Fe02

90716.4037
Ch

~~SeO, SeO2, FeO,~~
FeO_2, Fe_2O_3 (Do)

1968

K p. N 90716.4021 XII–151

Piacente Vincenzo, Malaspina Leopoldo, De Maria Giovanni. Proprietà termodinamiche dei sistemi binari appartenenti all' intergruppo VI_B del [illegible] sistema periodico. "Corsi e semin. chim. CNR e FG", 1968, N 13, 53–55 (итал.)

ОРИГИН.

1077 1078 1090 1103 ВИНИТИ

FeO_2 1975

Братушко Ю.В.

расчет геометр.

„Теор. и эксперим. химия" 1975, 11, №4, 461-469

(см NiN_2, III)

Fe·O_2 *is-9996 1975

Hildenbrand D.L.

Do

„Chem Phys Lett" 1975
34, N2, 352-354 (англ)

(см FeO, III)

отт. 15 в папке
Hildenbrand!

Fe_3O^{n+} Мичиньски О., 1976

Войцеховски В.

электр.
структ.
кластеров

„Ж. структур. химии"
1976, <u>17</u>, №1, 168-170

(см Cr_3O^{n+}; <u>III</u>)

FeO_2

1977

(Di)

2 Д365. **ИК-спектры матрично-изолированной** FeO_2: **свидетельство образования циклических комплексов «железо — кислород».** Abramowitz Stanley, Acquista Nicolo, Levin Ira W. Infrared spectra of matrix isolated FeO_2: evidence for a cyclic iron-oxygen complex. «Chem. Phys. Lett.», 1977, 50, № 3, 423—426 (англ.)

Ф. 1978
№ 2

Получены ИК-спектры соединения FeO_2 (**I**) и ряда изотопзамещенных продуктов **I**, изолированных в аргоновой матрице при т-ре 12—14° К. Проведено сопоставление ИК-спектров **I**, NiO_2, PdO_2 и PtO_2. ИК-полосы 945,9; 930,8 и 911,4 см$^{-1}$ приписаны валентным колебаниям связи O—O в $Fe^{16}O_2$, $Fe^{16}O^{18}O$ и $Fe^{18}O_2$ соответственно, тогда как частоты валентных колебаний связи Fe—O в этих соединениях составляют 517,1; 508,1 и 494,0 см$^{-1}$. Сделан вывод, что молекулы **I** в матрице образуют циклич. структуры с симметрией C_{2v}. Библ 18 И. В. А.

FeO_2 оттиск 5703 1977

87: 191509b Infrared spectra of matrix isolated FeO_2: evidence for a cyclic iron-oxygen complex. Abramowitz, Stanley; Acquista, Nicolo; Levin, Ira W. (Natl. Bur. Stand., Washington, D. C.). *Chem. Phys. Lett.* 1977, 50(3), 423-6 (Eng). IR matrix isolation techniques were used to study the reaction of Fe (vapor) with O mols. For various isotopically enriched O samples, spectral transitions at 945.9, 930.8 and 911.4 cm^{-1} were assigned on the basis of their relatively large frequency shifts to the O-O stretching modes of $Fe^{16}O^{18}O$ and $Fe^{18}O_2$, resp. The low frequency Fe-O stretching modes were assigned to features at 517.1, 508.1 and 494.0 cm^{-1} for the same 3-isotopically substituted dioxygen complexes. Both the frequency behavior and intensity patterns involving the dioxygen ligand indicate a cyclic isosceles model for the FeO_2 system.

Ir

И. К. спектр

C.A, 1977, 87, №24

оттиск 5703 1977

FeO2

молек. структ; ν_i

7 Б147. **Инфракрасные спектры изолированного в матрице FeO$_2$. Доказательство циклической структуры комплекса железо — кислород.** Abramowitz Stanley, Acquista Nicolo, Levin Ira W. Infrared spectra of matrix isolated FeO$_2$: evidence for a cyclic iron—oxygen complex. «Chem. Phys. Lett.», 1977, 50, № 3, 423—426 (англ.)

Методом матричной ИК-спектроскопии изучены стабилизированные в тв. аргоне продукты р-ции паров Fe и молекул O$_2$. Обнаруженные в спектрах различных изотопически обогащенных по кислороду образцов полосы поглощения 945,9/517,1; 930,8/508,1 и 911,4/494,0 см$^{-1}$ с учетом относительно больших сдвигов частот отнесены к вал. кол. O—O/Fe—O трех комплексов FeO$_2^{16}$, FeO^{16}O^{18} и FeO$_2^{18}$ соотв. На основании анализа поведения частот и интенсивностей ИК-полос полученных комплексов и лит. данных по колебательным спектрам комплексов Ni, Pd и Pt с O$_2$ сделан вывод, что структура системы FeO$_2$ соответствует циклич. равнобедренной модели.

