OCS am · 35516 1990.

Allen W. D., Yamaguchi Y.,
et al.

Chem. Phys. 1990, 145, N3,
427–466.

A systematic study of molecular
vibrational anharmonicity and

vibration-rotation interaction. by self-consistent-field higher-derivative methods. Linear polyatomic molecules.

OCS Оп. 34172 1990

сил. пост. Butayev B. S., Lyutsarev V. S., et al.,

J. Mol. Struct., 1990, 221, 149-157

The Morse-Like Potential model accounting for a stretch-bend interaction in linear XYZ molecules.

OCS 1990

Maki A.G., Wells J.S.
et al.

м. п.

J. Mol. Spectrosc. 1990.
144, N1. c. 224-229.

(см. CO; III)

OCS

1990

113: 240427q **Absolute carbonyl sulfide wavenumbers and analysis of bands in the region of the overtone $2\nu_2$.** Tolonen, A. M.; Horneman, V. M.; Alanko, S. (Dep. Phys., Univ. Oulu, SF-90570 Oulu, Finland). *J. Mol. Spectrosc.* 1990, 144(1), 18–26 (Eng). The IR spectrum of OCS in the region of the overtone $2\nu_2$ was studied with a Fourier transform spectrometer at a resoln. of 0.003 cm^{-1}. Calibration lines with high abs. wavenumber accuracy were produced in the spectral range of 1000–1–80– cm^{-1}. The overtone band $2\nu_2$ and the hot bands $3\nu_2-\nu_3$ and $4\nu_2-2\nu_2$ were analyzed, considering esp. the effects of l-type resonances. As a result, a set of mol. consts. for the vibrational levels $v_2 = 2$, $v_2 = 3$, and $v_2 = 4$ were derived.

Di

C.A. 1990, 113, №26

COS

Om 33573

1990

Вращат-постоян

112: 148142z **Heterodyne frequency measurements on carbonyl sulfide near 61.76 THz (2060 cm^{-1}).** Wells, J. S.; Schneider, M.; Maki, A. G. (Time Freq. Div., Natl. Inst. Stand. Technol., Boulder, CO 80303 USA). *J. Mol. Spectrosc.* 1990, 140(1), 170-6 (Eng). Heterodyne measurements were made on the 10^00-00^00 and 11^10-01^10 bands of $^{16}O^{12}C^{32}S$ and $^{16}O^{13}C^{32}S$ and the 10^00-00^00 band of $^{16}O^{12}C^{34}S$. These measurements were combined with earlier frequency measurements and FTIR measurements to obtain accurate calibration frequencies for 1985-2035 and 2550-2600 cm^{-1}.

C.A. 1990, 112, N 16

OCS

1990

113: 67546c **Infrared spectra, vibrational relaxation, and isotopically selective photodissociation of carbonyl sulfide in argon(l) and oxygen(l) cryogenic solutions.** Zittel, P. F.; Sedam, M. A. (Chem. Phys. Lab., Aerosp. Corp., Los Angeles, CA 90009 USA). *J. Phys. Chem.* 1990, 94(15), 5801-9 (Eng). Vibrational band centers of OCS between 500 and 4200 cm^{-1} were detd. for $^{16}O^{12}C^{32}S$ and the singly substituted ^{13}C, ^{17}O, ^{18}O, ^{33}S, and ^{34}S isotopic analogs in liq. Ar and liq. O_2 soln. Band strengths and band half-widths of the Lorentzian-shaped absorption features were also measured. The narrow spectral width of the absorption bands with respect to the isotopic band center shifts was exploited in a two-step, IR/UV laser photodissocn. technique to sep. oxygen isotopes with enrichment factors of 3-4. The dependence of the isotope enrichment factors on exptl. conditions provides some information about sulfur atom chem. and vibrational energy relaxation in the OCS/O_2/Ar cryogenic liq. system. A laser-induced fluorescence method was used to directly measure rates for relaxation of the ν_1 and ν_2 vibrational levels of OCS by Ar(l) and by O_2 in Ar(l) soln. at 84.4 K and place a lower limit on the rate for relaxation of the laser pumped $2\nu_2$ level.

ИК-спектр, Di

C.A. 1990, 113, N8

OCS

1990

20 Б4012. Изучение с разрешением по квантовым состояниям колебательно-вращательного возбуждения OCS горячими атомами водорода. Quantum state-resolved study of the rovibrational excitation of OCS by hot hydrogen atoms / Zhu Lei, Hershberger John F., Flynn George W. // J. Chem. Phys.— 1990.— 92, № 3.— С. 1687—1710.— Англ.

