Al-B

AlB_2 оттиск 5635 1977

Armstrong D. R
et al.

Электронная
структ.

J. chem. Soc. Faraday
Trans. II, 1977, 73,
952-57.

$Al(BH_4)_2CH_3$ оттиск 10198 1980

Barlow M; et al.

молекул.
структура

J. Chem. Soc. Dalton Trans., 1980, №8, 1374-78.

Кв. мех. расчетн
соедин. B и Al

1981

В- соединения

95: 225965e **MNDO calculations for compounds containing aluminum and boron.** Davis, L. P.; Guidry, R. M.; Williams, J. R.; Dewar, M. J. S.; Rzepa, H. S. (F. J. Seiler Res. Lab., USAF Acad., Colorado Springs, CO 80840 USA). *J. Comput. Chem.* 1981, 2(4), 433–45 (Eng). Parametrization of MNDO for Al and comparisons of calcd. mol. properties with exptl. values indicated the general usefulness of MNDO to study Al compds. Although results are not as good as for mols. contg. only C, H, N, and O, they are nevertheless accurate enough to be useful, esp. when predictive biases noted in this article are considered. Inclusion of the *d* orbital in the MNDO scheme may improve the Al results. Results for B compds. not previously reported are also reported.

(~~[illegible]~~)

C.A. 1981, 95, N 26.

$AlB_3^{\pm}$

оттиск 12815

1981

Bohm M.C., Gleiter R.

Theor. chim. acta, 1981, <u>59</u> (2), 153–179.

обзор,
теорий
расчетй,
молекул.
орбиталы,
геометрия

AlOB ОГТ 13559 1982

BAlO

теоретич. расчет стабильности изомеров

96: 223594e **Nonempirical calculations of the structure and stability of isomers in AlOB-BAlO-AlBO and BBO-BOB suboxides.** Zyubina, T. S.; Charkin, O. P.; Zyubin, A. S.; Zakzhevskii, V. G. (Inst. Nov. Khim. Probl., Chernogolovka, USSR). *Zh. Neorg. Khim.* 1982, 27(3), 558-64 (Russ). The potential surfaces of the title Al-B and B suboxide isomers were calcd. by the nonemipirical Hartree-Fock method. The equil. geometrical parameters, relative energies of the isomers, potential barriers sepg. the isomers, and ionization potentials and dipole moments of the isomers were estd. The results are compared with analogous data for HBO-BOH and HAlO-AlOH isomers (Z., T. S. and Ch., O. P., 1979).

⑭ ☒ BAlO; ● AlBO, BBO, BOB

С.А. 1982, 96, №26.

$AlBF_4$ 1982

Zakzhevskii V.D.,
Charkin O.P.
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геометр.,
структ.;
потенц.
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(см. B_2H_4; III)

$AlBF_4$ Оттиск 14606 1982

геометр., теорет. расчет.

Zakzhevskii V.G., Charkin O.P.,
Chem Phys. Lett., 1982,
<u>90</u>, N2, 117-121.

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1983

Nauryzbaeva B. K.,
Kopylova E. A., et al.

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Miner. Syr'ya 1983, (10),
42-45.

(см. $B(OH)_4^-$; III)

AlB_2

1986

105: 159021r **Electronic structure of transition-metal borides with the AlB_2 structure.** Burdett, Jeremy K.; Canadell, Enric; Miller, Gordon J. (Dep. Chem., Univ. Chicago, Chicago, IL 60637 USA). *J. Am. Chem. Soc.* 1986, 108(21), 6561-8 (Eng). A study of the electronic structure of solid metal borides with the AlB_2 structure type is presented. The interaction of the orbitals of the transition metal with those of a planar, graphite-like net of B atoms and the interaction with those of other metals are both important in influencing the properties of these species. The exptl. obsd. variation in the heat of formation of these species is dependent upon the extent of occupation of the metal-boron orbital set. The puckering of the B net in ReB_2 and RuB_2 structures is due not to the effects of charge transfer but to strong metal-metal repulsions perpendicular to the nonmetal sheets. In AlB_2, the strongest interactions are between the B atoms, which attain a graphite-like electron count, with its assocd. structural stability.

теор. расчет

㊷ ☒ ReB_2, RuB_2

C.A. 1986, 105, N18

AlOB
BAlO

деп. 24195

1986

Чаркин О.П.,
Зюбина Т.С.

расчёт
Еизом. и
барьер
изомер.

Координац. химия,
1986, <u>12</u>, N 8, 1011-1037.

(От. 33196) 1990

$AlB_5H_6^{2-}$ –
AlB_5H_7
структура,
теор. расчет

Мебель А.М., Чаркин О.П., Ж. неорган. химии, 1990, 35, N 2, 312–319.

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кубоднеех $AlB_5H_7^-$, CB_5H_7 и
SiB_5H_7

$Al_nB_m^-$

n= 5-30, m=1-3

электрон-
и геомет-
структ.

От. 36424

1991

Nakajima A., Kishi T., et al.,

Chem. Phys. Lett. 1991, 187, N 3, 239-244.

Electronic and geometric structures of aluminum-

boron negative cluster ions
$(Al_{\bar{n}} B_{\bar{m}})$.

