Co N2

CoN_2 1973

16 Б237. Поперечно-связанный азот в молекуле CoN_2, изолированной в матрице. Ozin G. A., Voet Vander A. «Sideways» bonded dinitrogen in matrix isolated cobalt dinitrogen, CoN_2. «Can. J. Chem.», 1973, 51, № 4, 637—640 (англ., рез. франц.)

Измерены спектры ИК-поглощения образца, полученного при одновременной соконденсации атомарного Co и смеси Ar/N_2 при M/A 250, 2000 на охлажденную подложку. В работе использовали изотопич. $N^{14}N^{15}$ и N_2^{15}. В ИК-спектре $N_2^{14}+Co$ обнаружена полоса поглощения 2101 $см^{-1}$. При использовании смеси $N_2^{14}+N_2^{15}$ в спектре появляется вторая полоса 2029 $см^{-1}$, а при использовании изотопич. смеси $N_2^{14}+N_2^{15}+N^{14}N^{15}$ дополнительно обнаружена третья полоса 2066,5 $см^{-1}$. Эти данные указывают на образование комплекса CoN_2 со связью Co...N_2, перпендикулярной тройной связи N_2. В аналогичном эксперименте с атомарным Ni, частоты $\nu_{NiN^{14}N}$ и $\nu_{NiN^{15}N}$ не эквивалентны, что указывает на линейное строение комплекса Ni···N≡N. Г. Кузьянц

Vi

Х. 1973 N16

CoN_2

1973

(Vi)

130144w Sideways bonded dinitrogen in matrix isolated dinitrogen cobalt. Ozin, G. A.; Vander Voet, A. (Erindale Coll., Univ. Toronto, Toronto, Ont.). *Can. J. Chem.* 1973, 51(4), 637–40 (Eng). The ir spectra are reported for matrix isolated $Co^{14}N_2$, $Co^{14}N^{15}N$ and $Co^{15}N_2$ formed in the co-condensation reaction of at. Co with dil N-Ar matrixes at 10°K. The data provided the 1st unambiguous spectroscopic evidence for a dinitrogen mol. bonded in a sideways fashion to a transition metal atom.

C. A. 1973. 78 N 20

CoN_2

1973

CoN_2^+ ; CoN_2^-

Vinogradova, S.N. Borod'ko, Yu.G.
Zh.Fiz.Khim. 1973, 47(4), 789-93.

Эл. структ. расчет

(см. TiN_2 ; III)

Со № 2 1975

Захаров И. И.
Авдеев В. И.

Электр.
строен.

„Докл. АН. СССР"
1975, 225, N 1, 126-129

(см № 1 № 2: III)

1978

CoN_2

Veillard H.

Nouv J. Chim. 1978, 2(3), 215-24

кв. мех. расчет

(см NiN_2^{III})

Co – N_2 1984

Гагарин С.Г., Шестерин Ю.А., и др.

расчёт ж. структур. земли, геомагн., 1984, 25, N1, 8–12. структ.

(сл. Alp – N_2; III)

CoN_2^+

1992

17 Б1055. Теоретическое изучение Cr^+ и Co^+, связанных с H_2 и N_2. Theoretical study of Cr^+ and Co^+ bound to H_2 and N_2 / Bauschlicher Charies W., (Jr.), Partridge Harry, Langhoff Stephen R. // J. Phys. Chem.— 1992.— 96, № 6.— С. 2475—2479.— Англ.

Модифицированным методом функционала связанных пар рассчитаны комплексы $Co(H_2)_n^+$ ($n=1$—3), CrH_2^+, CoN_2^+ и CrN_2^+. Использован базис атомных натуральных орбиталей, включающий наборы сгруппированных гауссовых ф-ций (20*s*15*p*10*d*6*f*)/[7*s*6*p*4*d*2*f*] на Cr и Co, (8*s*6*p*4*d*)/[4*s*2*p*1*d*] на H и (14*s*9*p*6*d*4*f*)/[7*s*6*p*4*d*1*f*] на N. Полученные энергии связи ионов Cr^+ и Co^+ с H_2 и N_2 хорошо согласуются с имеющимися эксперим. данными. Показано, что Co^+ не внедряется в связь H_2. Связь H_2 и N_2 с Co^+ существенно сильнее, чем с Cr^+. Несмотря на близость поляризуемости N_2 и Ar, связь в CrN_2^+ вдвое сильнее, чем в $CrAr^+$, что связано с вкладом вз-вия заряд — квадруполь. А. А. Сафонов

М.Л.

(43)

Х. 1992, N 17

CoN_2^+

1996

(Co–N связь, мол. расч.)