(Di)

Изучено колебат. возбуждение молекулы OCS атомами H при 2,3 эВ. Горячие атомы H получены путем фотолиза H_2S эксимерным лазером. Конечные состояния OCS определялись при помощи ИК-спектров поглощения. Определены поступат. и вращат. распределения высокочастотного (2062 $см^{-1}$) и низкочастотного (859 $см^{-1}$) колебат. состояний OCS. Результаты интерпретируются при помощи модели дышащих эллипсоидов. Показано, что двухквантовые возбуждение OCS соответствует удару атома H по двум концам линейной молекулы OCS. Объяснено также происхождение различий в поступат. и вращат. распределениях для двух колебат. мод. Библ. 48.

Л. В. Ленин

X. 1990, N20

OCS 1991

Aihara Jun-Ichi.

м.п. J. Mol. Struct. Theochem.

1991. 228. с. 277–283.

(См. $C_3H_5^-$; III)

OCS^+ 1991

115: 265645p The infrared laser spectrum of the ν_3 band of carbonyl sulfide ion (OCS^+) [Erratum to document cited in CA112(26):242350n]. Feher, M.; Salud, C.; Roesslein, M.; Maier, J. P. (Inst. Phys. Chem., Univ. Basel, CH-4056 Basel, Switz.). *J. Mol. Spectrosc.* 1991, 149(2), 562 (Eng). A reevaluation of the data has been provided. The error was reflected in the abstr.

ν_3

Erratum

C. A. 1991, <u>115</u>, N24

OCS 1991

Iachello F., Oss S.,
et al.

колебат.
спектры

J. Mol. Spectrosc. 1991.
<u>146</u>, N1. C. 56-78.

(См. ● N_2O; <u>III</u>)

OCS

Om. 35778

1991

Lang V.I., Winn J.S.,

J. Chem. Phys. 1991,
<u>94</u>, N8, 5270–5274

Matrix-isolated OCS: The high resolution infrared

Spectra of a cryogenically
solvated linear molecule.

OCS

1991

/ 114: 255977p High-resolution measurements of the bands of carbonyl sulfide between 2510 and 3150 cm⁻¹. Maki, A. G.; Wells, J. S.; Burkholder, J. B. (Mol. Phys. Div., Natl. Inst. Stand. Technol., Gaithersburg, MD 20899 USA). *J. Mol. Spectrosc.* 1991, 147(1), 173-81 (Eng). The 4 strongest absorption bands of OCS in the region from 2500 to 3150 cm⁻¹ were measured with FTS spectrometers with effective resolns. of about 0.010 cm⁻¹ or better. A total of 25 different vibrational transitions were identified in the spectrum and were analyzed to obtain improved band centers and rovibrational consts. Included in the bands identified are a few transitions due to the less abundant isotopomers, $^{16}O^{12}C^{34}S$, $^{16}O^{12}C^{33}S$, $^{16}O^{13}C^{32}S$, and $^{18}O^{12}C^{32}S$. Relative values are given for the transition moments of some of the overlapping bands.

М.Л.

C.A. 1991, 114, N26

OCS

1991

115: 59842x **Intracavity carbon monoxide laser Stark spectroscopy of the ν_3 band of carbonyl sulfide.** Masukidi, L. S.; LaHaye, J. G.; Fayt, A. (Mol. Spectrosc. Lab., Cathol. Univ. Louvain, B 1348 Louvain-la-Neuve, Belg.). *J. Mol. Spectrosc.* 1991, 148(2), 281-302 (Eng). Intracavity satn. Stark spectra with a CO laser are reported for the ν_3 band of OCS. The 137 Stark components measured between 2033 and 2063 cm-1 with an accuracy in the range of 1 MHz were assigned to $\Delta\nu_3 = 1$ transitions starting from the following levels: 00^00, 01^10, 10^00, 02^20, 02^00, 11^10, 03^30, and 12^20. Some complementary measurements on $\Delta\nu_3 = 2$ transitions, obtained with a CO_2 laser, are also reported. Some $\Pi \leftarrow \Pi$ and $\Delta \leftarrow \Delta$ transitions which do not follow the classical selection rules in l are discussed in detail. A global anal. was applied and statistical agreement with all data was obtained. An important result of this anal. is the first direct detn. of the dependence of the elec. dipole moment of OCS with the ν_3 mode. We have improved by an order of magnitude of the deduced value for the equil. dipole moment: μ_e = 0.71450(15) D. The effective dipole moments are calcd. for all vibrational states up to 5300 cm-1.

ν_3

C.A. 1991, <u>115</u>, N6

OCS

ЭМ 35862 1991

20 Б1078. Спектроскопические свойства OCS и $OCCl^+$, рассчитанные с помощью теории возмущений Мёллера — Плессета и методом конфигурац. взаимодействия. Spectroscopic properties of OCS and $OCCl^+$ by Møller — Plesset perturbation theory and configuration interaction / Peterson Kirk A., Mayrhofer Rudolph C., Woods R. Claude // J. Chem. Phys.— 1991.— 94, № 1.— С. 431—441.— Англ.

