C-O-S

8200

OCS_2 (α, газ, силовые постоянные) 1962

Kuchitsu K., Jijima T., Kopino Y.,
Tokyo, 1962, (C308), 4pp
Proc. Intern. Symp. Mol. Struct. Spectry.
Physicel...

CO_2; CS_2; OCS_2; N_2O; HCN; DCN; H_2O;
HDO; D_2O; H_2S; HDS; D_2S; CA, 1964, 61, N7, 7841h

CS_2O

1554

1963

CSO_3^- (силовые пост.,расчет)

Nagarajan G.
Potential constants of some XY_3Z type ions. "J.Scient.and Industr.Res.", 1962,B21, N 1, 42-43 (англ.)

РХ.,1963, 1, Б23

40892

O + OCS +

1976
4837

Manning Ronald G., Braun Walter, Kurylo Michael J. The effect of infrared laser excitation on reaction dynamics: $O+C_2H_4$ and O+OCS. "J. Chem. Phys.", 1976, 65, N 7, 2609-2615 (англ.)

60210.6664
Ch,Ph,TC,Ex-

96201
C C30S (и.п.)

XIV-7325
1976

Winnewisser Manfred, Christiansen Jørn Johs. Detection of the microwave spectrum of tricarbon oxide sulphide, C_3OS. "Chem. Phys. Lett.", 1976, 37, N 2, 270-275

(англ.)

0554 ПРИК

40

535 536

ВИНИТИ

OC_3S 1981

Winnewisser G., Yamada K.
et al.

спектр Laser Spectrosc. 5. Proc.
5 Int. Conf., Jasper, 29 Ju-
ne-3 July, 1981. Berlin e.a.,
1981, 268–271.

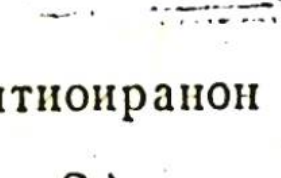
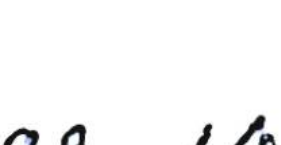
(см. HC_3N; III)

OCS_2

1982

18 Б12. Поверхность потенциальной энергии синглетного состояния молекулы OCS_2. Carlsen L. On the OCS_2 singlet potential energy surface. «J. Comput. Chem.», 1982, 3, № 1, 23—27 (англ.)

поверхность потенц. энергии

Теоретически изучена газофазная р-ция между $O(^3P)$ и CS_2. Рассмотрены возможные внутримолек. равновесия с образованием пяти различных продуктов р-ции. Путем расчета методом ППДП/В всевозможных энергетич. профилей для различных равновесий показано, что наиболее вероятными продуктами являются дитиоиранон  и оксатиран-тион  или дисульфидоксид $S{=}C{=}\overset{+}{S}{-}\overline{O}$. Построена полная схема внутримолек. перегруппировок в указанной системе.

С. Долин

Ж. 1982, 19, № 18.

C_3OS | Оттиск 15494 | 1982

Winnewisser M., Peau W.

Вращат. постоян., ф-ие дипольн. момента

Chem. Phys., 1982, 71, N 3, 377-387.

$(OCS)_2$

1984

Lolue James M.,
Rice Jane K., et al.

спектр.
(ошиб. мол.)
пучка

Chem. Phys. Lett.
1984, 112 (4), 376-80.

● (сл. $(CO_2)_2$; III)

$CS_2 + O$

1984

3 Б1124. Анализ. II. Фотоионизационная масс-спектрометрия. Washida Nobuaki. «Оё буцури, Oyo Buturi», 1984, 53, № 7, 608 (яп.)

Методом масс-спектрометрии при фотоионизации с помощью аргоновой лампы с фильтром из LiF (11,8; 11,6 эВ) и криптоновой лампы с фильтром из MgF_2 (10,6; 10,0 эВ) изучены продукты взаимодействия CS_2 с атомарным кислородом. В масс-спектрах продуктов р-ции обнаружены ионы $[S]^+$, $[CS]^+$, $[SO]^+$, $[COS]^+$, $[S_2]^+$. Ион $[S]^+$ удалось идентифицировать в присутствии O_2 при 10,6 эВ благодаря более высокому потенциалу ионизации O_2 (12,07 эВ). Приведены схема реакц. камеры, соединенной с ионным источником масс-спектрометра, а также масс-спектры продуктов р-ции CS_2 с O. Пред. сообщ. см. Washida N., Takagi H., «J. Am. Chem. Soc.», 1982, 104, № 1, 168. А. Кирюшкин

Х. 1985, 19, N 3.

OC3S от 20937 1984

6 Д60. Определение структуры трикарбооксисульфида (O-C-C-C-S) в зависимости от колебательного квантового числа v_7 методом изотопозамещения. The structure of tricarbon oxide sulfide, O-C-C-C-S, as a function of the vibrational quantum number v_7, determined by the isotopic substitution method. Winnewisser Manfred, Peau E. Walter. «Acta phys. hung.», 1984, 55, № 1—4, 33—44 (англ.)

м.л., геометр. структура

В диапазоне 26,5—40 ГГц исследованы МВ-спектры 5 изотопич. модификаций молекулы O-C-C-C-S. Идентифицированы линии вращательных переходов с J = =13—12 и 14—13 в колебательных состояниях с v_7 = =0, 1, 2. Определены значения равновесной вращательной постоянной B_e и постоянных α_7, γ_{77}, характеризующих зависимость B_e от v_7. Из полученных значений B_e вычислены структурные параметры OC_3S: OC = =1,1343, C_1-C_2 = 1,2696, C_2C_3 = 1,2540, C_3S = 1,5825 Å.

