2F

V 4820

H_2BF, H_2NO, H_2CF, H_2NF (структура) 1953

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The electronic orbitals, shapes, and spectra of polyatomic molecules.VI. H_2AB molecules

C.A., 1953, 11950c

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строение

(см. BH_3) III

1970

BH_2F

103997w Ab initio studies of the electronic structures of BH_3 BH_2F, BHF_2 and BF_3. Schwartz, Maurice E.; Allen, Leland Cullen (Frick Chem. Lab., Princeton Univ., Princeton, N.J.). *J. Amer. Chem. Soc.* 1970, 92(6), 1466–71 (Eng). The electronic structures of the mols. BH_3, BH_2F, BHF_2, and BF_3 have been studied by using the ab initio SCF-MO method. Of especial interest are changes of certain quantities through the series from no fluorination (BH_3) to complete fluorination (BF_3). These include const. at. charges for H and F atoms, linearly increasing total pos. charge of the central B atom, increase of the $2p\pi$-type population on B, increasing BF overlap (consisting of a balance between decreasing π overlap and increasing σ overlap, and linear increase of the orbital energy of the lowest unoccupied MO. Excluding the B $2p\pi$ from bonding yields directly a π energy of 27 kcal for BH_2F, and an estd. value of 59 kcal for BF_3, based on the π overlap populations. The 1st ionization

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C.A. 1970. 72. 20

potential is examd. for the series, and an explanation based on splitting of the degeneracy of the highest filled MO in BH_3 accounts for the decrease in the ionization potential upon initial fluorination. Consideration of calcd. and exptl. ionization potentials for BH_3 and BF_3 leads to an est. of 11.8 and 13.6 eV for the 1st ionization potentials of BH_2F and BHF_2. Comparisons of both inner-shell and valence-shell ionization potentials have also been made with the analogous series CH_4 to CHF_3, based on ab initio calcns. of Ha and Allen. The 1*s* binding energies of B and C correlate linearly with the Mulliken charge on the atom, and for multiple fluorination the changes in 1*s* binding energy are multiples of the change for a single fluorination.

RCJC

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● (см BF) III

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BH_2F Beirs 1993

118: 112101v Microwave spectroscopic detection of fluoroborane, BH_2F. Takeo, Harutoshi; Sugie, Masaaki; Matsumura, Chi (Natl. Chem. Lab. Ind., Tsukuba, Japan 305). *J. Mol. Spectrosc.* 1993, 158(1), 201–7 (Eng). Fluoroborane, BH_2F, has been detected as a transient chem. species in the reaction of diborane with trifluoroborane by a microwave spectroscopic technique. The rotational consts. obtained for three isotopic species of this mol. are (in MHz): $^{11}BH_2F$ A = 225096(304), B = 32044.881(43), C = 27926.901(43); $^{10}BH_2F$ A = 224511(208), B = 33249.928(88), C = 28837.887(100); $^{11}BD_2F$ A = 112517(88), B = 26622.0(16), C 21442.8(16) MHz. The dipole moment was μ_a = 0.82(5) D for $^{11}BD_2F$. The quadrupole coupling consts. and the mol. structure were also detd.

УФ спектр, A, B, C

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H_2BF

1994

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(Н) Х

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структурни параметри

H_2BCl

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$FB + H_2 \rightarrow FBH_2$

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поверхность потенц. энергии, теор. расч

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