125: 96540z **On the nature of the cobalt–nitrogen bond in the CoN_2^+ complex. A theoretical study.** Adamo, Carlo; Telesca, Rosanna; Lelj, Francesco (Dipartimento di Chimica, Universita della Basilicata, via N. Sauro 85, I–85100 Potenza, Italy). *Chem. Phys. Lett.* **1996**, 254(5,6), 314–320 (Eng). The interaction between Co^+ and a single N_2 mol. was studied by d. functional methods. The two lowest electronic states of the complex and two different coordination modes, namely end–on and side–on, were investigated. The results are in fair agreement with the exptl. ests., esp. concerning excitation and bonding energies. Unlike the suggestions arising from rotational spectra, the most stable electronic state has a linear arrangement. A natural bond orbital anal. underlines the importance of the charge transfer mechanism in the metal–nitrogen bond, strongly reducing the role played by electrostatic interactions.

C.A. 1996, 125, N 8

CoN_2^+

Adamo C., Telesko R., 1996.
Lelj F.,

Теор.
ден. и возб. сост.
наиболее реб.
линейная
структ.

Chem. Phys. Lett., 1996, 254,
N5/6, p. 314

Природа Co–N связи в CoN_2^+

1996

F: CoN2+
P: 3
16Б152. О природе связи кобальт-азот в комплексе CoN[2]{+}. Теоретическое изучение [методом функционала плотности]. On the nature of the cobalt-nitrogen bond in the CoN[2]{+} complex. A theoretical

1996

study / Adamo Carlo, Telesca Rosanna, Lelj Francesco [Chemical Physics Letters] // Chem. Phys. Lett. - 1996. - 254, N 5 - 6. - С. 314-320. - Англ.

РЖХ 1997

$Co(N_2)^+$

1996

124: 242847c **Ground State of $Co(N_2)^+$.** Heinemann, Christoph; Schwarz, Joseph; Schwarz, Helmut (Institut fuer Organische Chemie, Technischen Universitaet Berlin, D-10623 Berlin, Germany). *J. Phys. Chem.* **1996**, 100(15), 6088-92 (Eng). A combined exptl. (ion/mol. reactions in a Fourier transform ion cyclotron resonance mass spectrometer) and theor. (correlated ab initio calcns. using coupled-cluster and multireference CI wave functions) approach characterizes the electronic ground state of the cationic cobalt-dinitrogen complex $Co(N_2)^+$ as a linear species ($^3\Delta$) with a 0 K binding energy of 23.0 ± 1.7 kcal/mol. Recent speculation [J. Phys. Chem. 1995, 99, 1068] on a T-shaped ground state geometry of $Co(N_2)^+$ is repudiated on the basis of the measured binding energy as well as the calcd. potential energy surface for rotation of N_2 around its center of mass in the electrostatic potential of the Co^+ cation.

масс спектр, ионно мол. структ., энергия связи

С. А. 1996, 124, N 18

$Co(N_2)^+$

1996

21 Б133. **Основное состояние $Co(N_2)^+$.** Ground state of $Co(N_2)^+$ / Heinemann Christoph, Schwarz Joseph, Schwarz Helmut // J. Phys. Chem. .— 1996 .— **100** , № 15 .— С. 6088—6092 .— Англ. . Место хранения ГПНТБ

X. 1996, N 21

$Co(N_2)_4^-$ 1982

эл. структ., уровни энергии, теорет. расчет.

Wang Zhizhong, Shen Ezzhong, et al.

Fenzi Kexue Xuebao

1982, 2 (2), 47-56.

(см. $Ni(CO)_4$; I)

NH_4CoF_3 1987

Navarro R., Palacios E., et al.

Cp, Tr; Motions Solids. Proc. IIL-IFF Workshop, Grenoble, Sept. 24-26, 1986. Berlin e.a., 1987, 33-37.

(сем. NH_4ZnF_3; I)

NH_4CoF_3 (ат. 26698) "a" 1987

Smith D.

номера. J. Chem. Phys., 1987,

р-ции 86, N 7, 4055-4065.

$Co(CN)_6^{3-}$ (DM. 26698) 1987

Jameson C. J.,

колебат. анализ, средние амплитуды колебан.

J. Amer. Chem. Soc., 1987, 109, N 9, 2586–88.

$Co(CO)_3NO$ 1987

Mills I. M.

Mol. Phys. 1987, 61

Di; (3), 711-24.

(cf. $Ni(CO)_4$; III)

$Co(NH_3)_4^{2+}$ (ОМ-24201) 1986

Acevedo R., Diaz G.

(Td) Spectrosc. Lett., 1986,

нормальн. 19, N 6, 653-668.

координат.

аналу,

силовые

постоян.

