N6x

Nb_6
(кластеры
переход.
металлов).

1981

Mueller Hans.,
et al.

Z. Phys. Chem., (Leipzig
1981, 262(6), 1073-1088.

теорет.
расчёт

(см. Mo_6 ; III)

Nb_6

1984

24 Б1022. Сравнение распределения электронной плотности интермедиатных гидридных комплексов HNb_6J_{11} и интермедиатного гидрида HNb. Исследование аналогии кластер — объем. Vergleich der Elektronendichteverteilungen der Hydrido-Interstitialkomplexes HNb_6J_{11} und des Interstitialhydrids HNb. Ein Beitrag zur Cluster-bulk-Analogie. Fritsche H.-G., Dübler F., Müller H. «Z. anorg. und allg. Chem.». 1984, **513**, № 6, 46—56 (нем.; рез. англ.)

В рамках метода ССП—Xα—РВ проведены расчеты систем Nb_6, Nb_6H, $Nb_6J_8^{3+}$, Nb_6J_{11} и $HNb_6J_8^{3+}$, —систем, изучение к-рых необходимо для исследования моделей кластерного соединения HNb_6J_{11}, эксперим. обнаруженного и описанного в лит-ре. Для наглядности описания полученных решений построены карты электронной плотности (ρ) и дифференциальной ρ. Карты ρ показывают, что для всех кластеров распределение ρ компактно в областях вблизи ядер, а в областях связи ρ зна-

расчет структуры

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Х. 1984, 19, N24

чительно меньше. В кластере Nb_6J_{11} внутренний октаэдр Nb_6 характеризуется стабильным распределнием ρ, слабо зависящим от влияния окружения J. Атомарный водород даже внутри октаэдра Nb_2 характеризуется почти сферич. симм. распределением ρ. Связывание H—Nb в HNb и HNb_6J_{11} характеризуется переносом электронной плотности с металла на H.

М. Кузьминский

Nb_6

1985

10 Б1033. Электронное строение и механизм связывания водорода, внедренного в ниобий. Elektronenstruktur und Bindungsmechanismus für interstitiellen Wasserstoff in Niob. Opitz Christian, Grünler Bernd, Müller Hans. «Wiss. Z. Friedrich—Schiller—Univ. Jena. Natur—wiss. R.», 1985, 34, № 5—6: Beitr. theor. und phys. Chem., 667—672 (нем.; рез. нем., англ., рус.)

Расширенным методом Хюккеля рассчитано электронное строение октаэдрич. кластеров Nb_6 (I) и Nb_6H (II), моделирующих металлич. Nb и металл с внедренным в междоузлие водородом соотв. Для I и II найдены оптимизированные длины связей между ближайшими атомами Nb, 2,94 и 3,09 A соотв. Рассчитанная энергия связи атома H в II составила 2,2 эВ. Анализ заселенностей MO по Малликену в II показал, что внедрение водорода в ниобий приводит к ослаблению связи Nb—Nb из-за изменения электронной плотности на MO $1a_{1g}$.

И. А. Тополь

расчет структурн.

(71) XI

Х. 1986, 19, N 10

$Nb_x^{+,-}$ | Om. 23891 | 1985

Zheng L.-S., Brucat P.J., et al.,

J. Chem. Phys., 1985, 83, N8, 4273-4274.

$Nb_{\overset{\frown}{x}}$

(От · 23756)

1986

Brucat P.J., Zheng L.-S., et al.,

фотофрагменты

$x = 2 \div 10$

J. Chem. Phys., 1986, 84, N6, 3078-3088.

Nb_n (пп 24396) 1986

$n \geq 2$ Koutecky J., Fantucci P.,

теорет.
расчет
структ.
и энергет.

Chem. Rev., 1986, 86,
N 3, 539–587.

