Coñ

CO_4 от. 23876 1985

Holland G.F., Ellis D.E.,
et al.,

теорет. J. Chem. Phys., 1985,
расчет. 83, N7, 3507-3513.

Cr_6 От. 24842 1986

Datta N.C., Sen B.,

теорет. J. Chem. Soc. Faraday
расчёт. Trans., 1986, Pt. 2,
82, N7, 977-990.

Co_6

(от. 25306)

1986

Evans D. G.,

Inorg. Chem., 1986, 25, N 25, 4602–4604.

Роль d-электрон. в обр. связи.

Co_3^+

От. 23334

1986

Jacobson D. B., Freiser B. S.,

$\Delta_f H$, D_0,
I,

J. Amer. Chem. Soc.,
1986, <u>108</u>, N 1, 27-30.

Соп
n=2

(ОМ 24396)

1986

Koutecky J., Fantucci P.,

теорет.
расчет
структ.
и энергет.

Chem. Rev., 1986, 86,
N3, 539–587.

Co_n

1986

$n=3,4,5$

(теор. расчёт)

105: 197413e **Analysis of the reactivity of small cobalt clusters.** Rosen, A.; Rantala, T. T. (Dep. Phys., Chalmers Univ. Technol., Swed.). *Z. Phys. D: At., Mol. Clusters* 1986, 3(2-3), 205-9 (Eng). The electronic structure was calcd. of small Co clusters within the local spin d. approxn. by using the LCAO method. The calcns. were made for simple geometries with the optimized no. of interat. bonds, both for the bond length of Co_2 and the bulk metal. The Fermi energy is smaller for Co_n clusters with $n = 3, 4, 5$ and $n > 10$ than for other clusters. The variation of the Fermi energy with the cluster size correlates with the obsd. H_2 tendency for chemisorption, as found for Co clusters in a supersonic beam. Magnetic moments are somewhat smaller for these active clusters. The lowest unoccupied levels of majority spin appear close to the highest occupied levels of minority spin which is not the case for the inert clusters.

C.A. 1986, 105, N22

Кластеры Co 1986

Yamanouchi Kaoru.

Nippon Butsuri Gakkai-Shi 1986, 41 (11), 912-15.

(см. ● C_{60} ; III)

Co_6 1988

Opitz C., Mueller H., et al.

теор. расчет структ., стабильн.

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

(См. $V_{\overline{6}}$; $\overline{\underline{III}}$)

Co_n
$n<20$

1990

Энергии
связи

113: 65654n Binding energies of transition metal clusters measured with photodissociation. Zheng, Lansun; Yang, Shihe (Postdoctoral Stn. Phys. Chem., Xiamen Univ., Xiamen, Peop. Rep. China). *Wuli Huaxue Xuebao* 1990, 6(3), 272-6 (Ch). The binding energies of transition metal (Co, Nb, Fe, Ni, V, Ta, Pd) clusters have been measured as functions of cluster size and compn. with cluster size up to 20 atoms. The photodissocn. measurement showed that the binding energy is roughly const. with different cluster sizes but differs with different cluster compns. For almost all clusters measured, the primary one-photon fragmentation pathway is always found to be loss of a single metal from the cluster.

(76) ☒ Nb_n, Fe_n, Ni_n, V_n, Ta_n, Pd_n

C.A. 1990, 113, N 8

Co_n^+

1994

$n = 2 \div 18$

120: 174563x **Collision-induced dissociation of Co_n^+ (n = 2–18) with Xe: bond energies of cationic and neutral cobalt clusters, dissociation pathways, and structures.** Hales, David A.; Su, C. X.; Li, Lian; Armentrout, P. B. (Dep. Chem., Univ. Utah, Salt Lake City, UT 84112 USA). *J. Chem. Phys.* 1994, 100(2), 1049–57 (Eng). The kinetic energy dependence of collision-induced dissocn. (CID) of Co_n^+ (n = 2–18) with xenon is studied by using a guided ion beam mass spectrometer. Examn. of the general dissocn. behavior over a broad collision energy range shows that cobalt cluster cations dissoc. exclusively by loss of single atoms (cluster evapn.), with no evidence found for elimination of mol. cluster fragments. Bond dissocn. energies for cobalt cluster cations, Co_n^+ (n = 2–18), are detd. from measurements of the CID thresholds. Bond energies for neutral cobalt clusters, Co_n (n = 4–18), are derived by combining these cationic bond energies with ionization energies for Co_n from the literature. The dependence of binding energy on cluster size is similar to that obsd. for iron clusters, and inspires some speculation regarding cluster ion structures.