$Co(NH_3)_4^{2+}$

1983

/ 102: 35631h **Infrared spectrum and normal-coordinate analysis for tetraamminecobalt diperrhenate with nitrogen-14/nitrogen-15 and hydrogen/deuterium isotopic substitution.** Tellez, Claudio (Univ. Estad. Londrina, Parana, Brazil). *Acta Sud Am. Quim.* **1983**, 3(3-4), 139-44 (Port). The normal-coordinate anal. of the vibrational modes of $Co(NH_3)_4^{2+}$ was detd. from the IR spectra of the normal and isotopically substituted forms that are complexed with perrhenate. The force const f_{Co-N} = 1.59 mdyne/Å was compared to the force consts. for Zn-N and Cd-N of other authors.

H. Pomerance

сим. лосп, ик спектр

C. A. 1985, 102, N 4.

$Co \dots NH_3$ 1981

Itoh H., et al.

Z. Naturforch., 1981,
кв. хим. расчёт. A36, N4, 347-353.
эл. строение

(сем. $Cr \dots H_2O$, III)

$[Co(NH_3)_6]^{2+}$ | оттиск 10360 | 1980

Kai M., et al.

кв. мех. расчет, эн. связи

Int. J. Quant. Chem. 1980, <u>18</u>, 403–408

$Co(NO_2)_6^{-4}$ ОМ XVI – 6168 1980

Clack D. W., et al

Кв. мех. расчет

Solid State Commun., 1980, 34, N6, 395–99.

(см. $Cu(NO_2)_6^{-4}$) III

1980

$Co(NO_3)_3$

расчет электр. строения

Garner C.D., et al.,

J. Amer. Chem. Soc.,
1980, 102, N 13, 4325-4333

(см. $Ti(NO_3)_4$; III)

$CoNH_3^+$

$Co(NH_3)^{2+}$

1991

Langhoff S.R.,
Bauschlicher Ch.W. Jr.,
et al.

расчёт D_0,
структуры

J. Phys. Chem. 1991,
95 (26), 10677-81.

(сел. $ScNH_3^+$; III)

Co_2N_2 | Ом. 36153 | 1991

Siegbahn E. M.

Электрон. струк-тура

J. Chem. Phys. 1991, 95, N1, 364-372.

Side-on binding of the nitrogen molecule to first-row transition ●-metal dimers.

NO+Co (OM-38626) 1996

Gary L. Ruschel, Thomas M.
Nemetz et al.,
J. Mol. Struct., 1996,
384, N2-3, 101-114.
Matrix isolation and density
functional studies of
novel transition metal

complexes: NO + Fe, Co, Ni, Cu, and Zn in argon matrices.

CoNO (Om 39121) 1997

кобальт частоты — Julie L. C. Thomas, Charles W. Bauschlicher, Jr., et al.,

$CoNO^+$ — J. Phys. Chem. 1997, A101, 8530–39.

термич. свойства основн. сост. — Binding of Nitric Oxide to First-Transition-Row

$CoNH_3^+$ (Om 39122) 1997 [illegible]

$CoNH_2^+$

и др. M. Hendrickx, M. Ceulemans

et al.,

Журн. J. Phys. Chem. 1997, #101,

8540 – 8546

Ab Initio Study of the Activation of Ammonia by Co^+

128: 249962c **Reactions of Laser-Ablated Co and Ni Atoms with Nitrogen Atoms and Molecules. Infrared Spectra and DFT Calculations of Metal Nitride Molecular Species and Complexes.** Andrews, Lester; Citra, Angelo; Chertihin, George V.; Bare, William D.; Neurock, Matthew (Departments of Chemistry and Chemical Engineering, University of Virginia, Charlottesville, VA 22901 USA). *J. Phys. Chem. A* **1998**, 102(15), 2561–2571 (Eng), American Chemical Society. Laser-ablated Co and Ni atoms, co-deposited with pure N at 10 K, gave a strong new 795.3 cm^{-1} band with Co and a 838.8, 836.1 cm^{-1} isotopic doublet (2.5/1.0) with Ni, which exhibited 14/15 isotopic ratios appropriate for the diat. CoN and NiN mols. In solid Ar, CoN absorbs at 826.5 cm^{-1} and gives way on annealing to bands at 795.8 and 792.0 cm^{-1}, which are due to $(NN)_xCoN$ complexes. D. functional theory (DFT) calcns. predict quintet and quartet ground states for CoN and NiN, resp., and frequencies in reasonable agreement with the obsd. values. Evidence is presented for the dimetal dinitrides, $(CoN)_2$ and $(NiN)_2$, with rhombus structures and metal–metal bonding across the ring. DFT-based calcns. and revised assignments are presented for Ni–NN stretching modes in the dinitrogen complexes.