оп. 1985, 18, N6

C_3OS .Om. 20934 1984

102: 122258k **The structure of tricarbon oxide sulfide, O=C=C=C=C=S, as a function of the vibrational quantum number v_7, determined by the isotopic substitution method.** Winnewisser, Manfred; Poau, E. Walter (Phys. Chem. Inst., Justus-Liebig-Univ. Giessen, D-6300 Giessen, Fed. Rep. Ger.). *Acta Phys. Hung.* 1984, 55(1-4), 33-44 (Eng). The mol. structure of tricarbon oxide sulfide was detd. by the substitution method using the rotational consts. of 5 isotopic species. Since the lowest-lying bending mode v_7 in C_3OS is at 82.6 cm^{-1} the vibrational dependence of the mol. structure on this particular mode could be detd. By removing the vibrational dependence of the mol. structure on v_7 an effective equil. structure was obtained: O=(1.1343 Å)(C=(1.2696 Å)C=(1.2540 Å)C=(1.5825 Å)S. An interpretation of the pronounced vibrational dependence of the mol. structure on the excitation of the bending mode v_7 is presented in the light of the stretch-bend interaction introduced by P. R. Bunker (1980) in the semi-rigid bender anal. of the quasilinear mol. carbon suboxide, O=C=C=C=O.

(спрегнегра)

C. A. 1985, 102, N 14.

CO_2S^{4-2} Оп. 21631 1985

12 Л205. Изучение матрично-изолированных моно- и дитиокарбонатных анионов методом ИК-спектроскопии. Infrared matrix-isolation investigation of the mono- and dithiocarbonate anions. David Shelle J., Ault Bruce S. «Inorg. Chem.», 1985, 24, № 7, 1048—1051 (англ.)

Получены ИК-спектры (1500—550 $см^{-1}$) моно- и дитиокарбонатных анионов CO_2S^{2-} и COS_2^{2-} в составе комплексов с катионами Tl^+, а также их ^{13}C- и ^{18}O-изотопич. аналогов, изолированных в аргоновых матрицах при т-ре 12 К. Проведен анализ нормальных колебаний (К) матрично-изолированных анионов. Рассчитаны значения частот нормальных К и силовых постоянных связей в структуре этих анионов. Интенсивные ИК-полосы с малой шириной 1445 и 1202 $см^{-1}$ в спектре матрично-изолированных анионов CO_2S^{2-} приписаны валентным К связей С—О. Частота валент-

Ді, геометр., структ. ⊕ ⊗ Оф. 1985, 18, N12

COS_2^{2-}

ного К связи С—S в этих анионах равна 603 $см^{-1}$. Наиболее интенсивные ИК-полосы 1506 и 606 $см^{-1}$ в спектре анионов COS_2^{2-} отнесены к валентным К связей С—О и антисим. валентным К связей С—S, соответственно. Предположено, что при увеличении числа атомов серы в составе анионов происходит увеличение степени локализации π-электронной плотности в области связи С—О. Библ. 18. И. В. А.

CO_2S^{2-} ОМ. 24631 1985

22 Б1215. Исследование методом инфракрасной спектроскопии моно- и дитиокарбонатных анионов, изолированных в матрице. Infrared matrix-isolation investigation of the mono- and dithiocarbonate anions. David S., Ault B. «Inorg. Chem.», 1985, 24, № 7, 1048—1051 (англ.)

ИК спектры

Измерены ИК-спектры (1600—400 $см^{-1}$) продуктов соконденсации паров Tl_3O с OCS (I) и паров Tl_2O с CS_2 (II), изолированных в матрице Ar при т-ре 12 К. В спектре продуктов I наблюдаются интенсивные полосы при 1445, 1202 и 603 $см^{-1}$, отнесенные к вал. кол. иона CO_2S^{2-} ионной триады $Tl^+CO_2S^{2-}Tl^+$. Полосы при 1445 и 1202 $см^{-1}$ отнесены к кол. фрагмента CO_2, а полоса 603 $см^{-1}$ — к кол. связи C—S. В спектре продукта II имеются 2 полосы при 1506 и 606 $см^{-1}$, отнесенные к кол. ν(CO) и ν(CS) соотв. иона COS_2^{2-} ионной триады $Tl^+COS_2^{2-}Tl^+$. Отнесение подтверждено данными по изотопич. сдвигам полос при замещениях $^{16}O \rightarrow {}^{18}O$ и $^{12}C \rightarrow {}^{13}C$, а также данными расчета нормальных колебаний ионов CO_2S^{2-} и CO_2S^{2-}. И. А. Гарбузова

(71) ⊗

Х. 1985, 19, № 22

OC_3S 1986

Holland F., Winnewisser M., et al.

Proc. 9th Int. Conf. High Resolut. Infrared. Spectrosc.; Liblice near Prague, Sept. 8-12, 1986. Progr. Sess. Abstr. Pap. Prague, s.a.; 94. (cit. C_3S_2; III)

Оп. 24632

1986

$(OCS)_2$

Miller R.E.,

библиографии по спектроскопии

J. Phys. Chem., 1986, 90, N 15, 3301–3313.

(Оп. 27163) 1987

SO_2 – CO

(система) Пинковски Е., Сэлэгяну Е., Джанэ Д.,

расчет состава Rev. chim. (RSR), 1987, 38, № 2, 113–119.

[OCSk] (от. 27893) 1987

Вигасин А. А.,

структура, Di, сил. пост. (обзор)

Ж. структур. химии, 1987, 28, N5, 120–147.

OCS ... CO_2

1988

Оп. 29351

108: 84483u **Determination of the structure of the carbonyl sulfide-carbon dioxide complex (OCS CO_2).** Novick, Stewart E.; Fraser, R. D.; Lovas, F. J. (Dep. Chem., Wesleyan Univ., Middletown, CT 06457 USA). *J. Chem. Phys.* 1988, 88(2), 687-90 (Eng). The rotational spectrum of the weakly bound complex OCS-CO_2 was measured using a pulsed beam Fourier transform microwave spectrometer. The rotational consts. of the major isotopomer are (in MHz) A = 4454.606, B = 1517.778, and C = 1329.666. The mol. is planar with a slipped near parallel structure analogous to the structure of $(CO_2)_2$. The S atom occupies the inner position; this is the obtuse rather than the acute vertex of the O-C-O-S quadrangle. The distance from the center-of-mass (c.m.) of CO_2 to the c.m. of OCS is 3.552 Å.

Брашан. спектр A, B, C, спруж. параметр.

C. A. 1988, 108, N 10.

OCS—CO_2 Оп. 29351 1988

17 Б1311. Определение структуры OCS CO_2. Determination of the structure of OCS CO_2. Novick S. E., Seunram R. D., Lovas F. J. «J. Chem. Phys.», 1988, 88, № 2, 687—690 (англ.)