(энергии диссоциации)

C. A. 1994, 120, N 14

Co_3^+ (оп · 37606) 1994

Russon L.M., Heidecke S.A., et al.,

D_0^0 J. Chem. Phys. 1994, 100, N7, 4747-4755

Photodissociation measurements of bond dissociation energies: Ti_2^+, V_2^+, Co_2^+, and Co_3^+.

Соп 1994

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

J, структ., Comput. Phys.
теор, расчёт Proc. Int. Conf.,
2nd 1993 (Pub. 1994),
296-8. (см. Ni п, III)

Co_n

n=3-16

структура
кластеров

Ho J., Parks E.K., Zhu L., | 1995
Riley S.J. ~~[illegible]~~

Chem. Phys. 1995, 201, № 1, p 245-261

Reaction of small cobalt clusters with N_2: implications for cluster structure

Co_n

1995

$n=3-13$

124: 242739u Theoretical study on electronic structure of cobalt clusters. Li, Jun; Tong, Xiao-min; Li, Jia-ming (Inst. Physics, Academia Sinica, Beijing, Peop. Rep. China 100080). *Wuli Xuebao* 1995, 44(11), 1727–33 (Ch). Based on multiple-scattering self-consistent-field method, the authors have investigated the electron structure of Co_n cluster (n = 3–13). Comparing the calcd. ionization potentials for different geometries and electron configuration with the exptl. values, the authors can study the appropriate electron configuration and geometric structure of Co_n. From the occupation of local 3d valence electron in configuration, it was found, that the av. at. magnetic moment of Co clusters decreases as the no. of atoms increases. From the geometry of cobalt clusters, the possibilities of various ways of formation of Co_n cluster were also surmised.

теор. рас-
чет Э,
структ.
стабильн.

C. A. 1996, 124, N 18

Co_n^-

1995

$n=3,4,6$

123: 41132w Spin-polarized electronic structure of cobalt cluster anions studied by photoelectron spectroscopy. Yoshida, Hiroyuki; Terasaki, Akira; Kobayashi, Katsuyoshi; Tsukada, Masaru; Kondow, Tamotsu (Sch. Sci., Univ. Tokyo, Tokyo, Japan 113). *J. Chem. Phys.* 1995,. 102(15), 5960–5 (Eng). The photoelectron spectra of Co_n^- ($3 \leq n \leq 70$) were measured at the photon energy of 4.025 eV by use of a XeCl excimer laser. For Co_n^- with n=3, 4, and 6, the geometric and electronic structures were obtained from the spectra in comparison with the calcd. spectra by the spin-polarized DV–Xα method. The spectra obsd. are reproduced reasonably well by the calcn. with postulating the most probable geometrical structures. The 3d band with the majority spin is sepd. by 1.0–2.8 eV from that with the minority spin; the former is completely filled while the latter is partly filled and extends above Fermi level. The magnetic moments and the av. exchange energies of these cluster anions were estd. For Co_n^- with $n \geq 7$, the obsd. electron affinity depends linearly on the reciprocal of the cluster radius and approach the work function of a cobalt metal, as n increases. Below n=6, the electron affinity deviates from the linear dependence. This finding indicates that a size-dependent transition in the electronic structure occurs at $n \simeq 7$. The spherical conducting drop model suggests the presence of mobile electrons in Co_n^- with $n \geq 7$.

геометр. и
эл. стр-ра,
фотоэл.
спектр, Ae

C.A. 1995, 123, N4

Co(кластеры) 1996

Gou Q; et al.,

ИК, УФ спектры

Yuanzi Yu Fenzi Wuli
Xuebao 1996, <u>13</u>(2), 135-140

(см. Fe(кластеры); <u>III</u>)

Con

1996

Wang, Lai-Sheng;
Wu, Hongbin,

фотоэл.
спектр,
Ae

Proc. Sci. Technol.
At. Eng. Mater. 1995,
(Pub. 1996), 245-250.

(см. Tin; III)

Co_n 1996

(Э)
расчет

125: 19496n An analytic relationship between size and ionization potential of transition metal clusters. Zhao, Jijun; Chen, Xiaoshuang; Wang, Guanghou (Department of Physics and National Laboratory of Solid State Microstructures, Nanjing University, Nanjing, Peop. Rep. China 210093). *Chem. Phys. Lett.* **1996**, 254(1,2), 21–24 (Eng). Based on the effective-coordination-no. (ECN) model, we have constructed an analytic expression for the size dependence of ionization potentials (IPs) for transition metal clusters. An approx. formula of the surface ratio as a function of cluster size for the close-packed structures has been fitted from the icosahedral-like structures. The IPs of Co_n, Y_n, Nb_n, and Ni_n are calcd. and compared with expts. as well as with predictions of the conducting-spherical-droplet (CSD) model. It is found that the present approach agrees with expt. much better than the CSD model.

