$^1ScO_2$, $^3ScO_2^-$

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

(у Гурвич)

(тип осн. сост., структура)

ScO_2 925	Серебренников Л.В., 1980 Мальцев А.А.,
м.п. Дорофеева	Рук. деп. в ВИНИТИ № 54-80 Деп
14	ScO_2 м.п.

ScO_2 1982

Konnov S. A., Serebrennikov L. V., et al.

UK

спектр.

Vestn. Mosk. Univ., Ser. 2: Khim. 1982, 23 (2), 101-104.

(см. EuO_2; III)

ScO_2^- | Chim. 18785 | 1984

101: 43813p **Theoretical study of the geometry of triatomic oxides and oxide fluorides of 3d-metals.** Klimenko, N. M.; Musaev, D. G.; Charkin, O. P. (Inst. Novykh Khim. Probl., Moscow, USSR). *Zh. Neorg. Khim.* 1984, 29(4), 835–8 (Russ). The equil. geometrical parameters of ScO_2^-, TiO_2, VO_2^+, FScO, $FTiO^+$, and FCuO were calcd. by the Hartree-Fock method by using valence double-exponential Roos-Veillard-Vinot basis sets for 3*d* metals and double-exponential Oors-Siegbahn basis sets for O and F. The results were compared with available exptl. and theor. data. The calcns. favor angular structures for ScO_2^-, TiO_2, and VO_2^+ with a valence angle (OMO) = 126, 115, and 109°, resp., and for FScO and $FTiO^+$ θ(FMO) = 124 and 116°, resp. The FCuO mol. has a strongly sloping deformation potential and is assumed to be not rigid to deformation.

структура, параметры, пар. расч.

+5 ☒

C. A. 1984, 101, N 6

ScO2-

Оп. 18 Б5

1984

14 Б1021. Теоретическое исследование геометрии трехатомных окислов и оксифторидов 3*d*-металлов. Клименко Н. М., Мусаев Д. Г., Чаркин О. П. «Ж. неорган. химии», 1984, 29, № 4, 835—838

Выполнены хартри-фоковские расчеты равновесных геометрич. параметров ряда молекулярных систем диоксидов. ScO_2^-, TiO_2 и VO_2^+ и оксифторидов FScO, $FTiO^+$ и FCuO с использованием валентно-двухэкспонентного базиса Роса — Вейяра — Винота для атомов 3*d*-металлов и двухэкспонентного базиса Роса — Зигбана для атомов O и F. В соответствии с предположением, сделанным ранее («Ж. структ. химии», 1964, 5, 451, 921, 924) в рамках модели валентных состояний, расчеты свидетельствуют в пользу углового строения диоксидов ScO_2^-, TiO_2 и VO_2^+ [валентные углы $\theta(O\hat{M}O) = 126$, 115 и 109° соотв.], а также оксифторидов FScO и $FTiO^+$ [углы $\theta(F\hat{M}O) = 124$ и 116° соотв.]. Молекула FCuO имеет очень пологую деформац. потенциальную кривую и, по-видимому, может считаться деформационно нежесткой. Резюме

геометр., структура, потенц. кривая

(Б5)

X. 1984, 19, N 14

SCl_2^- Мусаев Д. Г., 1984

расчет равновес. геометр. структур

Автореферат диссертации на соискание ученой степени к.х.н., Москва, 1984.

Неэмпирические расчеты структур и относительных энергетических характеристик простых соединений 3d-элементов с заключенными оболочками.

SiO_2

(30353)

1988

Краснов К. С.,
Филиппенко Н. В.,
ОНИИТЭХИМ.

Деп. № 378-ХП-86,
Черкассы, 1988.

и. п.