С помощью микроволнового фурье-спектрометра измерен вращат. спектр слабосвязанных комплексов $OC^{32,34}S—CO_2$ образующихся в импульсном сверхзвуковом пучке. Значения спектроскопич. параметров комплекса ($OS^{32}S—CO_2$): $A=4454{,}606$ МГц, $B=1517{,}7781$ МГц, $C=1129{,}6662$ МГц, $\Delta_J=4{,}822$ кГц, $\Delta_K=20{,}3$ кГц, $\delta_J=1{,}390$ кГц, $\delta_K=13{,}7$ кГц (аналогичные данные приведены для $OC^{34}S—CO_2$). Из анализа штарковских сдвигов отдельных линий спектра определены значения μ_a, μ_b и μ_T равные, соотв., 0,125; 0,590 и 0,603 D. Комплекс имеет плоское строение, расстояние между центрами масс фрагментов OCS и CO_2, $R=3{,}552$ А, частота колебания — 47 $см^{-1}$, силовая постоянная $R_R=0{,}033$ мдн/А, углы θ_1 и θ_2 между R и направлениями OCO и OCS составляют соотв. 68,94 и 78,93°.

В. М. Ковба

М-л.

Х. 1988, 19, N 17.

$OCSCO_2$ Ом. 29351 1988

Ж 8 Л175. **Определение структуры** $OCSCO_2$. Determination of the structure of OCS CO_2. Novick Stewart E. «J. Chem. Phys.», 1988, 88, № 2, 687—690 (англ.)

С помощью микроволнового импульсного фурье-спектрометра (разрешение ~2 кГц) исследованы вращательные спектры поглощения слабо связанных молекул комплекса $OCSCO_2$ (I), получаемых в результате смешивания газовых пучков OCS (II) и CO_2 (III), при т-ре 1—2 К. Определены три главные вращательные постоянные основного изотопомера. Анализ данных показывает, что молекулы I имеют плоскую структуру с развернутой ориентацией осей групп молекул II и III. Для ряда линий основного изотопомера наблюдались штарковские сдвиги. Расстояние между центрами тяжести групп молекул II и III составляет 3,552 Å. Библ. 30.

К. Э. М.

М.П.

ф. 1988, 18, N 8

OCCCS (Dm-30910) 1988

110: 15300m Tricarbon oxide sulfide (OCCCS), cyanogen isothiocyanate (NCNCS), cyanogen isocyanate (NCNCO), and cyanogen azide (NCNNN) as semirigid benders. Ross, S. C. (Dep. Chem., Univ. Alberta, Edmonton, AB Can. T6G 2G2). *J. Mol. Spectrosc.* 1988, 132(1), 48–79 (Eng). The semirigid bender model was developed for a general planar mol. It was used to det. the ν_7 (linear convention) or ν_9 (bent convention) bending potential functions of the mols. OCCCS, NCNCS, NCNCO, and NCNNN by fitting the model to the obsd. microwave spectra. These 4 mols. illustrate the passage from a linear limit (OCCCS), through quasilinearity (NCNCS, NCNCO), to the bent limit (NCNNN).

(ν_7, ν_9)

(#3) IX

C.A. 1989, 110, N2

OCCCS

OM 30910 1988

5 Д43. Молекулы OCCCS, NCNCS, NCNCO и NCNNN как полужесткие деформируемые системы. OCCCS, NCNCS, NCNCO, and NCNNN as semirigid benders / Ross S. C. // J. Mol. Spectrosc.— 1988.— 132, № 1.— С. 48—79.— Англ.

Строится обобщенная модель гамильтониана полужесткой деформируемой плоской молекулы для изучения структуры ее колебательно-вращательного спектра при наличии внутримолекулярных колебаний большой амплитуды. Полученная модель используется для анализа низкочастотных деформац. колебаний перечисленных в названии молекул, имеющих различную равновесную геометрич. структуру (от линейной молекулы OCCCS до сильно изогнутой молекулы NCNNN). Потенц. ф-ции деформационных колебаний этих молекул определяются в рамках построенной модели по их наблюдаемым вращательным микроволн. спектрам: изменение вращательной структуры спектра при увеличении колебательного возбуждения деформационной моды позволяет определить параметры потенц. ф-ций с помощью написанной авторами программы.

В. М. Стрельченя

Л-Л.

(+3)

Ф. 1989, N5

$(COS)_2$

1989

111: 221866z Virbrational predissociation of carbonyl sulfide clusters excited near the ν_3 vibration of the monomer. Dueren, R.; Hillrichs, G.; Liesner, M.; Mohr, S. (Max-Planck-Inst. Stroemungsforsch., D-3400 Goettingen, Fed. Rep. Ger.). *Chem. Phys. Lett.* 1989, 160(5-6), 602-8 (Eng). OCS clusters were produced in a supersonic beam. Dissocn. spectra for these clusters were measured with a diode laser and a bolometer detector. Results are presented for large clusters with discrete sampling through a range of 80 cm^{-1} around the ν_3 monomer absorption. In this group the size distribution of the clusters varied with the stagnation pressure in the source. Broad spectra are obtained (between 20 and 40 cm^{-1} depending on the pressure) with a max. blue-shift of 12 cm^{-1} from the monomer absorption. For small clusters with a continuous scan, narrow (≈ 50 MHz) dissocn. lines are obsd., if the beam parameters are chosen so as to produce dimers preferentially.

предиссоци-
ация

C.A. 1989, 111, N 24

CSO

om. 32845

1989

структура, частоты ab initio расчет

Pyykkö P.,
Chem. Phys. Lett.,
1989, 162, N 4, 5,
349–354.

OCS

1989

6Б1506. Гетеродинные и фурье-спектроскопические измерения OCS вблизи 1700 $см^{-1}$. Heterodyne frequency and Fourier transform spectroscopy measurements on OCS near 1700 cm^{-1} / Wells J. S., Vanek M. D., Maki A. G. // J. Mol. Spectrosc.— 1989.— 135, № 1.— С. 84—88.— Англ.