О. Г. Гаркуша

Х-N7, 1978

FeO_2 Weltner W., Jr., 1979

Transition-metal molecules and Walsh's Rules-Rationalization of Optical and ESR data. 10th Materials Research Symposium on Characterization of High temperature, Vapors and Gases.

(тип осн. сост., структура)

NBS Special Publication 561 Volume 1, 1979, 587-607.

(у Гурвича)

FeO_2 Gingerich K. A., 1980

Current Topics in Materials
Sciene, Volume 6, edited
by Kaldes E.

Do; North-Holland Publishing
Company, 1980.

(есть оттиск в коробке оттисков Gingerich).

~~[illegible]~~ το Απρίλιο, 1973

FeO_2 1981

Chang Seihun, et al.

спектр Inorg. Chem., 1981, 20,
в матрице. N 9, 2813-2817.

(см. Fe_2; III)

FeO_2 | Оттиск 13561 | 1982

Blyholder G., Head J.,
Ruette F.,

Кв. мех-
расчёт

Theoret. Chim. Acta
(Berl.) 1982, 60, 429-444.

FeO_2^n

$n=0,\pm 1$

1982

Blyholder G., Head J.
et al.

геометр.,
структ.,
ΔH.

Inorg. Chem., 1982,
21, N 4, 1539-1545.

●

(см. FeO^n; III)

FeO_2 1982

Blyholder G., Head J.
Ruette F.

ν_i; геометр. структура.

Inorg. Chem., 1982, 21, N 4, 1539–1545.

●

(см. FeO; III)

FeO_2

1984

2 Д116. Современный уровень развития многоконфигурационного метода ССП с последующим учетом конфигурационного взаимодействия (МК—КВ) в применении к расчету молекул, содержащих атомы переходных металлов. Current status of the multiconfiguration—configuration interaction (MC—CI) method as applied to molecules containing transition-metal atoms. Siegbahn Per E. M. «Faraday Symp. Chem. Soc.», 1984, № 19: Symp. Mol. Electron. Struct. Calc. Meth. and Appl., Cambridge, 12—13 Dec., 1984, 97—107 (англ.)

Сформулированы проблемы расчетов молекул соединений элементов III и IV периодов при помощи метода КВ с получением 1-частичного базиса и набора исходных конфигураций многоконфигурац. методом ССП (МКССП). Показана целесообразность использования версии МКССП с полным учетом конфигураций в активном пространстве. Отмечено, что во многих случаях критич. значение имеет расширение активного простран-

теорет-
расчет

⑪

ф. 1986, 18, №2

ства на стадии МКССП. Описан эффективный метод решения задачи КВ, возникающей на каждой стадии процесса МКССП. Обсуждаются результаты применения описанного подхода к расчету электронного строения молекул FeO_2 и NiCO. А. В. Зайцевский

FeO_2 ОМ · 23334 1986

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

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

$\Delta_f H$, D_0,
I;

● работа бесценная

$Fe(O_2)$

1987

109: 239570s Infrared matrix-investigations of the interaction of oxygen with iron atoms and aggregates. Kettler, Ulrich L.; Barrett, Paul H.; Pearson, Ralph G. (Dep. Phys., Univ. California, Santa Barbara, CA 93106 USA). *NATO ASI Ser., Ser. B* 1987, 158(Phys. Chem. Small Clusters), 813-17 (Eng). IR absorption investigations are reported of the reactivity of Fe_n (n = 1,2, ...) with mol. O_2 in low temp. Ar matrixes. Besides the known $\nu_{o\text{-}o}$ IR line of iron peroxide $Fe(O_2)$ at 956 cm^{-1} the band at ≈873 cm^{-1} which has been reported for FeO becomes strong at higher Fe concns. So far the occurrence of FeO has only been reported when at. O is formed in the device or at the matrix surface, e.g. by the reaction of O_2 with excited rare-gas atoms from a hollow-cathode discharge. In this case also O_3 lines have been reported. As no O_3 lines are seen, it is believed that Fe_2 is capable of O-O bond rupture resulting in a reaction product of 2 FeO. A new band grows at moderate Fe concn. at the expense of $Fe(O_2)$. It is assigned to the $\nu_{o\text{-}o}$ mode of a FeO_2Fe mol. A band at 1098 cm^{-1} is attributed to $Fe(O_2)_2$.

ИК в матрице

(+3) ☒

C.A.1988, 109, N26

FeO, FeO_2Fe, $Fe(O_2)_2$

FeO_2 30353 1988

Краснов К.С.,
Филиппенко Н.В.,

ОНИИТЭХИМ.