потенциальн. поверхности, мол.пост

Рассчитаны потенциальные ПВ линейных конфигураций молекулы OCS и изоэлектронного иона $OCCl^+$. Расчеты проведены с помощью теории возмущений Мёллера — Плессета 4-го порядка и методом конфигурац. вз-вия с учетом однократных и двукратных возбуждений; в последнем случае введена поправка для размерной согласованности, что существенно повысило точность результатов. Использован базис сгруппир. гауссовых ф-ций $(13s9p3d1f)/[10s7p3d1f]$ на S и Cl и $(11s7p2d1f)/[8s5p2d1f]$ на C и O. Для потен-

☒ (+1)

Х.1991, N20

циальных ПВ получены аналитич. аппроксимации и вариац. методом решена колебат. задача. Для OCS рассчитанные энергии колебат. переходов согласуются с эксперим. данными с точностью 0,4%. Предсказаны спектроскопич. постоянные $OCCl^+$. Рассчитаны также ф-ции дипольного момента и определены интенсивности колебат. переходов. Рассчитаны константы квадрупольного взаимодействия. А. А. Сафонов

OCS

От 35862 1991

6- 9Д93. **Расчет спектроскопических характеристик OCS и $OCCl^+$ с помощью теории возмущений Меллера—Плессета и метода конфигурационного взаимодействия.** Spectroscopic properties of OCS and $OCCl^+$ by Møller—Plesset perturbation theory and configuration interaction / Peterson Kirk A., Mayrhofer Rudolph C., Woods R. Claude // J. Chem. Phys.— 1991.— 94, № 1. — С. 431—441.— Англ.

Неэмпирическим методом ССП МО ЛКАО в базисе гауссовых ф-ций 11*s*7*p*2*d*1*f*/13*s*9*p*3*d*1*f*, сгруппированном в 8*s*5*p*2*d*1*f*/10*s*7*p*3*d*1*f*, с учетом корреляции электронов в четвертом порядке теории возмущений Меллера—Плессета и методом конфигурац. взаимодействия исследовано электронное строение OCS (I) и $OCCl^+$ (II). Приведены равновесная геометрия, ф-ции потенц. энергии, различные спектроскопич. постоянные, ф-ции дипольных моментов, константы квадрупольного взаимодействия, энергии диссоциации и потенциалы ионизации. Полученные результаты согласуются с имеющимися эксперим. данными. В. Л. Лебедев

М-п.

☒

(Н)

ф. 1991, N9

CSO 1991

Prinslow Douglas A.,
Armentrout P. B.

(D_0) J. Chem. Phys. 1991, 94,
(5), 3563-7.

(см. CS_2^+ ; III)

OCS

1991

115: 81113g FTIR measurements on the $3\nu_2-\nu_2$ band of carbonyl sulfide. Tan, T. L.; Looi, E. C. (Fac. Sci., Natl. Univ. Singapore, Singapore, Singapore 0511). *J. Mol. Spectrosc.* 1991, 148(1), 262–4 (Eng). The $2\nu_2$ band of OCS is commonly used as a waveno. calibration std. in the 1050 cm^{-1} region and its first hot band $3\nu_2-\nu_2$ has been used as a secondary calibration std. Recently, the $3\nu_2-\nu_2$ band has been measured using the heterodyne frequency and Stark spectroscopic techniques. The measured frequencies, combined with calcd. data, give accurate mol. consts. An interest in OCS as an important mol. for calibration purposes is also shown by the work of Fayt et al. (5) who conducted a global rovibrational anal. on OCS based on different measurements. Good ests. of effective level consts. and their uncertainties were given for states up to 4950 cm^{-1}.

ИК спектр.

М.П.

C.A.1991, 115, N8

COS

1991

115: 81114h **Hot-band spectrum of carbonyl sulfide near 850 cm^{-1}.** Tan, T. L; Looi, E. C.; Lua, K. T. (Fac. Sci., Natl. Univ. Singapore, Singapore, Singapore 0511). *J. Mol. Spectrosc.* **1991**, 148(1), 265–9 (Eng). An anal. is presented of the hot-band spectra of COS near 850 cm^{-1} with spectral consts. derived in the anal.

м.л.

C.A. 1991, 115, N 8

COS

1993

118: 48265x **Hot-band spectrum of carbon dioxide near 700 cm^{-1} and the ν_1 band of carbonyl sulfide $OC^{34}S$.** Tan, T. L.; Lee, E. C.; Lee, K. K. (Fac. Sci., Natl. Univ. Singapore, Singapore, Singapore 0511). *J. Mol. Spectrosc.* 1993, 157(1), 261-7 (Eng). The IR spectra were measured for $CO^{34}S$ in the vapor phase. The line positions and mol. consts. are given.

ИК спектр,
М.П.