С использованием CO-лазера гетеродинным методом в области частот 49,4—52,1 ТГц с точностью 5—30 МГц и на ИК-фурье-спектрометре в области частот 1650—1736 $см^{-1}$ с разрешением 0,005 $см^{-1}$ выполнены измерения полос $00^02—00^00$, $01^12—01^10$, $00^03—00^01$ для $^{16}O^{21}C^{32}S$, $00^02—00^00$ для $^{16}O^{12}C^{34}S$ и $00^02—00^00$ для $^{16}O^{13}C^{32}S$. Из анализа с учётом микроволновых, субмиллиметровых и ИК-данных уточнены значения частот и вращат. постоянных колебат. полос вблизи 1700 $см^{-1}$. Полученные молекулярные постоянные использованы для расчета частот переходов полосы $00^03—00^00$ в области частот 2508—2577 $см^{-1}$ с точностью 0,00014—0,00093 $см^{-1}$.

С. Н. Мурзин

М.Л.

Х.1990, №6

OCCCS

OM 34010

1990

113: 122827x The far-infrared spectrum of tricarbon oxide sulfide (OCCCS): high-resolution Fourier-transform measurements. Holland, Frank; Winnewisser, Manfred; Johns, John W. C. (Phys.-Chem. Inst., Justus-Liebig-Univ., D-6300 Giessen, Fed. Rep. Ger.). *Can. J. Phys.* 1990, 68(4-5), 435-48 (Eng). High-resoln. far-IR gas-phase spectra of the linear cumulene-type mol. OCCCS have been measured between 50 and 660 cm^{-1}. Four band systems corresponding to the fundamental vibrations ν_4, ν_5, ν_6, and ν_7 were obsd. Anal. of the rotational structure of the two fundamental transitions 4_0^1 and 5_0^1 yielded the band origins and rotational consts. ν_4 = 593.640 432 (270) cm^{-1}, ν_5 = 544.101 238 (210) cm^{-1}, B_4 = 1414.370 33 (36) MHz and B_5 = 1415.186 10 (13) MHz. The very weak absorption of the bending vibration ν_5 was obsd. at lower resoln. around 438 cm^{-1}. The band system due to the low-lying CCC bending mode ν_7 was found as a weak absorption near 89 cm^{-1}. Despite the high resoln. of 0.004 cm^{-1} (apodized), the rotational structure of this band was not completely resolved. However, the band contour is in good agreement with the expected harmonic character of the bending potential. The ν_7 band systems of the three homologous mols. OCCCO, OCCCS, and SCCCS are compared in terms of their vibrational structure.

Uf creemp, M.N-

C.A. 1990, 113, N 14

$C(^3P) + OCS(X^1\Sigma^+) \rightarrow$

(ОП 34290) 1990

$CS(a^3\Pi_2, X^1\Sigma^+) + CO(X^1\Sigma^+)$

Nau-lin Ch., Costes M., et al.,

J. Chem. Soc. Faraday Trans. 1990, 86, N 5, 887-888.

A Pulsed Crossed Super-

Ionic Molecular Beam Study of the Reaction

$$C(^3P) + OCS(X\,^1\Sigma^+) \rightarrow CS(a\,^3\Pi_r, X\,^1\Sigma^+) + CO(X\,^1\Sigma^+).$$

$(OCS)_2$ ОМ 34370 1990

11 Б1276. **Инфракрасный колебательно-вращательный спектр и структура димера OCS.** Infrared vibration-rotation spectrum and structure of OCS dimer / Randall R. W., Wilkie J. M., Howard B. J., Muenter J. S. // Mol. Phys.— 1990.— 69, № 5.— С. 839—852. — Англ.

На ИК-спектрометре с перестраиваемым диодным лазером в области частот 2069—2075 $см^{-1}$ с точностью 0,001 $см^{-1}$ и импульсной молек. струей измерен колебательно-вращат. спектр димера $(OCS)_2$. Анализ ИК-спектра выполнен с учетом квартичного центробежного искажения и кориолисова вз-вия с плоской изгибной модой. Определены нулевая частота колебаний $\nu_0 = 2072{,}00664(4)$ $см^{-1}$, вращат. постоянные в основном и возбужденном состояниях, соотв., в МГц $A = 3074{,}8(2)$ и $3067{,}8(2)$, $B = 1262{,}7(2)$ и $1259{,}3(2)$, $C = 894{,}3(2)$ и $892{,}2(2)$. Полученные ИК-результаты отнесены к димеру симметрии C_{2h} с почти параллельным

М.Л.

Х.1991, N11

расположением фрагментов комплекса с расстоянием между центрами масс R(OCS—OCS)=3,648 А.

С. Н. Мурзин

/CO3/2

1991

115: 142858c **Potential energy functions and the carbonyl sulfide dimer.** Deakin, A. A.; Walmsley, S. H. (Dep. Chem., Univ. Coll. London, London, UK WC1H 0AJ). *J. Mol. Struct.* 1991, 247 89–92 (Eng). The structure is considered of the van der Waals dimer of carbonyl sulfide for no. of empirical potentials. The complex is planar with the mols. anti-parallel (the head to tail structure). A subsidiary min. for the head to head structure is usually found. These results are in general agreement with available exptl. evidence.

структура, расчет

C.A. 1991, 115, N 14

OCCCS

1991

115: 122729h The mid-infrared spectrum of tricarbon oxide sulfide (OCCCS): high-resolution Fourier-transform measurements. Holland, Frank; Winnewisser, Manfred (Phys.-Chem. Inst., Justus-Liebig-Univ., W-6300 Giessen, Fed. Rep. Ger.). *J. Mol. Spectrosc.* 1991, 149(1), 45-72 (Eng). The gas phase spectrum of the linear cumulene-type mol. tricarbon oxide sulfide, OCCCS, was measured between 700 and 2460 cm^{-1} with high resoln. using a Bruker Fourier-transform spectrophotometer. Three band systems corresponding to the stretching fundamentals ν_1, ν_2, and ν_3, as well as the band systems $\nu_2 + \nu_7$, $\nu_2 - \nu_7$, and $\nu_3 + \nu_5 + \nu_6$ were obsd. The rotational structure of 19 subbands was analyzed, among them the three fundamental transitions 1_0^1, 2_0^1, and 3_0^1, and the three bands $2_0^1 7_1^0$, $2_0^1 7_1^1$, and $2_0^1 7_0^1$. The anal. of the 4 bands involving ν_2 allowed two independent detns. of the energy of the first excited state of the low-lying CCC bending vibration ν_7. A simultaneous fit of all transitions starting from the vibrational ground state or the state $\nu_7 = 1$, including available rotational data, yielded a set of reliable term values and rotational consts. The first excited state of the low-lying CCC bending vibration ν_7 was found to be a 77.63094(20) cm^{-1}. Other consts. are ν_1= 2257.52915(20) cm^{-1}, B_1 = 1411.1578(54) MHz, ν_2 = 1961.96697(20) cm^{-1}, B_2 = 1409.3053(13) MHz, ν_3 = 1279.31516(20) cm^{-1}, B_3 = 1410.76050(41) MHz.