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1991

структ.
теор. расч.

Schleyer P.R.,
Boldyrev A.I.
J. Chem. Soc.
Chem. Commun.
1991, (21), 1536-8

см. Al_4O (III)

$SAlLi_3$ 1993

Zakrzewski V.G.; von Niessen W., et al.,

I, Ae, кв. мех. расчет.

Chem. Phys. 1993, <u>174</u>(2), 167-176.

(см. Al_2O; ● <u>III</u>)

AlB

ОМ. 37673

1994

121: 92421f **Theoretical study of the electronic states of AlB.** Baushlicher, Charles W., Jr.; Langhoff, Stephen R. (Ames Res. Cent., NASA, Moffett Field, CA 94035 USA). *J. Chem. Phys.* **1994,** 101(1), 80–5 (Eng). Potential-energy curves for the singlet, triplet, and quintet states of AlB below about 30,000 cm^{-1} were calcd. theor. to facilitate spectroscopic investigations, and for comparisons with analogs calcns. on the Al_2 and B_2 mols. The ground state of AlB is $X^3\Sigma^-$ with a dissocn. energy of 1.96 ± 0.06 eV. The $A^3\Pi$ state was calcd. to lie only 610 cm^{-1} above the ground state. Since transitions from the $(2)^3\Sigma^-$ state to both the $X^3\Sigma^-$ and $A^3\Pi$ states are predicted to be relatively strong, these transitions in the region of 17,000–18,000 cm^{-1} should be an excellent means of characterizing AlB and of detg. the X–A sepn. The adiabatic ionization potential to form the $X^2\Sigma^+$ ground state of AlB^+ was estd. to be 7.05 eV. Overall, the spectroscopy of AlB is much more similar to Al_2 than B_2.

Эл. состояние
м.п., De
теор. расчет

C.A. 1994, 121, N8.

AlB (см. 37773) 1994

Д,
Эксперим.,
теорет.
расчет

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Simons J.,

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98, N40, 9931-44.

$Al_nB_m^-$

1994

Kaya Koji,
Nakajima Atsushi.

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Adv. Met. Semicond.
Clusters 1994, <u>2</u>, 87-114.

(см. ● Li_nNa_m; I)

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1997

Int., B 1998, [illegible]

128: 146831e High resolution infrared and ab initio studies of aluminum and beryllium borohydrides. Williams, Darren Lee (Oregon State Univ., Corvallis, OR USA). 1997. 82 pp. (Eng). Avail. UMI, Order No. DA9805481. From *Diss. Abstr. Int., B* 1998, 58(8), 4244.

ИК спектр, теор. расчет

C.A. 1998, 128, N12

AlB_3

AlB_3^+

1997

128: 221869d Theoretical study on the structure and stabilization of AlB_3 and AlB_3^+. Xu, Xiaohong; Wu, Haishun; Zhang, Congjie Zhou, Weiliang (Dep. Chem., Shanxi Normal Univ., Linfen, Peop. Rep. China 041004). *Huaxue Wuli Xuebao* **1997**, 10(6), 535−539 (Ch), Zhongguo Kexue Jishu Daxue Chubanshe. Ab initio MO calcns. have been carried out with the GAUSSIAN−92 program. The structures of AlB_3 and AlB_3^+ were completely optimized within assumed symmetries using the RHF method and the unrestricted one. The effects of electron correlation were taken into account by using the Moller−Plesset perturbation theory to the second order. For singlet structures with $<s^2>$ values, a modified GAUSSIAN−92 version was used that annihilates spin−contamination (AUHF). Vibrational frequencies were calcd. anal. at HF/6−31G*. The HF/6−31G* geometrical parameters and total energies for AlB_3 and AlB_3^+ were calcd., along with MP2 total energies and frequencies. On the basis of all these results, the $C_{3v}(^1A_1)$ configuration is the most stable structure for AlB_3 and $C_{2v}(^2A_1)$ is the most stable one for AlB_3^+.

ab initio
расчет
стр-ры
и стабильн

CA-1998, 128, N18

AlB от. 39964 1999

AlB^- Gutsev G.L. et al.,

стр-ра J. Chem. Phys., 1999,
и 110, N 6, 2928-35
стабиль
ность

2001

F: AlB2
P: 3

134:331825 **Ab-initio investigation of the covalent bond energies in the metallic covalent superconductor MgB2 and in AlB2.** Bester, G.; Fahnle, M. Max-Planck-Institut fur Metallforschung, Stuttgart, Germany. Los Alamos Natl. Lab., Prepr. Arch., Condens. Matter (2001), 1-4, arXiv:cond-mat/0105107. Journal; Preprint Engl.

The contributions of the covalent bond energies of various atom pairs to the cohesive energy of MgB2 and AlB2 are analyzed with our recently developed energy-partitioning scheme for the d.-functional total energy. The covalent bond energies are strongest for the intralayer B-B pairs. In contrast to the general belief, there is also a considerable covalent bonding between the layers, mediated by the metal atom. The bond energies between the various atom pairs are analyzed in terms of orbital- and energy-resolved contributions.