C. A. 1993, <u>118</u>, N6

OCS

1993

118: 222325d **Rydberg spectroscopy of carbonyl sulfide: new assignments in the 70,000–74,000 cm^{-1} energy region.** Weinkauf, R.; Boesl, U. (Inst. Phys. Theor. Chem., Tech. Univ. Muenchen, 8046 Garching, Germany). *J. Chem. Phys.* 1993, 98(6), 4459–70 (Eng). The first Rydberg states of OCS were reinvestigated by applying a combination of several spectroscopic methods. The comparison of (2+1)- and (3+1)-multiphoton ionization (MPI) and one photon absorption spectra reveals quite different intensities indicating different symmetries of the involved Rydberg states. Assuming propensity rules for the ionization process and by measuring the ion ground state population with (2+1)-MPI photoelectron spectroscopy, it was possible to find new assignments for the spin-orbit components of the ion core and vibrational structures in the Rydberg states. Characteristic isotopic shifts in the (2+1)-MPI spectra confirm these assignments and deliver addnl. arguments for the identification of transitions to bending vibrations. In particular, for the bending vibration split by Renner-Teller interaction, ambiguities in the MPI photoelectron (PE) spectra could be solved by photodissocn. spectroscopy of the OCS$^+$ ions prepd. by (2+1)-MPI using the Rydberg transitions as intermediate resonances.

Ридберг. сост.

C.A. 1993, 118, N22

OCS

1994

122: 67093p Sub-Doppler frequency measurements on OCS at 87 THz (3.4 μm) with the CO overtone laser. Dax, A.; Wells, J. S.; Hollberg, L.; Maki, A. G.; Urban, W. (Time Frequency Division, National Institute Standards Technology, Boulder, CO 80303 USA). *J. Mol. Spectrosc.* **1994,** 168(2), 416–28 (Eng). Sub-Doppler frequency measurements have been made on three transitions of OCS in the 87-THz region (near 2900 cm^{-1}). The CO overtone laser was used as the satg. laser. Polarization spectroscopic techniques utilizing optical heterodyne detection were used to observe the features and subsequently provide the discriminant for locking the overtone laser to the OCS transitions. A CO_2 laser synthesizer was used to measure the frequency of the CO overtone laser and thereby measure the frequencies of the OCS lines. The resulting frequencies of the three new measurements are: 10^01-00^00 P(27), 87 117 278.496(50) MHz; $11^{1f}1-01^{1f}0$ R(14), 87 222 001.143(70) MHz for OCS; and for the $OC^{34}S$ 10^01-00^00 P(9), 87 010 586.667(75) MHz, where the nos. in parentheses are the uncertainties in the last digits. These new nos. have been fitted along with more than 5700 other data points in our OCS data bank and improved consts. have been obtained. These latest consts. are used to calc. updated calibration tables contg. values with much smaller uncertainties; three such tables are included.

уровни и (константы)

C. A. 1995, 122, N6

OCS

1994

122: 146126e Laser spectroscopy of mol. ions: the A–X transition in the OCS radical cation. Weinkauf, R.; Boesl, U. (Inst. fuer Phys. und Theoretische Chemie, Technische Universitaet Muenchen, 85747 Garching, Germany). *J. Chem. Phys.* **1994**, 101(10), 8482–93 (Eng). Spectroscopy of the OCS$^+$ ion in its ground and first excited states has been performed over a wide energy range using one–photon dissocn. spectroscopy. We used multiphoton ionization in the first step for state selective ion prepn. ion single well–defined vibrational and spin orbit states. This simplifies the ion spectra of the transition to the first excited A state considerably and delivers the information of the ion ground state by using hot ion prepn. For the stretching vibrations anharmonicities have been obsd. and for the first overtone of the bending vibration Fermi resonances have been found. Rotational consts. could be detd. for the vibrational ground states of the X and A ionic states in both spin–orbit components. A new double resonance technique was applied to measure vibrational frequencies in the ionic X ground state.

(A–X)

Вращ.
пост.

C.A. 1995, 122, N 12

1995

F: OCS
P: 3

2Б1227. Фурье-спектроскопия карбонилсульфида от 1800 до 3120 см{-1}. Нормальные образцы. Fourier transform spectroscopy of carbonyl sulfide from 1800 to 3120 cm{-1}: The normal species / Belafhal A., Fayt A., Guelachvili G. // J. Mol. Spectrosc. - 1995. - 174, N 1. - C. 1-19. - Англ.

На ИК-фурье-спектрометре в области частот 1800-3120 см{-1} с разрешением 0,007 см{-1} и точностью 3*10{-5} см{-1} измерены частоты и интенсивности 117 различных колебательных переходов карбонилсульфида. Выполнен глобальный анализ для образца {16}O{12}C{32}S. Полученные результаты могут быть использованы при составлении стандарта частоты. Библ. 33.

РЖХ 1997

OCS

1995

6Б1278. Абсолютные интенсивности переходов в $^{16}O^{12}C^{32}S$. Область 2500—3100 см$^{-1}$. Absolute intensities in $^{16}O^{12}C^{32}S$: The 2500—3100 cm^{-1} region / Errera Q., Auwera J. V., Belafhal A., Fayt A. // J. Mol. Spectrosc.— 1995 .— **173**, № 2 .— С. 347—369 .— Англ.