$\mathrm{Nb}_{\overline{x}}$ (om- 26548) 1986

Whetten R.L., Zakin M.R.,
Cox D.M. et al.,

J. Chem. Phys., 1986,
85, N3, ● 1697-98.

Nb_4

1987

107: 223544j Ab initio calculations of the electronic structure and effective magnetic moment of niobium(Nb_4). Wahnstroem, Tomas; Rosen, Arne (Dep. Phys., Chalmers Univ. Technol., S-412 96 Goeteborg, Swed.). *Surf. Sci.* 1987, 189–190, 788–94 (Eng). The electronic structure of Nb_4 clusters is calcd. within the spin-polarized local d. approxn. using the LCAO method. The calcns. were performed for a pyramidal and a planar structure with equal bond lengths extending from the value in the bulk to the value for the dimer. The position and symmetry of the HOMO and LUMO levels depend strongly on the bond length in the pyramidal as well as the planar structure. All clusters are diamagnetic except for the planar structure with a bond length longer than 4.85 au for which a net spin polarization is obtained.

(теор. расчет)

C. A. 1987, 107, N24

Nb_9, Nb_{11},
Nb_{12}

1988

(От. 29647)

109: 61672m **Evidence of structural isomerism in small niobium clusters.** Hamrick, Y.; Taylor, S.; Lemire, G. W.; Fu, Z. W.; Shui, J. C.; Morse, M. D. (Dep. Chem., Univ. Utah, Salt Lake City, UT 84112 USA). *J. Chem. Phys.* 1988, 88(6), 4095–8 (Eng). Evidence is presented of structural isomerism for clusters Nb_9, Nb_{11}, and Nb_{12}. The reactivity of Nb_n with N_2 and D_2 was used in detg. the isomers.

структ. изо-меризм

C. A. 1988, 109, № 8

Nb_4^+

От 31729

1988

156615j **Collision-induced dissociation processes of niobium iron tetraatomic monopositive ions: fission vs. evaporation.** S. K.; Lian, Li; Hales, David A.; Armentrout, P. B. (Dep. m., Univ. California, Berkeley, CA 94720 USA). *J. Chem. Phys.* 89(1), 610–11 (Eng). Cross sections for dissocn. of Nb_4^+ and induced by collisions with Xe were measured using guided -beam mass spectrometry. Sep. cross sections for different ducts were measured. The lowest-energy products are Nb_2^+ + and Fe_3^+ + Fe resp.

поперечн. сече-
ние диссоц.,
масспектр.

C.A. 1988, 109, N 18

Nb_4^+ (DM · 31345) 1988

Loh S.K., Li Lian,
Hales D.A. et al.,

D_0 J. Chem. Phys., 1988, <u>89</u>,
N 5, 3378– 3379.

Nb_6 1988

Opitz C., Mueller H.,
et al.

теор.
расчет
структ.,
стабильн.

J. Less-Common Met.
1988, 144(2), 257-64.

(См. V_6; III)

Nb XI (от 33190) 1989

Litzén U., Reader J.,

спектр,
энергет.
уровни

Phys. Scr., 1989, 39,
73-80.

Nb_3 1989

Loh S.K., Lian Li. et al.

J. Am. Chem. Soc. 1989,

111 (9), 3167–76.

(D_0)

(см. Nb_2; III)

Nb_n^+
$n=4,5,6$

1989

Loh S. K., Lian Li
et al.

(D_0)

J. Am. Chem. Soc. 1989,
111 (9), 3167-76.

(см. Nb_2; $\overline{\underline{III}}$)

Om. 35324

1990

Nb_n^+
(n=2-11)

Hales D.A., Lian L., et al.,

Int. J. Mass Spectrom. and Ion Process. 1990, 102, 26[illegible]9-80/

Collision-Induced Dissociati-

On of Nb_n^+ $(n=2-11)$: Bond Energies and Dissociation Pathways.