$Co^+ - N_2O$

1998

Элементарные осн. эл.-сост. d^2 + спектр. свойства, теор. расчет

129: 8783k **A quantum chemical ab initio study of the interaction between Co^+ and Ni^+ ions with CO_2 and N_2O.** Burda, Jaroslav V. (J. Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Rep. 182 23). *Chem. Phys.* **1998**, 230(1), 13–22 (Eng), Elsevier Science B.V.. Coordinations of monocations of Co^+ and Ni^+ to CO_2 and N_2O were calcd. using the CCSD(T) method and 6–31G(3d, f) basis sets for C, N, and O atoms, and Stuttgart's pseudopotentials for metal cations. The strongest interaction (125.1 kJ/mol) was found for Co^+–N_2O when the ion is bound to the nitrogen end of the oxide, establishing the linear complex in the triplet state ($^3\Delta$). The coordination of Ni^+ to the same N–end of N_2O has a very similar stabilization. The ground state symmetry of the linear Ni^+–N_2O complex

(+1)

$Ni^+ - N_2O$

С. А. 1998, 129, N 1

is $^2\Sigma^+$. The interaction energy of the metal cations with the oxygen end of N_2O is more than 40 kJ/mol weaker than with the nitrogen end of the mol. The linear structure of the ions bound to the oxygen of carbon dioxide are more stable than similar structures of metal–ion oxygen–ended N_2O. Stabilization energies of $Co^+–CO_2$ and $Co^+–N_2O$ in quintet states are more than 25 kJ/mol smaller than the corresponding energies in triplets, and a similar relationship holds in the case of $Ni^+–CO_2$ and $Ni^+–N_2O$.

$Co(H_2O)NO^+$ | Dm. 40401 | 1999

Huiping Chen, Denley B. Jacobson et al.,

cmp-pc

J. Phys. Chem. A1999, 103, 10884-10892

Structure and Studies of CoH^+ Reactivity NO^+ in the Gas Phase

F: Co(NO)x

2000

P: 3

132:285593 Reactions of Laser-Ablated Fe, Co, and Ni with NO: Infrared Spectra and Density Functional Calculations of MNO+ and M(NO)x (M = Fe, Co, x = 1-3; M = Ni, x = 1, 2), and M(NO)x- (M = Co, Ni; x = 1, 2). Zhou, Mingfei; Andrews, Lester Department of Chemistry, University of Virginia Charlottesville, VA 22904-4319, USA

J Phys Chem A, 104(17), 3915-3925

(English) 2000

C.A. 2000

Laser-ablated Fe, Co, and Ni atoms, cations, and electrons were reacted with NO mols. during condensation in excess Ne and Ar. The end-on bonded Fe(NO)1-3, Co(NO)1-3, and Ni(NO)1-2 nitrosyls and side-bonded Fe-(.eta.2-NO), Co-(.eta.2-NO), and Ni-(.eta.2-NO) species are formed during sample deposition or on annealing. The FeNO+, CoNO+, and NiNO+ mononitrosyl cations are also produced via metal cation reactions with NO. Evidence is also presented for the Ni(NO)1,2- and Co(NO)1,2- anions. The product absorptions are identified by isotopic substitution (15N16O, 15N18O, and mixts.), electron trapping with added CCl4, and d. functional calcns. of isotopic frequencies. This work provides the 1st vibrational spectroscopic characterization of Fe, Co, and Ni nitrosyl cations and anions.

F: CoNO+
P: 3

DM.40601 2000

132:285593 Reactions of Laser-Ablated Fe, Co, and Ni with NO: Infrared Spectra and Density Functional Calculations of MNO+ and M(NO)x (M = Fe, Co, x = 1-3; M = Ni, x = 1, 2), and M(NO)x- (M = Co, Ni; x = 1, 2).

Zhou, Mingfei; Andrews, Lester Department of Chemistry, University of Virginia Charlottesville, VA 22904-4319, USA J. Phys. Chem. A, 104(17), 3915-3925 (English) 2000

Laser-ablated Fe, Co, and Ni atoms, cations, and electrons were reacted with NO mols. during condensation in excess Ne and Ar. The end-on bonded Fe(NO)1-3, Co(NO)1-3, and Ni(NO)1-2 nitrosyls and side-bonded Fe-(.eta.2-NO), Co-(.eta.2-NO), and Ni-(.eta.2-NO) species are formed during sample deposition or on annealing. The FeNO+, CoNO+, and NiNO+ mononitrosyl cations are also produced via metal cation reactions with NO.

C.A. 2000

Evidence is also presented for the Ni(NO)1,2- and Co(NO)1,2- anions. The product absorptions are identified by isotopic substitution (15N16O, 15N18O, and mixts.), electron trapping with added CCl4, and d. functional calcns. of isotopic frequencies. This work provides the 1st vibrational spectroscopic characterization of Fe, Co, and Ni nitrosyl cations and anions.

CoN

2003

Takayoshi Yamaki et al.,

электрон. стр-ра, теорет. Chem. Phys. Lett., 2003, 376, 487-492.

A theoretical study on lower electronic states of CoN