ИК-спектр.

М.Л.

C.A. 1991, 115, N 12

$(COS)_2^+$

1991

115: 57596w **Ab initio study of the carbonyl sulfide ion-molecule complex ($(COS)_2^+$).** McKee, Michael L. (Dep. Chem., Auburn Univ., Auburn, AL 36849 USA). *Chem. Phys. Lett.* 1991, 179(5-6), 559-62 (Eng). The ion-mol. complex $(COS)_2^+$ is predicted to be bound by a two-center-three-electron (2c-3e) bond between two sulfur atoms. The lowest energy structure has C_2 symmetry with a S-S distance of 2.866 Å at the UHF/6-31 G* level. The calcd. binding energy at the [spin-projected MP4(PMP4)/6-31 + G*] + zero-point-energy corrections(ZPC) level (19.9 kcal/mol) is in good agreement with a photoionization measurement (17.2 kcal/mol), and an est. based on measured COS^+CO_2 and COS^+N_2O binding energies (19.5 kcal/mol). An alternative structure bound by an O-O interaction is 13.5 kcal/mol higher in energy due to an unfavorable 2c-4e destabilizing interaction.

спутница, газ

C. A. 1991, 115, N 6

$(COS)_2^+$

1991

20 Б1135. Неэмпирическое изучение комплекса $(COS)_2^+$. Ab initio study of the $(COS)_2^+$ complex / McKee Michael L. // Chem. Phys. Lett.— 1991.— 179, № 5—6.— С. 559—562.— Англ.

Неограниченным методом Хартри—Фока в базисе 6-31G* рассмотрены 4 геометрич. конфигураций комплекса $(COS)_2^+$. В найденных точках энергии определены с учетом корреляц. поправок. Наиболее устойчивой оказалась конфигурация с точечной группой симметрии C_2 и равновесным расстоянием S—S равным 2,866 А. Энергия связи (19,9 ккал/моль) хорошо согласуется с имеющимися эксперим. результатами и теор. оценками. Отмечено, что стабилизация этой конфигурации обусловлена образованием двухцентровой трехэлектронной хим. связи между двумя атомами серы.

В. Б. Павлов-Веревкин

М.П.

Х. 1991, N 20

(COS)$_2^+$

1991

9 Д158. Неэмпирическое исследование комплекса $(COS)_2^+$. Ab initio study of the $(COS)_2^+$ complex / McKee Michael L. // Chem. Phys. Lett.— 1991.— 179, № 5—6.— С. 559—562.— Англ.

С использованием пакета программ Гауссиан-88 проведены исследования ион-молекулярного комплекса $(COS)_2^+$ (I). В рамках неограниченного метода Хартри—Фока в базисе 6-31 ГФ+ найдено, что наиболее стабильная структура I имеет симметрию C_2 с расстоянием S—S, равным 2,866 Å, и связью $2c$—$3e$ между двумя атомами S. Рассчитанная энергия связи (19,9 ккал/моль) согласуется с эксперим. значением, полученным в измерениях фотоионизации (17,2 ккал/моль), и с оценкой, основанной на измерениях энергий связи комплексов COS^+CO_2 и COS^+N_2O (19,5 ккал/моль). Альтернативная структура, связанная взаимодействием O—O, оказалась выше по энергии на 13,5 ккал/моль вследствие дестабилизирующего взаимодействия $2c$—$4e$. Рассчитанные колебательные частоты комплекса I согласуются с экспериментом. Т. Д.

М.Л.

сф. 1991, N 9

$(OCS)_2$

1993

118: 261361k An investigation of the structure of weakly bound carbon oxido sulfido dimer $(OCS)_2$. Bone, Richard G. A. (Department of Chemistry, McMaster University, 1280 Main St. West, Hamilton, Ontario, Can.). *Chem. Phys. Lett.* 1993, 206(1-4), 260-70 (Eng). Ab initio calcns. confirm that there is a stable structure of the van der Waals dimer of OCS having C_{2h} symmetry, with the S atoms occupying the inner positions in the complex, in accordance with a recent exptl. observation. Second-order Moeller-Plesset perturbation theory (MP2) calcns. with a TZ2P basis set find that this structure is the global min. Three other stationary points, predicted by the electrostatic model, have been located. Two of these have the monomer axes parallel, but staggered, with respect to one another; in the other the monomers are collinear. A comparison of SCF and MP2 results demonstrates that although the obsd. form is an electrostatically favored structure, dispersion interactions are crucial in detg. its energy relative to the other isomers. What becomes abundantly clear is that basis sets of the size of double-zeta with a single shell of polarization functions are inadequate to describe species such as $(OCS)_2$.

структура и спектроскопия, теоретическая

C. A. 1993, 118, N26

COS_2

1993

21 Б1158. Поверхность потенциальной энергии COS_2. Вид поверхностей потенциальной энергии низших синглетного и триплетного состояний для реакции атомов кислорода с дисульфидом углерода. The COS_2 potential energy surface: Aspects of the lowest singlet and triplet potenial energy surfaces for the reaction of oxygen atoms with carbon disulfide /Froese Robert D. J., Goddard John D. //J. Chem. Phys .—1993 .—98 ,№ 7 .—С. 5566—5578 .—Англ.

Рассчитаны участки потенциальных поверхностей низших синглетного и триплетного состояний молекулы COS_2, характеризующие р-ции $O(^3P)+CS_2(^1\Sigma_g^+ \rightarrow CS(^1\Sigma^+)+$ $+SO(^3\Sigma^-)\rightarrow OCS(^1\Sigma^+)+S(^3P)\rightarrow CO(^1\Sigma^+)+S_2(^3\Sigma^-_g)$. Расчеты проведены по теории возмущений Меллера—Плессета второго (при оптимизации геометрии) и четвертого (при расчете энергий в стац. точках) порядков в базисе 6-31ГФ*. Показано, что основным путем р-ции является прямое образование продуктов CS и SO. Результаты расчетов подтверждают экспериментально наблюдавшееся отношение ветвления. Наиболее стабильна синглетная структура, представляющая собой кольцо CSS с карбонильной группой. Библ. 46.