Nb_9
Nb_{10}

1990

113: 121185z **Isomers of niobium clusters: direct spectroscopic evidence.** Knickelbein, Mark B.; Yang, Shihe (Chem. Div., Argonne Natl. Lab., Argonne, IL 60439 USA). *J. Chem. Phys.* 1990, 93(2), 1476-7 (Eng). The existence is conformed of Nb cluster isomers displaying different reactivities. Photoionization efficiency spectra are presented of Nb_{12} measured under conditions where: a) the reactive form is the predominant isomer, and b) the reactive form has been eliminated leaving mostly the unreactive form. The ionization potentials are also detd. for Nb_9 and Nb_{10} clusters.

J;

C.A. 1990, 113, N14

$Nb_2 - Nb_{76}$ Оп. 35377 1990

Knickelbein M.B.,
Yang S.,

I;

J. Chem. Phys., 1990,
93, N8, 5760–5767

Photoionization Studies of

niobium clusters: Ionization potentials for Nb_2 – Nb_{76}.

Nb_3 (ОМ 34521) 1990

Sellers Harrell.

струк-
тура
D_0, I,
расчёт

J. Phys. Chem. 1990,
94 (4), 1338–43.

(● см. Nb; I)

Nbп

От. 34521

1990

Sellers H.,

ab initio
расчет

J. Phys. Chem. 1990, <u>94</u>, N4,
1338 - 1343.

Ab Initio and Relativistic
Effective Core Potential

Studies of Niobium – Nitrogen
and Niobium Cluster Systems.

$\mathrm{Nb}_{\overset{\frown}{n}}$ 1990

$n < 20$

Zheng Lansun,
Yang Shihe.
Wuli Huaxue Xuebao
1990, 6(3), 272-6.

Энергии
связи

(см. $\mathrm{Co}_{\overset{\frown}{n}}$; III)

Nb_n^+ Оттиск 35677 1991

Radi P.P., von Helden G.,
Hsu M.T. et al.,

Chem. Phys. Lett. 1991,
179, N 5,6, 531-538.
Observation of small
doubly charged niobium

Nb_n

1993

118: 132598r **Density-functional study of niobium clusters.** Goodwin, Leif; Salahub, Dennis R. (Fac. Arts Sci., Univ. Montreal, Montreal, PQ Can. H3C 3J7). *Phys. Rev. A* 1993, 47(2), R774-R777 (Eng). Local- and nonlocal-GTO-spin-polarized-d.-functional calcns. were done for Nb clusters having two to seven atoms. The most stable geometries, found with geometry optimization, have a high at. coordination. The trends in the exptl. binding energies, bond dissocn. energies, and ionization potentials were well reproduced, with the exception of the pentamer bond dissocn. energy which was too low. The possible causes are discussed. These are the most extensive state-of-the-art calcns. to date for the clusters of a transition metal.

(теор. расч)

C.A. 1993, 118, N6

Nbп 1993

Zhao J.J., Han M., et al.,

(У) Phys. Rev. B: Condens. Matter 1993, 48(20), 15297–300.

(см. Niп; ● III)

Nb_3

ИК в

матрице

1996

J. Chem. Phys, 1996, <u>105</u>, №13
p. 5355

Nb_n^-

1996

$n = 3-8$

126: 163804z Photoelectron spectra and geometric structures of small niobium cluster anions. Kietzmann, Hardy; Morenzin, J.; Bechthold, Paul S.; Gantefoer, Gerd; Eberhardt, Wolfgang; Yang, Dong-Sheng; Hackett, Peter A.; Fournier, Rene; Pang, Tao; et al. (Inst. Festkorperforschung, Forschungszentrum Juelich, 52425 Juelich, Germany). *Phys. Rev. Lett.* **1996**, 77(22), 4528–4531 (Eng), American Physical Society. Photoelectron spectroscopy measurements and d. functional theory calcns. are combined to det. structures of Nb_n^- (n = 3–8) clusters. A detailed comparison between obsd. and calcd. electronic binding energies shows that the clusters have low-symmetry compact 3-dimensional structures and the lowest possible total spin, except for the three- and five-atom clusters which are in triplet states. The authors find evidence for the coexistence of two isomers of Nb_8^- under some exptl. conditions. This approach shows great promise for structural characterization of small clusters.