В области 2500—3100 см$^{-1}$ с высокой точностью измерены абс. интенсивности около 400 отдельных линий вращат. структуры полос $3\nu_1$, $\nu_2^1+\nu_3$, $2\nu_1+2\nu_2^0$, $\nu_1+4\nu_2^0$, $\nu_1+\nu_3^1$ и $2\nu_2^0+\nu_3$ $^{16}O^{12}C^{32}S$. Рассчитаны интегральные интенсивности полос, дипольные моменты переходов, значения факторов Германа—Уоллиса. Рассмотрены проявления различных резонансов (ангармонических, l-типа) между верхними колебат. состояниями. В. М. Ковба

М.П.

Х. 1997, N6

OCS 1995

Martin Jan M. L.,
Francois Jean-Pierre,
et al.

ab initio,
сил. пост.,
Vi

J. Mol. Spectrosc. 1995,
169 (2), 445-57.

(см. H_2S; III)

OCS 1995

Walker A. R., Hight,
Chen Wei, et al.

вращат. пост.

J. Chem. Phys. 1995,
<u>102</u>(19), 7298–305.

(см. HBr; III)

OCS

OM 37820

1995

122: 199866c Sub–Doppler frequency measurements on OCS near 1689 and 1885 cm^{-1}. Wells, J. S.; Dax, A.; Hollberg, L.; Maki, A. G. (Time and Frequency Div., Nat'l. Inst. Standards Technology, Boulder, CO 80303 USA). *J. Mol. Spectrosc.* **1995,** 170(1), 75–81 (Eng). We have used an optical polarization heterodyne technique to measure the frequencies of two OCS lines, one near 5.3 μm and the other near 5.9 μm. These sub–Doppler measurements gave 56,533 766.125 ± 0.035 MHz for the $2\nu_2 + \nu_3$ P(16) transition and 50,627 632.013 ± 0.100 MHz for the $2\nu_3$ P(48) line. The P(16) measurement is in excellent agreement (20 kHz) with a new result obtained with an alternate technique by a group at the University of Bonn. The $2\nu_3$ measurement was combined with other frequency measurements to produce an improved calibration table for the $2\nu_3$ OCS band near 1700 cm^{-1}. These and other sub–Doppler frequency measurements in different spectral regions give improved frequencies for a no. of OCS bands. These new frequencies will soon be incorporated into calibration data that will be available over the Internet.

(Pi)

C.A. 1995, 122, N 16

1995

F: OCS
P: 3

6Б166. Гиперсферические кинематические колебательные координаты линейных трехатомных молекул. Hyperspherical kinematic vibrationa coordinates for linear triatomic molecules / Zuniga Jose, Bastida Adolfo, Alaci Mercedes, Requena Alberto // J. Phys. Chem. - 1995. 99, N 28. - C. 11051-11060. - Англ.

Для описания молек. колебаний линейных трехатомных молекул использован набор гиперсферич. кинематич. координат. Величины внутренних ортогональных векторов и угол между ними определяют набор кинематич. колебательных координат, к-рые затем преобразуются в обобщенные гиперсферич. координаты. В результате гиперсферич кинематич. система содержит три параметра оптимизации. Для линейной трехатомной молекулы с помощью подходящего выбора параметров смещения эту систему можно свести к криволинейной нормальной системе. В качестве иллюстрации приведены расчеты уровней колебательной энергии молекул OCS и N[2]O. Результаты сопоставлены с эксперим. значениями. Библ. 78.

Р.ЖХ. N 6, 1996

OCS

1996

125: 259889m Resonance enhanced multiphoton ionization spectroscopy of carbonyl sulfide. Morgan, Ross A.; Orr–Ewing, Andrew J.; Ascenzi, Daniela; Ashfold, Michael N. R.; Buma, Wybren Jan; Scheper, Connie R.; de Lange, Cornelis A. (Sch. Chem., Univ. Bristol, Bristol, UK BS8 1TS). *J. Chem. Phys.* **1996**, 105(6), 2141–2152 (Eng). Rydberg excited states of the OCS mol. in the energy range 70500–86000 cm^{-1} were studied via the 2 and 3 photon resonance enhancements they provide in the mass resolved multiphoton ionization (MPI) spectrum of a jet–cooled sample of the parent mol. Spectral interpretation was assisted by companion measurements of the kinetic energies of the photoelectrons that accompany the various MPI resonances. The earlier conclusions of R. Weinkauf and U. Boesl (1993) are supported regarding 5 Rydberg origins of 70,500–73,000 cm^{-1} energy, attributable to, resp., states of $^3\Pi$, $^1\Pi$, $^3\Delta$, $^1\Delta$, and $^1\Sigma^+$ symmetry arising from the $4p\lambda \leftarrow 3\pi$ orbital promotion. A further 21 Rydberg origins are identified at higher energies. These partition into clumps with quantum defects ~3.5 and 4.5, which are assocd. with the orbital promotions $np\lambda \leftarrow 3\pi$ (n = 5,6), and others with near integer quantum defect which are interpretable in terms of excitation to s, d, and (possibly) f Rydberg orbitals. MPI

