SiO 1990

Peterson Kirk A.,
Woods R. Claude.

потенц.
энергия,
μ, расчет

J. Chem. Phys. 1990. 92,
N 10. С. 6061–6068.

(См. AlF; III)

SiO 1990

Wong, Ming Wah.,
Radom, Leo,

J. Phys. Chem., 1990,
Расчет м.п., 94 (2), 638-44.
потенц.
кривые Isoelectronic analogs of
phosphorus nitride.

C.A. 1990, 112, N 8, 62958h.

remarkably multiply
charged cations.

SiO Оп. 35796 1991

$A^1\Pi - X^1\Sigma^+$

Hynes A.J.,

Chem. Phys. Lett. 1991, 181, N2-3, 237-244.

Laser - induced fluorescence of silicon monoxide in a glow discharge and an atmospheric pressure flame.

SiO

ОМ 35510 1991

20 Б1055. Неэмпирический расчет дипольного момента и динамической поляризуемости монооксида кремния и его аниона. Ab initio calculation of the dipole moment and frequency-dependent polarizability for silicon monoxide and its anion / Inoue Toshihiro, Iwata Suehiro // J. Mol. Struct.— 1991.— 243, № 1—2.— С. 147—162.— Англ.

Методом ССП и конфигурац. взаимодействия (КВ) в расширенном базисе гауссовых ф-ций рассчитаны потенциальные кривые и ф-ции дипольного и квадрупольного моментов, статич. и динамич. поляризуемости основного $X^1\Sigma^+$ состояния SiO и низших состояний $^2\Sigma$ и $^2\Pi$ аниона SiO^-. Получено, что состояния аниона лежат близко к основному состоянию нейтр. молекулы (рассчитанное методом КВ адиабатич. сродство к электрону составляет для $^2\Sigma$ и $^2\Pi$ состояний —1,11 и —1,60 эВ, соотв.). Проанализированы результаты расчетов поляризуемостей методами КВ и ССП в конечном поле.

А. А. Бучаченко

М. П.

Х. 1991, N 20

SiO

От 3567Н

1991

114: 195529g The millimeter-wave spectrum of highly vibrationally excited silicon monoxide. Mollaaghababa, R.; Gottlieb, C. A.; Vrtilek, J. M.; Thaddeus, P. (Div. Appl., Harvard Univ., Cambridge, MA 02138 USA). *Astrophys. J.* 1991, 368(1, Pt. 2), L19-L22 (Eng). The millimeter-wave rotational spectra of SiO in high vibrational states (v = 0-40) in its electronic ground ($X^1\Sigma^+$) state were measured between 228 and 347 GHz in a lab. discharge through SiH_4 and CO. On ascending the vibrational ladder, populations decline precipitously for the first few levels, with a vibrational temp. of about 1000 K; at $v \approx 3$, however, they markedly flatten out, and from there to $v \approx 40$ the temp. is of the order of 10,000 K. With the Dunham coeffs. detd. here, the rotational spectrum of highly vibrationally excited SiO can now be calcd. into the far-IR to accuracies required for radioastronomy (i.e., $\lesssim 1$ km s^{-1}). Possible astronomical sources of highly vibrationally excited SiO are certain stellar atmospheres, ultracompact H II regions, very young supernova ejecta, and dense interstellar shocks.

Мв спектр, высокие колебат. уровни

М.Л.