(обзор)

ScO_2

1992

116: 159264z Gas-phase thermochemistry of the Group IIIB dioxides: scandium, yttrium, and lanthanum oxides (ScO_2, YO_2, and LaO_2). Clemmer, D. E.; Dalleska, N. F.; Armentrout, P. B. (Dep. Chem., Univ. Utah, Salt Lake City, UT 84112 USA). *Chem. Phys. Lett.* 1992, 190(3-4), 259-65 (Eng). Gas-phase ScO_2, YO_2, LaO_2 and the singly charged cations of these species are formed in endothermic reactions between MO^+ (M = Sc, Y, and La) and NO_2 in a guided ion beam mass spectrometer. The cross sections of these reactions are measured as a function of kinetic energy and are interpreted to give the following bond energies (in eV): D^0(OSC-O) = 3.95 ± 0.33, D^0(OYO) = 4.14 ± 0.22, D^0(OLa-O) = 4.20 ± 0.33, D^0(OSc^+-O) = 1.72 ± 0.19, D^0(OY^+-O) = 1.76 ± 0.16, and D^0(OLa^+-O) = 0.99 ± 0.31. Values for the MO_2 ionization energies (in eV) are detd. to be IE (ScO_2) = 8.56 ± 0.20, IE(YO_2) = 8.23 ± 0.16 and IE(LaO_2) = 8.11 ± 0.35. The differences between these values and [illegible] in the literature are discussed by considering the nature of the bonding in MO_2 and MO_2^+.

D(OSc-O),
D(OSc^+-O),
Y

+2

C. A. 1992, 116, N 16

OScO.   1997

Chertikin, G.V. et al.,

ИК в   J. Phys. Chem. A 1997,
Ar мат-   101 (48), 9085–9091
рице,
Di,
структура   (см. ● ScO; III)

ScO2 (Dm-39708) 1998

Hongbin Wu and Lai-Sheng Wang*

M.N.

J. Phys. Chem. 1998, A102, 9129-9135

ScO_2

1998

Rosi, Marzio; Bauschlicher Charles W., et al.,

(Di) Theor. Chem. Acc. 1998, 99 (2), 106-112.

(au. CaO_2; ● III)

F: ScO2-
P: 3

of.40136

1999

131:162645 A Further Study of the Products of Scandium and Dioxygen React Bauschlicher, Charles W., Jr.; Zhou, Mingfei; Andrews, Lester; Johnson, R. Tobias; Panas, Itai; Snis, Anders; Roos, Bjoern O. (NASA Ames Research Center, Moffett Field, CA 94035, USA). J. Phys. Chem. A, 103(28), 5463-5 (English) 1999 The products of the reaction of Sc and dioxygen were re-studied. By adding the electron-trapping mol. CCl4, addnl. information about the IR s was obtained, as well as the observation of new bands. New ab initio cal are also performed on possible products of the Sc plus O2 reaction. The previously obsd. band at 722.5 cm-1 is assigned as the b2 mode of ScO2-. arising from ScO+, Sc(O2)+, and (O2)ScO are also assigned. The authors a still unable to assign any bands to OScO. The problems assocd. with the computational study of ScO2 are discussed.

1999

F: (O2)ScO
P: 3
131:162645 A Further Study of the Products of Scandium and Dioxygen React Bauschlicher, Charles W., Jr.; Zhou, Mingfei; Andrews, Lester; Johnson, R. Tobias; Panas, Itai; Snis, Anders; Roos, Bjoern O. (NASA Ames Research Center, Moffett Field, CA 94035, USA). J. Phys. Chem. A, 103(28), 5463-5 (English) 1999 The products of the reaction of Sc and dioxygen were re-studied. By adding the electron-trapping mol. CCl4, addnl. information about the IR s was obtained, as well as the observation of new bands. New ab initio cal are also performed on possible products of the Sc plus O2

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of. 40136

1999

F: Sc(O2)+
P: 3
131:162645 A Further Study of the Products of Scandium and Dioxygen React Bauschlicher, Charles W., Jr.; Zhou, Mingfei; Andrews, Lester; Johnson, R. Tobias; Panas, Itai; Snis, Anders; Roos, Bjoern O. (NASA Ames Research Center, Moffett Field, CA 94035, USA). J. Phys. Chem. A, 103(28), 5463-5 (English) 1999 The products of the reaction of Sc and dioxygen were re-studied. By adding the electron-trapping mol. CCl4,

addnl. information about the IR s was obtained, as well as the observation of new bands. New ab initio cal are also performed on possible products of the Sc plus O2 reaction. The previously obsd. band at 722.5 cm-1 is assigned as the b2 mode of ScO2-. arising from ScO+, Sc(O2)+, and (O2)ScO are also assigned. The authors a still unable to assign any bands to OScO. The problems assocd. with the computational study of ScO2 are discussed.