Ридберг.
состоян

C. A. 1996, 125, N 20

resonance attributable to CO ($X\ ^1\Sigma^+$) fragments and to S atoms in both their ground (^1P) and excited (^1D) electronic states are identified. Anal. of the former of the former resonances confirms that the CO(X) fragments resulting from 1 photon dissocn. of OCS and excitation wavelengths ~230 nm are formed with a highly inverted, bimodal rotational state population distribution, while the latter are consistent with previous reports of the wavelengths dependence for forming ground and excited state S atoms in the near UV photolysis of OCS.

OCS

1996

6Б1275. **Субдоплеровские гетеродинные измерения частот вблизи 5 мкм с лазерной системой на боковой полосе CO. Улучшенные калибровочные таблицы для переходов карбонилсульфида.** Sub-Doppler heterodyne frequency measurements near 5 μm with a CO-laser sideband system: Improved calibration tables for carbonyl sulfide transitions / Saupe S., Wappelhorst M. H., Meyer B., Urban W., Maki A. G. // J. Mol. Spectrosc.— 1996 .— **175**, № 1 .— С. 190—197 .— Англ.

На субдоплеровском гетеродинном (смешение частот двух CO_2-лазеров) CO-лазерном спектрометре на боковой полосе в области частот около 2050 см$^{-1}$ или 61 ТГц с точностью 21—84 кГц измерены колебательно-вращат. переходы семи колебат. полос $^{16}O^{12}C^{32}S$ и трех полос $^{16}O^{12}O^{34}S$. Определены уточненные значения молекулярных постоянных и на основе их составлены калибровочные таблицы в области частот от 860 до 3100 см$^{-1}$ для основного изотопич. образца карбонилсульфида.

С. Н. Мурзин

М·П.

X. 1997, N6

OCS

1997

ближний ИК спектр

127: 72337d Vibrational overtone transitions of OCS in the near infrared. Yang, Xiaoke; Noda, Chifuru (Dep. Chemistry, Univ. New Hampshire, Durham, NH 03824 USA). *J. Mol. Spectrosc.* 1997, 183(1), 151–156 (Eng), Academic. Vibrational overtone transitions of OCS in the near IR, 10,000–14,000 cm^{-1}, are obsd. for the 1st time by the photoacoustic technique. The spectra are analyzed using mol. parameters and Hamiltonians derived for energy levels <5000 cm^{-1}. The mol. parameters of OCS for the low vibrational states can be extended to higher vibrational states within exptl. accuracy. A total of 14 transitions in three polyad groups were assigned. Strong perturbations were obsd. in these highly excited states of OCS.

C.A. 1997, 127, N5

OCS OM · 38947 1997

Спектроск.
постоян.

Youngshang Pak and
R. Claude Woods,

J. Chem. Phys.,
1997, 107 (13),
5094–5102

OCS

1998

Gutsev G.L. et al.,

J. Chem. Phys. 1998,

(Ae, стр-ра) 108 (16), 6756-62

(см. CO_2; III)

OCS^- 1998

Gutsev G.L. et al.,

(Ae, стр-ра) J. Chem. Phys. 1998,
108 (16), 6756-62

(см- CO_2; III)

OCS

Оп 39557 а'' 1998

130: 73146q **Fourier transform spectroscopy of carbonyl sulfide from 3700 to 4800 cm^{-1} and selection of a line-pointing program.** Naim, S.; Fayt, A.; Bredohl, H.; Blavier, J.-F.; Dubois, I. (Lab. Spectroscopie Mol., Chem. Cyclotron, Univ. Catholique Louvain, B1348 Louvain-la-Neuve, Belg.). *J. Mol. Spectrosc.* 1998, 192(1), 91-101 (Eng), Academic Press. The authors have measured the Fourier transform spectrum of natural OCS from 3700 to 4800 cm^{-1} with a near Doppler resoln. and a line-position accuracy between 4 and 8 × 10^{-5} cm^{-1}. For the normal isotopic species, 37 vibrational transitions were analyzed for both frequencies and intensities. The authors also report 15 bands of $OC^{34}S$, eight bands of $O^{13}CS$, nine bands of $OC^{33}S$, and two bands of ^{18}OCS. Important effective Herman-Wallis terms are explained from eigenvectors. A comparison of different line-pointing programs is also presented. (c) 1998 Academic Press.