фотоэл-спектр. структура, энергии связи

С. А. 1997, 126, N12

1996

Nb_3

спектр в Ar матрице
ωe, Ri

126: 52303r Spectroscopy of mass–selected niobium trimers in argon matrixes. Wang, Huaiming; Craig, Robert; Haouari, Hanae; Liu, Yifei; Lombardi, John R.; Lindsay, D. M. (Dep. Chem. Cent. Anal. Structures Interfaces, City Coll. New York, New York, NY 10031 USA). *J. Chem. Phys.* **1996**, 105(13), 5355–5368 (Eng), American Institute of Physics. The absorption (scattering depletion) spectrum and Raman spectra for Nb_3 in an Ar matrix prepd. by the mass selected ion deposition technique were obtained. The absorption spectrum in the visible region shows 3 overlapping transitions, centered at 20,300 cm^{-1} (A), 18,800 cm^{-1} (B), and 17,000 cm^{-1} (C), resp. Resonance Raman spectra obtained with excitation into these bands display two distinct fundamental frequencies at $227.4 \pm 2.9(e')$ and $334.9 \pm 2.8(a'_1)$ cm^{-1} which indicate that the ground state of the Nb_3 mol. has a nearly equilateral triangular geometry (D_{3h}). The f_r (bond stretch) and f_{rr} (stretch–stretch interaction) force consts. for Nb_3 are 1.95 and 0.05 mdyn/Å, resp. The Raman excitation profiles bear a strong resemblance to the triniobium absorption spectrum, but the peaks seem more closely spaced than the absorption spectrum. Both a'_1 and e' vibration are obsd. with the same intensity near the peak A, while the a'_1 vibration dominates the profile at the peak B. Neither displays much intensity near the peak C.

C. A. 1997, 126, N 4

$Nb_{\hat{n}}$ 1996

Zhao Jijun, Chen Xiaoshuang, et al.

(Т) Chem. Phys. Lett.

расчет 1996, <u>254</u> (1, 2), 21-24.

(см. $Co_{\hat{n}}$; <u>III</u>)

Nb$_{\hat{n}}$ 1994

Zhao J. J., Han M., et al.

I, структ., теор. расчёт

Comput. Phys., Proc. Int. Conf., 2nd. 1993 (Pub. 1994), 296–8.

(См. Ni$_{\hat{n}}$; III)

Nb_n^-

$(n=3\div8)$

1998

129: 45512s Structural characterization of niobium−cluster anions from density−functional calculations. Fournier, Rene; Pang, Tao; Chen, Changfeng (Department of Physics, University of Nevada, Las Vegas, NV 89154 USA). *Phys. Rev. A: At., Mol., Opt. Phys.* 1998, 57(5), 3683−3691 (Eng), American Physical Society. We did an extensive search for the lowest−energy isomers of Nb_n^- (n = 3−8) with a local−spin−d. method. We report the calcd. optimum geometries for various cluster isomers, and their vibrational frequencies and electron binding energies. We describe two simple ways to account for final−state effects on electron binding energies, based on Slater's transition state method, which yield results consistent with one another and with expt.

(теорет. расчет)

CA-1998, 129, N4

Nb_n

1998

n = 8, 9, 10

130: 100942e Structural, electronic, and vibrational properties of neutral and charged Nb_n (n = 8, 9, 10) clusters. Gronbeck, Henrik; Rosen, Arne; Andreoni, Wanda (Department of Physics, Goteborg University and Chalmers University of Technology, S−41296 Goteborg, Swed.). *Phys. Rev. A: At., Mol., Opt. Phys.* 1998, 58(6), 4630−4636 (Eng), American Physical Society. We present a theor. study of the structural, vibrational, and electronic properties of small niobium clusters (Nb_8, Nb_9, and Nb_{10}) using d.−functional theory with local as well as gradient−cor. exchange correlation d. functionals. For Nb_8 and Nb_9, several low−energy structures were obtained, whereas for Nb_{10} there seems to be only one isomer that is energetically preferred. Vibrational spectra are in the range 100−300 cm^{-1} and are sensitive to the structure. Electronic properties are investigated by means of the densities of states, which depend strongly on the geometry. The theor. results for the ionization potentials and vertical detachment energies are in good agreement with available exptl. data.