А. А. Сафонов

Ж. 1993, №21

$UCCS^{2+}$
$SCCS^{2+}$

Um · 37995

1995

Ling Wah Wong,

стабильн.. структура, ab initio расчет

J. Mass Spectrometry, 1995, 30, 1144-1148

CO–OCS

1996

125: 207169g **The structure of CO–OCS: a spectroscopic and theoretical investigation.** Brookes, M. D.; Clift, D. J. M.; Low, R. J.; Brown, J. M.; Howard, B. J. (Physical Chem. Lab., Oxford Univ., Oxford, UK OX1 3QZ). *Mol. Phys.* 1996, 88(4), 899–914 (Eng). The spectrum of the weakly bound complex CO–OCS has been measured in the IR using direct absorption diode laser spectroscopy in a supersonic jet, and in the microwave region using a pulsed nozzle Fourier–transform instrument. In addn., microwave spectra of the two isotopomers ^{13}CO–OCS and CO–OC^{34}S were recorded. A T shaped structure has been detd. with the carbon atom in CO closest to the OCS (RMS angle ± 20.5° with respect to the intermol. axis) and the sulfur end of OCS pointing away from CO (vibrationally averaged angle 105.7°). The ground state center of mass sepn. is 4.17 Å. The effective structure is rationalized by a simple potential incorporating a distributed multipole anal. of the electrostatic charge distribution, distributed dispersion contribution and a cylindrical hard core repulsion, with discussion of the implications for the potential of including correlation effects in the CO multipole.

(ИК спектр, структура)

C. A. 1996, 125, N16

$(OCS)_3$

1996

125: 207170a **Internal motion effects in the microwave spectrum of OCS trimer.** Connelly, James P.; Bauder, Alfred; Chisholm, Alan; Howard, Brian J. (Laboratorium Physikalische Chemie, CH-8092 Zurich, Switz.). *Mol. Phys.* 1996, 88(4), 915-929 (Eng). The microwave spectrum of OCS trimer, measured between 6 GHz and 18 GHz using Fourier-transform microwave spectroscopy, is consistent with a very asym. rotor, $\kappa = 0.18$. A- and c-type transitions are obsd. with many lines showing a fine doubling of <20 kHz. A fit of av. line positions to Watson A redn. (I^R) rotational parameters gives; A = 847.97958(2), B = 736.17579(2), C = 574.32591(1) MHz, $\Delta_J = 0.45440(9)$, $\Delta_{JK} = 0.1572(5)$, $\Delta_K = 0.3010(5)$, $\delta_J = 0.06797(4)$, $\delta_K = 0.0339(3)$ kHz. From a sum of equil. structures are chiral, suggesting the obsd. splitting is the result of tunneling interconversion between enantiomers. A scheme employing the recursion relation for assocd. Legendre polynomials is used to extend the distributed multipole method for the electrostatic interaction between linear mols. to include multipole moments up to the highest order available from ab initio calcns.

MB спектр, A, B, C.

C.A. 1996, 125, N16

$CO_2 - SO_2$ комплекс

1996

125: 21342c **The microwave spectrum and structure of the carbon dioxide–sulfur dioxide complex.** Sun, Linghong; Ioannou, Ioannis I.; Kuczkowski, Robert L. (Department Chemistry, University Michigan, Ann Arbor, MI 48109–1055 USA). *Mol. Phys.* .1996, 88(1), 255–268 (Eng). The rotational spectra of nine isotopomers of the carbon dioxide–sulfur dioxide van der Waals complex were obsd. with a pulsed mol. beam Fourier transform microwave spectrometer. All odd K energy levels were missing in the sym. isotopic species, but were present in the singly substituted $C^{18}O^{16}O$ or $S^{18}O^{16}O$ isotopomers. No inversion splittings were obsd. in any of the isotopic species. The obsd. frequencies for each isotopomer were fit to obtain rotational and centrifugal distortion consts. Consideration of the moments of inertia, selection rules and missing levels indicate that the complex has a cross structure with C_{2v} symmetry. The C_2 axis of SO_2 is perpendicular to the C_∞ axis of CO_2. The neg. end of the SO_2 dipole moment points to the carbon atom. The center of mass distance between the two monomers is 3·29(5) Å. The dipole moment is 1·771(2) D. Distributed multipole electrostatic calcns. support the cross structure.

(МВ спектр)

C. A. 1996, 125, N 2

OCCCS

1996

125: 21319a **The low-lying bending vibration system ν_7 of OCCCS observed at Doppler-limited resolution.** Wagener, V.; Winnewisser, M.; Bellini, M. (Physikalisch-Chemisches Institut, Justus-Liebig-Universitaet, D-35 392 Giessen, Germany). *J. Mol. Spectrosc.* **1996**, 176(2), 425-438 (Eng). Parts of the gas-phase spectrum of the linear cumulene-type mol. tricarbon oxide sulfide, OCCCS, were recorded in the region of its lowest-lying CCC bending vibration ν_7 around 2.4 THz. The Doppler-limited spectrum was obtained at low temps. using a tunable far-IR spectrometer. The rotational spectrum was recorded between 78 and 118 GHz with microwave techniques at room temp. The anal. of 412 rotational transition frequencies obtained during this and previous work allowed the authors to assign 71 resolved rovibrational transitions of the ν_7 band system in the far-IR region. They are distributed among 16 subbands of the fundamental band and the 1st three hotbands. The center of the fundamental band is at 2,325,894.20-(30) MHz. Forty-five spectroscopic consts. describing the vibrational states $\nu_7 = 0-4$ were obtained by fitting all data simultaneously to an effective Hamiltonian for polyat. linear mols. The anharmonicity coeff. x_{77}^{0} of the bending vibration is only −0.2% of the harmonic frequency ω_7^0, which is $\omega_7^0 = 2{,}320{,}995(13)$ MHz.

(ν_7)

C.A. 1996, 125, N 2

1996

F: OCCCS

P: 3

5Б1295. Низколежащая изгибная колебательная система 'ню'[7] OCCCS при ограниченном Допплером разрешении. The low-lying bending vibration system 'ню'[7] of OCCCS observed at Doppler-limited resolution / Wagener V., Winnewisser M., Bellini M. // J. Mol. Spectrosc. - 1996. - 176, N 2. - C. 425-438. - Англ.