C.A. 1991, 114, N 20

^{29}SiO

^{30}SiO

в

спектре

звёзд

1992

116: 183940n Silicon oxide (^{29}SiO and ^{30}SiO) maser emission from evolved stars. Alcolea, J.; Bujarrabal, V. (Cent. Astron. Yebes, Guadalajara, Spain E-19080). *Astron. Astrophys.* **1992,** 253(2), 475–86 (Eng). Presented is the first systematic study of the $\upsilon = 0$ emission of ^{29}SiO and ^{30}SiO (the rare isotopic substitutions of SiO) in evolved stars. Obsd. were the $\upsilon = 0$ $J = 1$–0 ^{29}SiO line in 38 objects, reporting the detection of this transition in 8 new sources. The $\upsilon = 0$ $J = 1$–0 line of ^{30}SiO was obsd. in 13 stars, including one new detection. From the observational characteristics of both ^{29}SiO and ^{30}SiO lines are confirm that they are produced by maser amplification. These masers seem to be nonsatd. Also studied was the variation of the ^{29}SiO maser, that has been found to be similar to those of the $\upsilon = 1, 2$ ^{28}SiO ones i.e. following the IR variation of the star. The $\upsilon = 0$ $J = 1$–0 ^{29}SiO and ^{30}SiO masers present very narrow lines, with an equiv. width of ~2 km s^{-1}, at velocities very close to that of the star. This result is not compatible with the theor. predictions of the only proposed mechanism to produce $\upsilon = 0$ SiO masers. The obsd. ^{29}SiO variability and the good correlation of it6s intensity with the 8 μm flux indicate that this maser is probably pumped by the stellar radiation. From the comparison with the $\upsilon = 1$ $J = 1$–0 ^{28}SiO maser are ob5ained that this line is much stronger (~85 times) than the $\upsilon = 0$ $J = 1$–0 ^{29}SiO one. Also searched for $\upsilon = 1$ ^{29}SiO masers, but with neg. results, concluding that, if they are present, these lines must be at least ~130 times weaker than those of ^{28}SiO.

C.A. 1992, 116

N 18

SiO 1992

McLean A.D., Liu B.,
et al.,

Ф-ии
потенц.
энергии,
r_e, ω_e,
T, D_e, расчет

J. Chem. Phys. 1992,
<u>97</u>(11), 8459-64

(см. B_2^+; <u>III</u>)

SiO 1993

Molaaghababa, R.,
(Harvard Univ., Cambridge,
MA USA). 1993, 125 pp.

мм
спектр

(см. SiC; III)

SiO

1993

118: 243667g **Measurement of the $A^1\Pi - X^1\Sigma^+$ electronic transition moment of oxosilylene using a shock tube.** Park, Chung S.; Crosley, David R.; Eckstrom, Donald J.; Heere, Karen R. (Mol. Phys. Lab., SRI Int., Menlo Park, CA 94025 USA). *J. Quant. Spectrosc. Radiat. Transfer* 1993, 49(4), 349–60 (Eng). The reflected-shock-heated gas in a shock tube was used to measure the electronic transition moment, R_e^2, for the $A^1\Pi - X^1\Sigma^+$ band system of SiO. The absorption spectra of several different gas mixts. were recorded using an optical multichannel analyzer in the 220–310 nm wavelength range. Synthetic spectra were compared with exptl. spectra to det. the R_e^2 as a function of internuclear distance, r. Best agreement was achieved if the theor. values of Langhoff and Arnold are multiplied by a const. value of 1.3, or if they are shifted by 0.25 Bohr toward larger r. However, both the authors results and the theor. values are in disagreement with two recent laser-induced fluorescence detns. A transition moment was found that decreases with increasing r, having a value $R_e^2 = 1.3 \pm 0.17$ at. units at the equil. internuclear distance of 3.0 Bohr.

$A^1\Pi - X^1\Sigma^+$

электр. мом. перехода

спектр в УТ

C.A. 1993, 118, N24

SiO

1993

118: 132567e **Quasirelativistic studies of molecular electric properties: dipole moments of the Group IVA oxides and sulfides.** Kello, Vladimir; Sadlej, Andrzej J. (Chem. Cent., Univ. Lund, S-221 00 Lund, Swed.). *J. Chem. Phys.* 1993, 98(2), 1345-51 (Eng). Dipole moments of SiO, GeO, SnO, PbO, and of the corresponding sulfides were computed by using a variety of high-level correlated methods and polarized basis sets of Gaussian functions. The contribution of relativistic effects was accounted for by the first-order quasirelativistic approach based on mass-velocity and

(M)

(+3) ☒

C.A. 1993, 118, N14

Darwin terms. The results for sulfides are in good agreement with expt. while for oxides seem to show a progressive deterioration with the increase of the heavy atom nuclear charge. The discrepancies between the calcd. and exptl. dipole moments for oxides were carefully analyzed for the PbO mol. in terms of the basis set choice and reliability of the calcd. electron correlation and relativistic corrections. The pattern of relativistic corrections computed in the present study is compared with that which follows from recent quasirelativistic and fully relativistic calcns. of Dyall. Some complementary calcns. of the dipole moment of PbSe and PbTe seem to indicate that both the polarized basis sets and computational methods used in this study should not fail to predict correct values of the dipole moment of PbO and other oxides of the group IVa atoms. The rather unexpected discrepancies have no plausible explanation within the range of methods employed in this study and offer a challenge for more advanced, fully relativistic mol. calcns. at the correlated level of approxn.

