BCM

1980

$B_{13}C_2$,

23 Б333. Природа химической связи в карбиде бора $B_{13}C_2$. III. Статические деформационные плотности и иллюстративное представление. Kirfel A., Gupta A., Will G. The nature of the chemical bonding in boron carbide, $B_{13}C_2$. III. Static deformation densities and pictorial representation. «Acta crystallogr.», 1980, B36, № 6, 1311—1319 (англ.)

Химич. связь

Продолжено изучение природы хим. связи в карбиде бора. С этой целью построены сечения статич. деформац. электронной плотности (ДЭП), синтезированной в рамках модели мультипольного разл. Гиршфельда. Рассмотрение проводится в сравнении с аналогичными динамич. ДЭП и сопровождается анализом погрешностей. Найдено, что в цепи C — B — C имеется смещение заряда по направлению к атомам C. Это указывает на непригодность приближения нейтр. атомов для описания электронного распределения в $B_{13}C_2$,

Х. 1980 N 23

а также на необходимость учета асферичности атомной электронной плотности при уточнении структур такого рода. В икосаэдре B_{12} из-за наличия внешних хим. связей идеальная симметрия нарушается и Пв икосаэдра оказывается состоящей из треугольников 3 типов. Ковалентные связи между атомами В делокализованы и носят трехцентровый характер. Результаты иллюстрируются пространственным представлением ДЭП в виде Пв равной плотности. Кроме того, исследована степень деформации полной электронной плотности атомов, вовлеченных в хим. связь. Сделан вывод о полезности аналитич. мультипольного представления ДЭП для изучения электронного распределения. Сообщ. II. см. Kirfel A. и др. Acta Cryst., 1979, B35, 2291.

В. Г. Цирельсон

BC_n

$n = 1 \div 14$

1986

Olah Ruben,
Cormides Istvan,
et al.
Shitsuryo Bunseki
1986, 34(5), 257-66.

структура

(cel. SiC_n, III)

Карбид Гора

$B_n^- C_m^+$

(масспектр)

Оп. 29195

1988

Becker S., Dietze H.-J.,

Int. J. Mass Spectrom. and Ion Processes, 1988, 87, N 3, 287–298.

$^{0}B_{n}^{+}$
$(n = 1-4)$

1989

Bernardo Dan N.,
Morrison G. H.

Surface. Sci. 1989.
223, N3. C. L913-L919

ii. n.

(cfr. $Si\,B_{n}^{+}$, III)

CB_n^+ 1991

Bernardo Dan N.,
Morrison G.H.
Surface Sci. 1991. 223
N.
N.C. L 913 - L 919.

(au. SiB_n^+ ; III)

C_nB^-

1992

117: 55084f **Mass spectrometry of linear carbon boride (C_nB^-) generated with laser vaporization.** Huang, Rongbin; Zhang, Peng; Su, Zhaohui; Su, Jianrui; Zheng, Lansun (Dep. Chem., Xiamen Univ., Xiamen, Peop. Rep. China 361005). *Wuli Huaxue Xuebao* 1992, 8(2), 145–7 (Ch). The time–of–flight mass spectrum of C_nB^- was recorded on a selfbuilt instrument with laser vaporization of tetraphenylboron sodium. By anal. of the compn. of the anions, it was found that the no. of the boron atoms in any of these ions equals the no. of the charges carried by the anion, and the sum of the nos. of the carbon and boron atoms in these species are always odd nos. The exptl. results show that boron atom has a strong tendency to attract an electron so that those C_nB^- will have similar electronic structures as C_n, and carbon clusters with odd members are always more stable than their even neighbors.