М.п.

(обзор)

Деп. N 378-ХП-86,
Черкассы, 1988.

$Fe^+O_2^-$

1988

109: 82195y AB initio MO studies on structure and reactivity of superoxo transition metal complexes. Yamaguchi, K.; Takahara, Y.; Fueno, T. (Fac. Eng. Sci., Osaka Univ., Osaka, Japan 560). *Stud. Org. Chem. (Amsterdam)* 1988, 33(Role Oxygen Chem. Biochem.), 263–8 (Eng). Ab initio MO calcns. were carried out to elucidate structure and reactivity of superoxo transition-metal complexes. The superoxide character for mol. oxygen involved in these species is parallel to the electron donating ability of ligands and is sensitive to environmental effects such as the H bond. The terminal O atom exhibits dual properties, electrophilic and nucleophilic, and the radical character is not negligible for the former case. The anion (θSH) is particularly effective for the formation of Fe^+OO^-, indicating the important role of the thiolate ligand for the iron-oxo formation in biol. systems.

ab initio
расчет.

C. A. 1988, 109, N 10

FeO_2 от. 30487а 1988

110: 65926r IR spectra of the reaction products of iron atoms with oxygen molecules in a matrix. Serebrennikov, L. V. (USSR). *Vestn. Mosk. Univ., Ser. 2: Khim.* 1988, 29(5), 451–5 (Russ). The IR spectra were obtained for the Fe + O_2 system in the presence of Ar and also Kr. The interpretation of the bands of the IR spectra are given. In the Fe + O_2 system, 3 types of dioxides can be formed: asym. (C_s or C_{2v}), cyclic (C_{2v}), and curved (C_{2v}). It is not clear why, in calcg. the FeO_2 mol. without an O–O bond, a linear mol. is obtained, since the expt. gives an angle of $a \approx 150°$.

ИК в мат-рице, структура

С.А. 1989, 110, N8

FeO_2 1992

Rudnyi E.B., Kaibicheva E.A. et al.
12th IUPAC Conf. Chem. Thermodyn. [and] Jt Meet. 47th
(Ae) Calorim. Conf., Snowbird,
Utah 16-21 Aug., 1992; Program. Abstr. and Repts. S.l.
(1992) c. 229
(см. PtO_2; III)

OFeO

ν_3= 945.8

ИК в Ar.

Цис-FeO$_2$

O-O вал. кол.

ИК в Ar..

ν_{O-O}=956,0

[illegible]

1992

Fanfarillo M., Downs A.J.
Greene T.M., Almond M.J. -
Inorg. Chem. 1992, 31, p.2973

FeO_2 1995

Fan, Jiawen; Wang,
Lai-Sheng,

(Ae) J. Chem. Phys., 1995, 102 (22),
8714-17.

(calc. FeO; ● $\overline{\underline{III}}$)

FeOO

O-O колеб.
в Ar. ИК:
1204.5 $см^{-1}$.
в O_2 ИК:
1209.8 $см^{-1}$

Chertihin G.V., Saffel W., Yustein J.T., Andrews L., Neurock M., Ricca A., Bauschlicher, Jr., J. Phys. Chem. 1996, 100, 5261.

1996

Cyc-FeO_2

ν_{OO} = 956.0 ИК в Ar
954,5 ИК в O_2
νORO = 548,4 ИК в Ar
549,7 ИК в O_2.

FeOO

Andrews B.V., Chertihin G.V., Citra A., Neurock M. 1996

O-O колеб.
в N_2 ИК.
1204.2 $см^{-1}$

J. Phys. Chem. 1996, 100, p.11235

7

F: FeOO
P: 3

1999

132:16651 Determinants of the FeXO (X = C, N, O) Vibrational Frequencies Heme Adducts from Experiment and Density Functional Theory. Vogel, Kathle M.; Kozlowski, Pawel M.; Zgierski, Marek Z.; Spiro, Thomas G. Department of Chemistry, Princeton University Princeton, NJ 08544, USA J. Am. Chem. Soc., 121(43), 9915-9921 (English) 1999

Vibrational spectra of CO, NO, and O2 adducts of heme proteins contain information on interactions of the heme and its bound ligands with the surrounding protein matrix that may help in elucidating the mechanism of small-mol. activation. Whereas the heme-CO system is well studied and a framework exists for the interpretation of such interactions, heme-NO and complexes were not systematically studied. Resonance Raman spectra were