SiO 1994

Andrews Lester, Mielke Zofia et al.

ИК в матрицах, ab initio расчёты

$A\,^2\Sigma_u^+ - X\,^2\Pi_g$

J. Phys. Chem. 1994, 98 (42), 10706–9.

● (см. PNP ; III)

SiO 1994

Barandiarán Zoila,
Seijo Luis.

структура,
частоты
колебан.

J. Chem. Phys. 1994.
<u>101</u>, N5. C. 4049-4054.

(см. SiH_2; <u>III</u>)

SiO (от. 37773) 1994

Boldyrev A.I., Gonzalez N.,
Simons J.,

$^1\Sigma^+$, J. Phys. Chem., 1994,
D,
эксперим., <u></u>98, N 40, 9981–44
теорет.
расчет

SiO OM 38132 1995

124: 70049a Infrared absorption and emission spectra of SiO. Campbell, J. M.; Klapstein, D.; Dulick, M.; Bernath, P. F.; Wallace, L. (Centre for Molecular Beams and Laser Chemistry, University of Waterloo, Waterloo, ON Can. N2L 3G1). *Astrophys. J., Suppl. Ser.* 1995 (Pub. 1995), 101(1), 237–54 (Eng). High–resoln. FTIR spectra of SiO were recorded from 2 sources, the umbral region of a sunspot and a high–temp. lab. cell. Rovibrational transitions in the sunspot absorption spectrum were measured in consecutive vibrational bands from (1, 0) to (13, 12) with J values ≤141 for $^{28}\mathrm{Si}^{16}\mathrm{O}$ (1258 lines) and (1, 0) to (6, 5) for $^{29}\mathrm{Si}^{16}\mathrm{O}$ and $^{30}\mathrm{Si}^{16}\mathrm{O}$ (455 lines). In the lower temp. lab. emission spectrum only 387 rotational lines in the (1, 0) to (5, 4) bands were measured exclusively for $^{28}\mathrm{Si}^{16}\mathrm{O}$. The lab. spectrum served primarily to calibrate the lines in the sunspot spectrum to abs. rest frequencies. An improved set of Dunham consts. for the $^{1}\Sigma^{+}$ ground state was obtained from a global fit of a combined data set consisting of the IR data and all the previously reported microwave and millimeter–wave data. An internuclear potential for the $^{1}\Sigma^{+}$ ground state, as a parameterized modified–Morse function, was obtained by fitting the data directly to the eigenvalues of the radial Schroedinger equation.

ИК спектр
поглощение
и спектр
испускание

C.A. 1996, 124, N6.

1995

F: SiO
P: 3
3Б1165. Суммы по состояниям для молекул CS и SiO. Partition functions for the CS and SiO molecules / Chandra S., Sharma A. K. // Indian J. Pure and Appl. Phys. - 1995. - 33, N 6. - C. 345-346. - Англ.

РЖХ: 1997

SiO 1995

Wang, S.G., Schwarz, W.H.E.,

D_0, сил. пост., ω_e, теор. расчет

THEOCHEM 1995, <u>338</u>, 347-62

(см. CO; <u>III</u>)

SiO 1997

Bernath, Peter F.,

lek, Symp. – Int. Astron. Union
obzor 1997, 178, 281–286

(Cell. Astr.; ● III)

SiO 1999

Brinkmann, N.R.; et al.,

J. Chem. Phys., 1999, 110, (13),

(Ae) 6240–45.