(масс спектр, стабильность)

C. A. 1992, 117, N6

$C_{59}B$

1992

117: 220164d Molecular structures, binding energies and electronic properties of dopyballs $C_{59}X$ (X = B, N and S). Kurita, Noriyuki; Kobayashi, Kinya; Kumahora, Hiroki; Tago, Kazutami; Ozawa, Kunio (Energy Res. Lab., Hitachi Ltd., 1168 Moriyamacho, Hitachi-shi, Ibaraki, Japan 316). *Chem. Phys. Lett.* 1992, 198(1-2), 95-9 (Eng). When optimized by a MO method with Harris functional and spin-restricted approxns., the mol. structures of $C_{59}B$ and $C_{59}N$ are found to be almost the same as that of C_{60}, while that of $C_{59}S$ is different from that of C_{60}. The binding energies calcd. self-consistently are 6.05 (C_{60}), 6.03 ($C_{59}B$), 6.00 ($C_{59}N$) and 5.91 ($C_{59}S$) eV/atom. The energy gaps between the LUMO and the HOMO or the half-occupied MO are 1.50 (C_{60}), 1.06 ($C_{59}B$), 0.30 ($C_{59}N$) and 0.63 eV ($C_{59}S$), and the Mulliken charges of the doped B, N and S atoms are 4.5, 7.2 and 15.5, resp., meaning the N atom exists as an acceptor, while the B and S atoms exist as donors in these dopyballs.

(мол. структ., энергия связи) теор. расчет

(+2) $C_{59}N$, $C_{59}S$

C.A. 1992, 117, N 22

B_nC_n 1995

$n=12, 16$

теор. расчёт структ. парам., I, Δ, H

Stankevich I.V., Chistyakov A.L., et al.

Zh. Strukt. Khim. 1995, 36(6), 976-82.

(см. B_nN_n, III)

C_nB^-

$n < 13$

1995

123: 209315j C_nB^- ($n < 13$): laser generation and ab initio calculations. Wang, Chun-Ru; Huang, Rong-Bin; Liu, Zhao-Yang; Zheng, Lan-Sun (The State Key Laboratory for Physical Chemistry of Solid Surface, Department of Chemistry, Xiamen University, Xiamen, Peop. Rep. China 361005). *Chem. Phys. Lett.* 1995, 242(3), 355–60 (Eng). C_nB^{1-} cluster anions with n = 1–12 were generated from direct laser vaporization (of graphite doped with $Na_2B_7O_4$), and studied by mass spectrometry. Ab-initio calcns. were performed on the clusters to optimize their geometries, and to obtain their electron detachment energies and fragmentation energies. The calcd. results show that C_nB^{1-} with even n are much more stable than those with odd n, in agreement with the mass-spectrometry exptl. observation. Qual. MO diagrams have been drawn which relate the no. of total valence electrons of the cluster anions to their electronic features.

ab initio расчет спектров, спр-ра

C.A. 1995, 123, N 16

1996

F: B2C3
P: 3
16Б159. Теоретическое изучение структуры и колебательных спектров кластера B[2]C[3] [с использованием неэмпирического метода] / Ge Mao-Fa, Feng Ji-Kang, Huang Xu-Ri, Yang Cheng, Sun Chia-Chung [Gaodeng xuexiao huaxue xuebao] // Gaodeng xuexiao huaxun xuebao = Chem. J. Chin. Univ. - 1996. - 17, N 9. - С. 1458-1461. - Кит.; рез. Англ.

РЖХ 1997

B_2C_3

1996

125: 341524x **Theoretical studies on the structure and vibrational spectra of B_2C_3 cluster.** Ge, Mao-Fa; Feng, Ji-Kang; Huang, Xu-Ri; Yang, Cheng; Sun, Chia-Chung (Department of Chemistry, Jilin University, Changchun, Peop. Rep. China 130023). *Gaodeng Xuexiao Huaxue Xuebao* 1996, 17(9), 1458-1461 (Ch). The B_2C_3 cluster was studied by using quantum chem. ab initio method. Various possible structures, related vibrational spectra and binding energies were calcd. The electronic structure of the most stable configuration of the B_2C_3 cluster was analyzed and discussed.