На микроволновом спектрометре в области частот 78-118 ГГц с точностью 4 кГц измерен вращат. спектр и на перестраиваемом ИК-спектрометре в области частот вблизи 2,4 ТГц с допплеровским разрешением измерен спектр низколежащей CCC изгибной 'ню'[7] колебат. моды линейной молекулы OCCCS. С помощью эффективного гамильтониана определено 45 спектроскопич. постоянных для колебат. состояний v[7]=0, 1, 2, 3 и 4. Измерен центр фундаментальной колебат. полосы 2325894,20(30) МГц.

РЖХ 1997

$CO_2 \cdot CS_2$

1998

кол. вр. спектр
и
структура

129: 251844e **The Rovibrational Spectrum and Structure of the Weakly Bound CO_2–CS_2 Complex.** Dutton, C. C.; Dows, D. A.; Eikey, R.; Evans, S.; Beaudet, R. A. (Department of Chemistry, University of Southern California, University Park, CA 90089–0482 USA): *J. Phys. Chem. A* 1998, 102(35), 6904–6909 (Eng), American

C. A. 1998, 129, № 19

Chemical Society. The rovibrational spectrum of the weakly bound complex CO_2–CS_2 was obsd. by exciting the asym. stretch of the CO_2 moiety near 2349 cm^{-1}. The complex was formed by the supersonic expansion of a 1:2 mixt. of CO_2 and CS_2 in He and had a nonplanar X–shaped structure. The intermol. distance is 3.392 Å with a dihedral angle of 90°. The band center is located at 2346.5448 cm^{-1}, with ground–state rotational consts. of A" = 0.08590 cm^{-1}, B" = 0.04634 cm^{-1}, and C" = 0.03546 cm^{-1} and centrifugal distortion consts. of D_j" = -1.37×10^{-7} cm^{-1}, D_k" = 1.06×10^{-6} cm^{-1}, and D_{jk}" = -1.01×10^{-6} cm^{-1}. The excited–state consts. are similar to the ground–state consts. A portion of the potential energy surface was modeled through the use of a Buckingham atom–atom potential and a quadrupole–quadrupole electrostatic potential. Calcns. for the CO_2–CS_2 and $(CO_2)_2$ complexes produced structures in agreement with exptl. results. Although the CO_2–CS_2 configuration is controlled by the quadrupole–quadrupole interactions, the atom–atom interactions predominantly det. the energy of the dimer. Because the magnitude of the CS_2 quadrupole was increased in the electrostatic potential, the structure shifted from nonplanar X–shaped to a planar parallel configuration.

$OCS(CO_2)_2$ 1998

тример

128: 328139t **Rotational spectrum and structure of the OCS–$(CO_2)_2$ trimer.** Peebles, Sean A.; Kuczkowski, Robert L. (Department of Chemistry, The University of Michigan, Ann Arbor, MI 48109–1055 USA). *Chem. Phys. Lett.* 1998, 286(5,6), 421–424 (Eng), Elsevier Science B.V.. The rotational spectrum of the OCS–$(CO_2)_2$ trimer was assigned. The rotational consts. and dipole moment components are consistent with a nonplanar, barrel–like structure which approx. aligns the 3 mol axes in a parallel fashion. This conformation is in good agreement with rotational consts. predicted from a distributed multipole electrostatic interaction which includes atom–atom terms representing dispersion and repulsion contributions.

(гр. симм.)

C.A. 1998, 128, N26

OCS(CO2)2

1998

129: 282734y **Rotational spectrum and structure of the OCS-$(CO_2)_2$ trimer.** Peebles, Sean A.; Kuczkowski, Robert L. (Department of Chemistry, The University of Michigan, Ann Arbor, MI 48109-1055 USA). *J. Chem. Phys.* 1998, 109(13), 5276-5282 (Eng), American Institute of Physics. The rotational spectra of 9 isotopes of the mixed trimer, OCS-$(CO_2)_2$, were assigned using pulsed nozzle FTMW spectroscopy techniques. The structure resembles a distorted triangular cylinder. It can be thought of as the slipped $(CO_2)_2$ dimer with the OCS above the dimer and crossed -23° to the axis of each CO_2. The distance between the C atoms on the CO_2 is 3.68(5) Å. The distance between the C on each CO_2 and the C on the OCS is 3.59(5) and 3.66(5) Å, resp. The axes of the linear mols. are tilted 30°-35° from perpendicular relative to the edges of the C-C-C plane. The dipole moment components for the trimer are μ_a=0.63(2) D, μ_b=0.16(10) D and μ_c=0.21(2) D. The structure and dipole moment components are consistent with an interaction model, which includes a distributed multipole moment electrostatic anal. and atom-atom terms describing dispersion and repulsion. The structure is compared to other related dimers and trimers contg. CO_2, OCS, and N_2O.

вращат. спектр, спец. конфигур. параметр

C. A. 1998, 129, N 21

$(OCS)_2\ CO_2$

1998

129: 267121c **Rotational Spectrum and Structure of the $(OCS)_2$–CO_2 Trimer.** Peebles, Sean A.; Kuczkowski, Robert L. (Department of Chemistry, The University of Michigan, Ann Arbor, MI 48109–1055 USA). *J. Phys. Chem. A* **1998**, 102(42), 8091–8096 (Eng), American Chemical Society. The rotational spectra of seven isotopes of the CO_2–$(OCS)_2$ mixed trimer were assigned using pulsed nozzle FTMW spectroscopy techniques. The structure resembles a distorted triangular cylinder with the three monomers aligned roughly parallel. The trimer may be thought of as a slightly perturbed $(OCS)_2$ dimer with the CO_2 lying above the dimer and crossed at 12° and 20° to the axes of the two OCS mols., resp. The distance between the C atoms on the OCS is 3.757(9) Å. The distance between the C on each OCS and the C on the CO_2 is 3.574(6) and 3.773(8) Å, resp. The dipole moment components for the trimer are $\mu_a = 0.40(1)$ D, $\mu_b = 0.21(7)$ D, and $\mu_c = 0.206(1)$ D with $\mu_{total} = 0.50(4)$ D. The structure and dipole moments are close to those predicted by an interaction model which includes a distributed multipole moment electrostatic contribution and atom–atom terms to describe the dispersion and repulsion interactions.