(см. AlO; III)

$^{28}Si^{18}O$

1998

128: 287828w **Microwave spectrum of a silicon monoxide isotopomer: $^{28}Si^{18}O$.** Cho, Se-Hyung; Saito, Shuji (Korea Astronomy Observatory, Daejc, 305-348 S. Korea). *Astrophys. J.* **1998**, 496(1, Pt. 2), L51-L52 (Eng), University of Chicago Press. The rotational transitions of $^{28}Si^{18}O$ in the ground vibrational state were obsd. by lab. microwave spectroscopy for astronomical use. The SiO mols. were generated in a free-space absorption cell by dc-glow discharge in a mixt. of tetra-Me silane, $Si(CH_3)_4$, and $^{18}O_2$. Ten rotational transitions were precisely measured in the 40-444 GHz region. The rotational and centrifugal distortion consts. were detd. by a least-squares anal. of measured line frequencies: $B_0 = 20176.4394(43)$ and $D_0 = 0.025809(32)$ MHz, with the 3 σ deviations in parentheses.

(м/в спектр)

C.A. 1998, 128, N23

SiO

1998

Decker, Stephen A.,
et al.,

THEOCHEM 1998, 451 (1-2),
215-226

теорет.
расчет
стр-ры
и
стабильн.

(см. N_2; ● III)

SiO

1998

$(A^1\Pi - X^1\Sigma^+)$
$(E^1\Sigma^+ - X^1\Sigma^+)$
теорет.
расчет

129: 33804a **Theoretical study of the $A^1\pi - X^1\Sigma^+$ and $E^1\Sigma^+ - X^1\Sigma^+$ bands of SiO.** Drira, I.; Spielfiedel, A.; Edwards, S.; Feautrier, N. (Departement Atomes et Molecules en Astrophysique et URA812 du CNRS section de Meudon, Observatoire de Paris, 92195 Meudon, Fr.). *J. Quant. Spectrosc. Radiat. Transfer* **1998**, 60(1), 1–8 (Eng), Elsevier Science Ltd.. Franck–Condon factors and radiative lifetimes of the $A^1\pi - X^1\Sigma^+$ and $E^1\Sigma^+ - X^1\Sigma^+$ transitions of the SiO mol. were calcd. from accurate ab initio MRCI calcns. including electronic transition moment variations. A comparison of the present results with the RKR potentials shows a good agreement and the deduced spectroscopic consts. agree reasonably well with the exptl. values. The variations of the electronic transition moment of the two bands are compared with the few exptl. data and critically discussed.

С.А. 1998, 129, N3

SiO

1998

129: 181515x **The c $^3\Sigma^+$–b $^3\Pi_r$ and g $^3\Sigma^+$–b $^3\Pi_r$ transitions of the SiO molecule.** Dubois, Iwan; Bredohl, Harald (Institute of Astrophysics and Geophysics, University of Liege, B–4000 Liege, Bulg.). *J. Phys. B: At., Mol. Opt. Phys.* **1998**, 31(12), 2805–2807 (Eng), Institute of Physics Publishing. The c $^3\Sigma^+$–b $^3\Pi_r$ transition of SiO was obsd. in emission in a microwave discharge through He with traces of $SiCl_4$ and O_2 with a Bruker IFS 120 at high resoln. The rotational anal. yields more precise mol. consts. for the 2 states involved than the previous study of Nagaraj and Verma. Using the new consts. for the b $^3\Pi_r$ state, better consts. are also obtained for the g $^3\Sigma^+$ (4sδ) state analyzed by Singh et al.

$c\,^3\Sigma^+ - b\,^3\Pi_r$,

$g\,^3\Sigma^+ - b\,^3\Pi_r$

М.Л.

CA, 1998, 129, N14

SiO (Оп 39599) 1998

Iwan Dubois and Harald Bredohl,

J. Phys: At. Mol. Opt. Phys. 1998, <u>31</u>, 2805–2807.

The $c^3\Sigma^+ - b^3\Pi_2$ and $g^3\Sigma^+ -$

$b\ ^3\Pi_2$ transitions of the SiO molecule.