③ ☒ Y_n, Nb_n, ● Ni_n.

C. A. 1996, 125, N2

Co_n, Y_n, Nb_n,
N_n

IP

Zhao J., Chen X., Wang G. 1996
Chem. Phys. Lett., 1996, 254,
N1/2, p.21-24.
Эмпирическ. соотн. между
размером и потенц. ионизации
кластеров перех. металлов.

$Co_{\overline{n}}$
$n \leqq 5$

1997

Castro M., Jamorski Ch.,
et al.

структ.,
энергия
связи,
теор.
расчёт.

Chem. Phys. Lett.
1997, $\underline{271}$ (1, 2, 3), 133–
142.

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

Co_n^- Оп. 38902 1997

(n=2-8)

Hong-Jun Fan, Chen-Wan Liu et al.,

геометр, стр-ра

Chem. Phys. Lett., 1997, <u>273</u>, 353-59.

Соп | От. 39062 | 1997

n≤5 Miguel Castro,
Christine Jamorski et al.;

стр-ра,
св-ва Chem. Phys. Lett.
1997, 271, 133–
142.

1999

F: Con
P: 3
131:303468 Electronic states of transition metal clusters. Fujima, Nobuhisa; Yamaguchi, Tsuyoshi Faculty of Engineering, Shizuoka University Shizuoka 432-8561, Japan Mesosc. Mater. Clusters, 249-258. Edited by: Arai, Toshihiro. Springer: Berlin, Germany. (English) 1999. A review with 19 refs. We calcd. the electronic states of the 3d transition metal clusters by using the local d.

functional method, and clarified their extraordinary characteristics, which are mainly caused by the chem. bonding 3d electrons in the clusters. We first clarify the structure of chem. bonding in Mn clusters and its size dependence, and discuss the origin of the magic no. which has been obsd. in the cationic clusters. Second, we calc. the electronic states of binary Co-V clusters and discuss the extraordinary stability to the hydrogen-adsorption of Co1 cluster.

Co_n

$n \leq 5$

2001

потенц.
ф-ии

135: 294221r **Model potential nonlocal density functional calculations of small cobalt clusters, Co_n, $n \leq 5$.** Pereiro, M.; Man'kovsky, S.; Baldomir, D.; Iglesias, M.; Mlynarski, P.; Valladares, M.; Suarez, D.; Castro, M.; Arias, J. E. (Facultad de Fisica, Departamento de Fisica Aplicada, Universidade de Santiago de Compostela, Santiago de Compostela, Spain). *Comput. Mater. Sci.* 2001, 22(1÷2), 118–122 (Eng), Elsevier Science B.V. Small cobalt clusters Co_n ($2 \leq n \leq 5$) are studied by using self–consistent nonlocal generalized gradient approxn. (GGA) d. functional methods. An emphasis is made on a proper treatment of exchange and correlation effects. The enhancement of the magnetic moments as well as the bonding properties of these clusters are discussed in terms of the cluster size and symmetry. We compare some results from deMon–KS (D) module release 3.2 and the computational scheme of Sambe–Felton and Dunlap (SFD).

С. А. 2001, 135, N20

F: Co2
P: 3

1999

132:127966 Global potential energy surfaces for the CO2 and CS2 molecules Zuniga, J.; Bastida, A.; Alacid, M.; Requena, A. Departamento de Quimica Fisica, Universidad de Murcia Murcia 30100, Spain Chem. Phys. Lett., 313(3,4), 670-678 (English) 1999 Global potential energy surfaces for the ground electronic states of the CO2 and CS2 mols. are detd. We use the many-body single-value surfaces previously constructed by Murrell and Guo (J. Chem. Soc. Faraday Trans. 2 83, 683) and refine their parameters by the nonlinear least-squares metho order to reproduce the obsd. vibrational frequencies of each mol. The fi made by computing variationally the vibrational frequencies using sets of optimal generalized internal coordinates. The quality of the potentials checked by computing vibrational frequencies of isotopic species and high excited vibrational energies not included in the fits.

C.A. 2000, 132

Co_2

2001

Gutsev G.L., Khanna S.N., et al.,

Chem. Phys. Lett., 2001, <u>345</u>, 481-489

Magnetic excitations of Co_2 dimer