C. A. 2000, 132

examd. of all 3 classes of adducts, combining literature values with new for FeIINO porphyrins having both electron-donating and electron-withdraw substituents. Neg. linear correlations are obsd. for all 3 adducts betwe their Fe-XO and X-O stretching frequencies. The slopes of these correlat lines are -0.4 for 5-coordinate FeCO and FeNO porphyrins and -0.8 for 5- coordinate FeO2 adducts. Fe-NO and Fe-O2 bonds are equally or even more sensitive than Fe-CO bonds to electronic influences that affect metal-to-ligand .pi. back-bonding. The responses of the NO and O2 adducts to tran ligand binding are very different from those for CO complexes. Ligands t to CO displace the plot to steeper slopes and lower Fe-CO frequencies, reflecting competition of the ligand lone pairs for the .sigma. acceptor orbital, dz2. No displacement of the line is obsd. for 6-coordinate FeNO FeO2 adducts, but only a shift to, higher positions on the line, indicatin greater back-bonding. The authors infer that trans ligand competition fo the dz2 orbital is not as effective for NO and O2 as for CO, reflecting t lower energy of the N and O orbitals relative to that of the C orbitals. These results are discussed with the aid of a simple bonding model involv FeXO valence isomers. To examine this model, the authors applied d. functional theory to 5- and 6-coordinate XO adducts of Fe(II) porphine. Geometries were in good agreement with expt., as were vibrational frequen for CO adducts. DFT overestimated the Fe-NO bond extension on binding a trans ligand and predicted a decrease in the Fe-NO stretching frequency, whereas an increase is obsd. The predicted frequency change was likewise the wrong direction for Fe-O stretching in 6- vs. 5-coordinate FeO2 adduc Probably DFT captures the essential features of back-bonding, but not of .sigma. competition with the trans ligand, in the cases of NO and O2.

FeO_2

2000

Gutsev G.L. et al.,

электрон.
и
геометр.
стр-ра
осн. и
возб.
сост.

J. Phys. Chem. A 2000,
104 (51), 11961-71.

(Cu-Se ● O_2; III)

FeO_2
FeO_2^+
FeO_2^-

2000

134: 47111n Density functional study of FeO_2, FeO_2^+, and FeO_2^-. Garcia-Sosa, Alfonso T.; Castro, Miguel (Departamento de Fisica y Quimica Teorica, Facultad de Quimica, Universidad Nacional Autonoma de Mexico, Del. Coyoacan, Mexico, Mex. 04510). *Int. J. Quantum Chem.* 2000, 80(3), 307–319 (Eng), John Wiley & Sons, Inc. The lowest energy structures of FeO_2 were detd. by means of d. functional theory techniques as implemented in the program DGauss 3.0.1. The calcns. performed were of the all-electron type using two levels of theory, namely the local spin d. approxn. with the use of the Vosko-Wilk-Nusair (VWN) functional and the generalized gradient approxn. (GGA) in the form of the Becke (1988) exchange and Perdew (1986) correlation functionals. Results were visualized by means of the program UniChem. Bond distances and angles as well as total energies were calcd. for several states of the moieties: $Fe(O)_2$, C_{2v}; $Fe(O)_2$, $D_{\infty h}$; $Fe(\eta^2-O_2)$, C_{2v}; $Fe(\eta^1-O_2)$, C_s; and $Fe(\eta^1-O_2)$, $C_{\infty v}$. MO and harmonic vibrational analyses were carried out for these species, in addn. to Mulliken population analyses. Singly pos. and neg. charged species were also considered and fully geometry optimized in a SCF (SCF) gradient method. Accurate ionization potentials and electron affinities (both vertical, v, and adiabatic,

структура,
ν, теор.
расчет

C.A. 2001, 134, N4.

a, detns.) were thus able to be computed. The results show the following for the ground state (GS) $Fe(O)_2$, C_{2v}, $M = 3$: $OFeO = 138.1°$ ($133.6°$) [values in parentheses are for local spin d. approxn. (LSDA)−VWN, while the others are at the GGA−B88/P86 level]. Here, R_e Fe−O = 1.60 Å (1.57 Å), ET = −1414.2064 au (−1,410.5047 au), EA_a = 2.47 (2.60) eV, IP_a = 10.6 (10.5) eV, EA_v = 2.41 (2.20) eV, IP_v = 10.67 (10.63) eV, and EA_{exp} = 2.349 eV (in agreement with related studies). In the GS the dioxygen mol. is found to be dissocd., compared to those states which have coordination modes where the O_2 mol. formally persists. A 3d4sp configuration for the iron atom is found to be esp. relevant in Fe−O bond formation. The iron−oxygen and oxygen−oxygen bonds involved are characterized. A direct relationship is obsd. between these electronic and structural properties, influencing also the total energy for a given mol.