SiO
SiO_2

От. 40073

1999

Nicole R. Brinkmann
et al.,

Ae,
теор.
расчет

J. Chem. Phys., 1999,
110, N13, 6240–45

1999

F: SiO
P: 3
131:357735 RKRV potential energy curves, dissociation energies, .gamma.- centroids and Franck-Condon factors of YO, CrO, BN, ScO, SiO and AlO mole
Reddy, R. R.; Ahammed, Y. Nazeer; Gopal, K. Rama; Azeem, P. Abdul; Anjaneyulu, S. Department of Physics, Sri Krishnadevaraya University Anantapur 515 003, India Astrophys. Space Sci., Volume Date 1998-1999, 262(2), 223-240 (English) 1999 The potential energy curves for the electronic ground states of astrophy important YO, CrO, BN, ScO, SiO and AlO mols. are constructed techniques the 5-parameter Hulburt-

Hirschfelder function. The estd. dissocn. energi 7.235 .+-. 0.15, 4.337 .+-. 0.09, 3.917 .+-. 0.09, 6.899 .+-. 0.14, 8.181 0.17 and 5.202 .+-. 0.11 eV for YO, CrO, BN, ScO, SiO and AlO, resp. The D0 values are in reasonably good agreement with literature values. The r Centroids and Franck-Condon factors for the bands of B2.SIGMA.+ - X2.SIGM YO, B5.pi. - X5.pi. of CrO, A3.pi. - X3.pi. of BN, B2.SIGMA.+ - X2.SIGMA. ScO, E1.SIGMA.+ - X1.SIGMA.+ of SiO and D2.SIGMA.+ - X2.SIGMA.+ and B2.SI X2.SIGMA.+ of AlO mols. were detd. The Franck-Condon factors are evaluat the approx. anal. method of Jarmain and Fraser. The absence of the bands these systems is explained.

F: SiO
P: 3

?

131:176578 SiO flame emission spectroscopy from a silane/hydrogen/oxygen/ diffusion flame. Wooldridge, M. S.; Danczyk, S. A.; Wu, J. (Department of Mechanical Engineering and Applied Mechanics, University of Michigan, Ann MI 48109-2125, USA). Proc. - Electrochem. Soc., 98-23(Fundamental Gas-Ph Surface Chemistry of Vapor-Phase Materials Synthesis), 135-140 (English) As part of a study of SiH4 combustion in particle producing flames, spontaneous emission from an atm. pressure SiH4/H2/O2/Ar diffusion flame examd. The expts. were conducted using a flat-flame burner where SiH4 di Ar was injected through the center of the burner. Si, SiH and SiO interm were identified from the spectral emission signature. The electronic spe the SiO A1.PI. - X1.SIGMA.+ band were analyzed. Comparison of the exptl. with an emission model for SiO indicated significant vibrational nonequil level of vibrational excitation was quantified in terms of a vibrational independent of a translational temp. The best-fit model results obtained comparison with the exptl. data yielded a translational temp. of T = 3250 a vibrational temp. of Tvib = 15000 K. The vibrational temp. corresponds changes in fractional population of over an order of magnitude from equil distributions for some vibrational levels.

SiO

Оп. 40755

2001

Hermann J., Coursimault F.,
O. Motret et al.,

J. Phys. B: At. Mol. Opt.
Phys., 2001, 34, 1917-1927.

Investigation of silicon
oxide emission spectra obser-

ved in a pulsed discharge and a laser – induced plasma.

SiO

2001

(Вак УФ спектр)

135: 378024s The VUV Absorption Spectrum of SiO: Three New Ionization Limits. Esteva, J. M.; Breton, J.; Bredohl, H.; Dubois, I.; Remy, F. (LURE Universite de Paris-Sud, F-91405 Orsay, Fr.). *J. Mol. Spectrosc.* **2001**, 208(2), 166–168 (Eng), Academic Press. The absorption spectrum of SiO was obsd. down to 250 Å. Besides the Rydberg series reported by M. A. Baig and J. P. Connerade (1979, J. Phys. B: At. Mol. Phys. 12, 2309–2318), 3 new groups of Rydberg series were obsd. converging at 18.59, 22.64, and 37.07 eV. These new limits are compared to theor. calcns. (K. L. Cai and J. P. Francois, 1999, J. Mol. Spectrosc. 197, 12–18) and to the isovalent mol. CO. (c) 2001 Academic Press.

C.A. 2001, 135, N26.