(FTIR (спектр))

C.A. 1999, 130, N6

OCS

1998

(FTIR-спектр, νi)

129: 267224p **Fourier transform spectroscopy of carbonyl sulfide from 4800 to 8000 cm^{-1} and new global analysis of $^{16}O^{12}C^{32}S$.** Rbaihi, E.; Belafhal, A.; Auwera, J. Vander; Naim, S.; Fayt, A. (Faculte des Sciences, Universite Chouaib Doukkali, El Jadida, Morocco). *J. Mol. Spectrosc.* **1998**, 191(1), 32–44 (Eng), Academic Press. The authors have measured the FT spectrum of natural OCS from 4800 to 8000 cm^{-1} with a near Doppler resoln. and a line-position accuracy between 2 and 8×10^{-4} cm^{-1}. For the normal isotopic species $^{16}O^{12}C^{32}S$, 37 vibrational transitions were analyzed for both frequencies and intensities. The authors also report 6 bands of $^{16}O^{12}C^{34}S$, 5 bands of $^{16}O^{13}C^{32}S$, 2 bands of $^{16}O^{12}C^{33}S$, and 2 bands of $^{18}O^{12}C^{32}S$. Important effective Herman–Wallis terms are explained by the anharmonic resonances between closely spaced states. As those results complete the study of the Fourier transform spectra of natural carbonyl sulfide from 1800 to 8000 cm^{-1}, a new global rovibrational anal. of $^{16}O^{12}C^{32}S$ was performed. The authors detd. a set of 148 mol parameters, and a statistical agreement is obtained with all the available exptl. data. (c) 1998 Academic Press.

C.A. 1999, 129, N20.

OCS

1998

130: 17418t Probing molecular site structure in low-temperature matrixes: An EXAFS study of carbonyl sulfide in solid argon. Roubin, P.; Varin, S.; Crepin, C.; Gauthier-Roy, B.; Flank, A.-M.; Delaunay, R.; Pompa, M.; Tremblay, B. (P2IM, Centre Saint-Jerome, Universite de Provence, 13 397 Marseille, Fr.). *J. Chem. Phys.* 1998, 109(18), 7945–7948 (Eng), American Institute of Physics. The authors present here an EXAFS (extended x-ray absorption fine structure) expt. performed at the K edge of the S atom of OCS isolated in an Ar matrix. The aim was to elucidate the structure of the trapping site of the mol. The Ar atoms are located at a mean distance of 3.78 Å from the S atom, with a root mean square variation of the S–Ar distances of ~0.08 Å. Results indicate that the host atoms occupy a statistical set of positions around the mol., rather than well-defined sites.

структура,
в Ar матрице

C. A. 1999, 130, N2

OCS

1998

FTIR-спектр

93 полосы

впервые

проанализированы

129: 101338d Fourier transform spectroscopy of ^{18}O–enriched carbonyl sulfide from 1825 to 2700 cm^{-1}. Strugariu, T.; Naim, S.; Fayt, A.; Bredohl, H.; Blavier, J. F.; Dubois, I. (Molecular Spectroscopy Lab., Catholic Univ. Louvain, B 1348 Louvain–la–Neuve, Belg.). *J. Mol. Spectrosc.* 1998, 189(2), 206–219 (Eng), Academic Press. The authors have measured the Fourier transform spectrum of carbonyl sulfide from 1825 to 2700 cm^{-1}, using a sample enriched in both ^{18}O (94.0%) and ^{17}O (1.54%). A careful calibration yields a line–position accuracy between 1.5 and 3.0 10^{-5} cm^{-1}. The authors obsd. and analyzed 118 IR bands of which 93 are measured for the 1st time: 55 for $^{18}O^{12}C^{32}S$, 20 for $^{18}O^{12}C^{34}S$, 11 for $^{18}O^{12}C^{33}S$, 1 for $^{18}O^{12}C^{36}S$, 12 for $^{17}O^{12}C^{32}S$, 4 for $^{17}O^{12}C^{34}S$, 2 for $^{17}O^{12}C^{33}S$, and 13 for $^{18}O^{13}C^{32}S$. Intensities are also reported and analyzed for all those bands. The intensity accuracy is better than 10%, and the precision of ~1% allows one to det. some Herman–Wallis coeffs.

CA 1998, 129, №8

OCS 1999

Zheng, Yujun; et al.,

теорет.
расчет
колебат.
уровней

Phys. Lett. A 1999,
256 (2,3), 197–204

(См. HC N; III)

2000

F: OCS
P: 3
133:35539 Terahertz Measurements of Rotational Transitions in Vibrationally Excited States of OCS. [Erratum to document cited in CA132:228857].
Morino, I.; Yamada, K. M. T.; Maki, A. G.
National Institute Advanced Interdisciplinary Research (NAIR) Tsukuba, Ibaraki 305-8562, Japan J. Mol. Spectrosc., 200(2), 290 (English) 2000