кол. спектр, стр-ра, теор. расч

С.А. 1996, 125, N 26

B_4C_2
B_2C_4

1997

128: 106571p **Ab initio study of B_4C_2 and B_2C_4 clusters.** Ge, Mao-Fa; Huang, Xu-Ri; Feng, Ji-Kang; Yang, Cheng; Sun, Chia-Chong (Dep. Chem., Inst. Theoretical Chem., Jilin Univ., Changchun, Peop. Rep. China 130023). *Gaodeng Xuexiao Huaxue Xuebao* **1997**, 18(11), 1838-1841 (Ch), Gaodeng Jiaoyu Chubanshe. Various geometric configurations of B_4C_2 and B_2C_4 clusters were studied by quantum-chem. ab initio methods, and their vibrational spectra were calcd. The stable configurations of B_2C_4 are linear or planar; while those of B_4C_2 are linear, planar or three-dimensional. Therefore, B_4C_2 is similar to B_6 and B_2C_4 is similar to C_6. It is an important effect of stability that B_4C_2 and B_2C_4 have B-C and C-C multiple-bonds, and a strong conjugated effect.

ab initio расчет стабильн. и спр-ти

C.A. 1998, 128, N9

B2 C3 (Dm. 40069) 1999

Комплекс José Domingo Presilla-Márquez et al.,
и
Аналог J. Chem. Phys., 1999, 110, N12, 5702-5709

(C59B)2 и др.

2000

Batsev I.F. et al.,

J. Phys. Chem. Solids
2000, 61 (5), 695-699

теорет. расчет структуры, параметр, энергии связи

(см. ● (C59N)2; III)

C2B

2000

134: 34423r **Large amplitude vibrations in the X $2A_1$ state of C_2B.** Leonard, C.; Chambaud, G.; Rosmus, P.; Carter, S.; Handy, N. C.; Wyss, M.; Maier, J. P. (Laboratoire de Chimie Theorique, Universite de Marne la Vallee, 77454 Champs sur Marne, Fr.). *J. Chem. Phys.* 2000, 113(13), 5228–5234 (Eng), American Institute of Physics. A three-dimensional potential energy function (PEF) of the $^2A_1$ electronic ground state of C_2B was generated by electronic structure calcns. The PEF possesses a min. in an isosceles triangular structure which lies 2204 cm−1 below two equiv. min. having linear equil. geometry. The barrier height between the min. relative to the triangular structure was calcd. to the 2383 cm−1. The nuclear motion problem was solved variationally in Jacobi coordinates for J = 0 and 1. Ten vibrational states of A_1 and nine of B_2 symmetry lie below the linear min. The permutational splitting between the $(000)^+$ and $(000)^-$ states in the linear $^{12}C_2$ ^{11}B is 0.064 cm−1, in $^{12}C^{13}C^{11}B$ this is 0.530 cm−1. Above the energy of the barrier to linearity there are large amplitude vibrations with triangular structure character. In the dense stack of such states vibrational modes of the linear structure are discernible, including their permutational splittings.

(X2A1 спектр

C.A. 2001, 134, N3

C_{70}-x Bx

$x = 2 \div 10$

2001

Chen Zhongfang;
et al.,

стр-ра
стабилн.;
теор. расч

J. Phys. Chem. A 2001,
105 (34), 8105-8110

(см. C_{70}-x [redacted] Nx; II)

$C_{35}B$

2001

135: 185728r **Relationship between the geometries, electronic structures, and dopant atom of $C_{35}B$ and $C_{35}N$.** Ding, Changgeng; Yang, Jinlong; Han, Rongsheng; Wang, Kelin (Open Laboratory of Bond Selective Chemistry and Center for Fundamental Physics, University of Science and Technology of China, Hefei, Peop. Rep. China 230026). *J. Chem. Phys.* 2001, 114(21), 9375–9379 (Eng), American Institute of Physics. The geometrical and electronic structures of substitutionally doped fullerenes $C_{35}B$ and $C_{35}N$ have been studied using the d.–functional theory with the local spin d. approxn. and generalized gradient approxn. methods. The dopant atom has a tendency to substitute the site where the substituted carbon atom has a significant contribution to the frontier orbitals of C_{36}; and the ground state of $C_{35}B$ is the D_{2d} structure whereas $C_{35}N$ prefers the D_{6h} structure. The reactivities towards a nucleophile or electrophile attack are discussed and the binding energies, vertical ionization potentials, electron affinities and chem. hardnesses are predicted for all the clusters.

структура, стабильн.-, теор. расч

☒ (A) $C_{35}N$

C.A. 2001, 135, N13

C_3B_2 | Om 41472 | 2002

Jalbout A.F.*,

ab initio
анализ

J. Mol. Struct. (Theochem) 2002, 593, 49–54.