Di, структ. парам., теор. расчет

C. A. 1999, 130, N 8

Nb_3
Nb_4

От. 40103

1999

Joseph E. <u>Fowler</u>, América Garcia et al.,

Phys. Rev. 1999, <u>A60</u>, N4, 3058– 3070

Many low-lying isomers of the cationic and neutral niobium trimer and tetramer.

Nb_n (OM 39970) 1999

$n=22$

Masaki Sakurai et al.,

J. Chem. Phys., 1999, 111, N1, 235 - - -

Magic numbers in transition metal (Fe, Ti, Zr, Nb and Ta) clusters

1999

F: Nbn+
P: 3

132:171728 FT-ICR study on hydrogenation of niobium cluster cations Nbn+ (n=2-15) in seeded supersonic jet and multiple-collision-induced dissocia of NbnHm+ hydrides. Vakhtin, Andrei B.; Sugawara, Ko-ichi

National Institute for Advanced Interdisciplinary Research Tsukuba 305-8562, Japan

J. Chem. Phys., 111(24), 10859-10865 (English) 1999 Hydrogenation of niobium cluster cations Nbn+ (n=2-15) in a seeded supersonic jet of H2/He and multiple-collision-induced dissocn. (MCID) of resulting NbnHm+ hydrides have been studied using a Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometer. The nascent NbnHm+ hydri trapped in the FT-ICR cell have broad m distributions with no apparent

C. A. 2000, 132

prevalence of odd or even m. A pulse of argon applied to the trapped clusters causes a dramatic squeezing of the initial m distribution (throu the collision-induced removal of weakly bound H2 mols.), favoring several particular hydrides for each cluster size n, e.g., Nb7H8+, Nb7H11+, and Nb7H12+ for n=7. The max. m values of these stable hydrides are close to stoichiometric compn. of NbH2 for the clusters with n<13, and approach th of NbH at larger n. The hydrides obsd. in our expts. are different from products of the Nbn++H2 reactions performed in the FT-ICR cell at room te which show only even and strongly n-dependent m values. The MCID of the NbnHm+ clusters occurs through the sequential desorption of H2 mols. yiel NbnH+ and Nbn+ as final dissocn. products for odd and even m, resp. Base the expts. on the MCID of Nb12H18+, an explanation is suggested for diffe reactivities of the Nb12+ clusters toward H2 in the ICR and fast-flow-rea expts.

F: Nb8
P: 3

2000

132:129556 A vibrationally resolved negative ion photoelectron spectrum o Nb8. Marcy, Timothy P.; Leopold, Doreen G. Department of Chemistry, University of Minnesota Minneapolis, MN 55455, USA Int. J. Mass Spectrom., 195/196, 653-666 (English) 2000 The 488 nm neg. ion photoelectron spectrum of Nb8, obtained at an instrumental resoln. of ~5 meV, displays a clear vibrational progression mode with a frequency of 180 .+-. 15 cm-1 in neutral Nb8 and 165 .+-. 20 in Nb8-. The normal mode displacement of 0.4 .+-. 0.1 u1/2 A indicates a very small geometry change upon electron detachment. The electron affini of Nb8 is 1.513 .+-. 0.008 eV. These results are discussed in light of previous neg. ion photoelectron spectroscopic and d. functional studies o Nb8 and Nb8.

C.A. 2000, 132

Nb_n^+ (Dm. 40860) 2001

(n = 3-5) Majumdar D.,
геометрия, Balasubramanian K.,
длина связи,
энерг. диссо-
циации J. Chem. Phys., 2001,
115, N2, 885–898
Theoretical study of the

electronic states of small cationic niobium clusters, Nb_n^+ $(n=3-5)$