C. A. 2000

OCS

2000

134: 199895j More Sub–Doppler Heterodyne Frequency Measurements on OCS between 56 and 63 THz. Murtz, M.; Palm, P.; Urban, W.; Maki, A. G. (Institut fur Angewandte Physik der Universitat Bonn, D–53115 Bonn, Germany). *J. Mol. Spectrosc.* **2000**, 204(2), 281–285 (Eng), Academic Press. By using tunable microwave sidebands added to CO–laser lines, the authors have made more sub–Doppler heterodyne frequency measurements on OCS. Three new

(спектр)

C.A.-2001, 134, N14

rotational transitions were measured for each of 3 absorption bands $10^{0}0-00^{0}0$, $02^{0}1-00^{0}0$, and $03^{1}1-01^{1}0$. The abs. uncertainties of th measurements are on the order of ±25 kHz. New calibration tables ar given for the region 1860−1925 and 2020−2085 cm^{-1} based on the mos recent OCS measurements. (c) 2000 Academic Press.

2000

F: OCS
P: 3
133:301513 Excited vibrational states and potential energy function for OCS determined using generalized internal coordinates. Zuniga, Jose; Bastida, Adolfo; Alacid, Mercedes; Requena, Alberto Departamento de Quimica Fisica, Universidad de Murcia Murcia 30100,

Spain J. Chem. Phys., 113(14), 5695-5704 (English) 2000. Variational calcns. of excited vibrational states for the OCS mol., using generalized internal coordinates properly optimized, are presented. The calcns. are made for two empirical and one ab initio potential energy surfaces previously reported. It is shown that the computed vibrational frequencies differ considerably from the exptl. values for the three potential surfaces employed. Consequently a new and much more accurate potential surface is detd. for OCS by nonlinear least-squares fitting to the obsd. vibrational terms. The surface is expressed as a Morse-cosine expansion in valence coordinates and its quality is checked by computing the vibrational frequencies of three isotopic species of the mol.

OCS От. 40967 2001

Koichiro Mitsuke* and Masakazu Mizutani;

Bull. Chem. Soc. Jpn., 2001, <u>74</u>, 1193–1201.

UV and Visible Emission

Spectra from the Photodissociation of Carbonyl Sulfide Using Synchrotron Radiation at 15-30 eV.

OCS^+ 2001

OCS^-

ИК спектр в Ne матр.

135: 233162a **The infrared spectra of OCS^+ and OCS^- trapped in solid neon.** Lugez, Catherine L.; Thompson, Warren E.; Jacox, Marilyn E. (Optical Technology Division, National Institute of Standards and Technology, Gaithersburg, MD 20899−8441 USA). *J. Chem. Phys.* 2001, 115(1), 166−173 (Eng), American Institute of Physics. When a Ne:OCS sample was codeposited at approx. 5 K with a beam of neon atoms that were excited in a microwave discharge, the IR spectrum of the resulting deposit included absorptions which can be assigned to OCS^+, OCS^-, and one or more dimer ions. Detailed isotopic substitution studies support the assignments offered for OCS^+ and OCS^-. The CO−

C.A. 2001, 135, N16.

and CS−stretching absorptions obsd. for OCS$^+$ isolated in a neon matrix lie close to the corresponding gas−phase band centers. The CO− and CS−stretching fundamentals of OCS$^-$ isolated in solid neon were obsd. for the first time at 1646.4 and 718.2 cm−1, resp. These frequencies are in good agreement with values previously calcd. using ab initio and d. functional methods. The least−squares force const. fit to the data obtained in isotopic substitution expts. supports the proposed assignment. Dimer ions were also stabilized, but IR data for these species were insufficient to provide definitive assignments.

2001

F: OCS
P: 3

134:302349 **Doppler-Free Two-Photon Millimeter Wave Transitions in OCS and CHF3.** Surin, L. A.; Dumesh, B. S.; Rusin, F. S.; Winnewisser, G.; Pak, I. I. Physikalisches Institut, Universitat zu Koln, Koln, Germany. Phys. Rev. Lett. (2001), 86(10), 2002-2005. in English.

Doppler-free 2-photon rotational transitions J = 13 ←← 11 and J = 12 ←← 10 of OCS and J = 8 ←← 6 and J = 7 ←← 5 of CHF3 were detected in the frequency range 134-156 GHz, using a novel, highly sensitive intracavity-jet technique. The sub-Doppler narrowing of the obsd. peaks (down to 40 kHz full width at half max. as compared to 300 kHz of the Doppler width) demonstrates the potential of this new technique for high precision millimeter wave spectroscopy. The possibilities of the further redn. of the 2-photon absorption line widths are considered.

OCS – orthoH_2 Om 41 228 2002
OCS – paraH_2
OCS – paraD_2 Jian Tang and A.R.W McKel-
OCS – orthoD_2 lar,

J. Chem. Phys., 2002,
116, N 2, 646 – 653

Infrared spectra ~~of~~ OCS –

hydrogen complexes.