Raman. спектр, структури. параметри

C.A. 1999, 129, N20

1999

F: SO2-OCS
P: 3 131:278481 Rotational spectrum, structure and modeling of the SO2-OCS com
Peebles, S. A.; Sun, L. H.; Ioannou, I. I.; Kuczkowski, R. L. Department of Chemistry, The University of Michigan Ann Arbor, MI, USA J. Mol. Struct., 485-486, 211-223 (English) 1999
The microwave spectra of the SO2-OCS complex and three of its isotopomers were obsd. wi Fourier transform microwave spectrometer. The rotational consts. of the species were detd. as A = 4841.4187(17) MHz, B = 974.7763(4) MHz and C = 960.5389(4) MHz. Centrifugal distortion terms up to HKJ were necessary f satisfactory fit of the rotational transitions. The dipole moment compon are .mu.a=0.4834(14) D and .mu.b=0.437(4) D for a

total dipole moment of 0.652(4) D. The dimer has Cs symmetry with the oxygens of the SO2 straddl OCS. The C2 axis of SO2 is nearly parallel to the OCS orienting the dipo moments of the monomers approx. antiparallel. The centers of mass of the monomers are sepd. by 3.7471(4) A. The angle made by the S atom of OCS, center of mass of the OCS, and the center of mass of the SO2 is 123.8(5).degree.. The angle made by the center of mass of the OCS, the c of mass of the SO2, and the S atom of the SO2 is 142(5).degree.. A semi- empirical model including electrostatic, dispersion and repulsion contrib was applied to the system and has reproduced the structure close to the uncertainty in the structural parameters.

1999

F: (OSC)3
P: 3
131:189913 The OCS Trimer: Isotopic Studies, Structure, and Dipole Moment Peebles, Rebecca A.; Kuczkowski, Robert L. (Department of Chemistry, University of Michigan, Ann Arbor, MI 48109-1055, USA). J. Phys. Chem. A 103(32), 6344-6350 (English) 1999 The rotational spectra of (18OCS)3 and (O13CS)3 have been assigned using pulsed-nozzle Fourier transform microwave spectrometer. The data for the isotopic species have been combined with normal species data from a paper

Connelly et al. [Connelly, J. P., et al. Mol Phys. 1996, 88, 915] to det. nine structural parameters of the trimer. The carbon atoms form a triang the axes of the monomer units roughly parallel to each other (barrel-like structure). The monomers have an antiparallel-like arrangement, with the moment of one monomer opposing those of the other two monomers. The dipo moment of the complex has been measured, giving values of .mu.a = 0.537(1 .mu.c = 0.373(2) D, and .mu.total = 0.653(8) D. The b component of the d moment was too small to det. from our data but is predicted to be about 0 The structure of (OCS)3 has been compared with similar trimers involving triat. mols. and with the OCS dimer

1999

F: C4O2S2m
P: 3
131:248498 Ab initio study of the relative stability of C4O2S2m- (m = 0, 3, 4). Zhou, Lixin; Huang, Zunxing; Tian, Anmin; Wu, Liming; Li, Junqian Department of Chemistry, Fuzhou University Fuzhou 350002, Peop. Rep. China Fenzi Kexue Xuebao, 15(1), 11-15 (Chinese) 1999 An ab initio SCF MO approach was used to investigate the equil. geometry and relative stability of the C4O2S2m- (m = 0,1,2,3,4) ions. The series anions studied goes through a change from non-arom. structure to arom. st to anti-arom. structure. The relative stability decreases in the order: > C4O2S22- > C4O2S2 > C4O2S23- > C4O2S24-.

CO-OCS

Om. 40495

2000

Changhong Xia et al.,

Ukcnexp

Mol. Phys., 2000,
98, N20, 1669-1672

Infrared spectrum of the
CO-OCS van der Waals complex
in the carbon monoxide

stretching band

F: C2OS
P: 3
133:49168

DM. 40476

2000

Extensive ab Initio Study of the C2O2, C2S2, and C2OS Systems: Stabilities and Singlet-Triplet Energy Gaps. Talbi, D.; Chandler, G. S. Laboratoire d'Etude Theorique des Milieux Extremes, ENS Paris 75005, Fr. J. Phys. Chem. A, 104(24), 5872-5881 (English) 2000 [illegible] Society. [illegible] Physical Chem. [illegible]

Ab initio MO theory has been used to study the three lowest open shell states of ethylenedione, C2O2, 2- thiooxoethen-1-one, C2OS, and ethylenedithione, C2S2. To treat the singlet and triplet states in an even-handed manner, MC-SCF theory (MCSCF), which included all the important configurations for a quant. description of these states, was used as the basis of the investigation. Further correlation effects have been included using a

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multireference CI (MRCI) approach. Basis sets of triple-.zeta. quality with d- and f-polarization functions were employed. Equil. geometries were obtained from d. functional theory (DFT) calcns. using the B3LYP exchange correlation functional and are presented for the 3.SIGMA.g-, 1.DELTA.g states of all three mols. Harmonic frequencies are also presented for these states and were calcd. at the MCSCF and DFT levels. The reported relative energies for the states were obtained from MRCI calcns. As expected from previous work, the ground states are confirmed to be of 3.SIGMA.g- symmetry for all mols., but it is only for the C2S2 that this state lies below the energy of the dissocn. products in their own ground states. For C2OS, though, this energy gap is small (5.7 kcal/mol). In contrast to a no. of other calcns., the 1.DELTA.g states for all three mols. are also shown to be min. on the MCSCF potential energy surfaces. The 1.DELTA.g states are all close to the ground states (<10 kcal/mol). Consequently, with C2S2, this singlet state also lies below the ground state of the dissocd. products. The relative energies of the 1.SIGMA.g+ states at the optimized geometries for the 1.DELTA.g states have also been detd.

F: C2OS
P: 3
133:49168

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Extensive ab Initio Study of the C2O2, C2S2, and C2OS Systems: Stabilities and Singlet-Triplet Energy Gaps. Talbi, D.; Chandler, G. S. Laboratoire d'Etude Theorique des Milieux Extremes, ENS Paris 75005, Fr. J. Phys. Chem. A, 104(24), 5872-5881 (English) 2000 Ab initio MO theory has been used to study the three lowest open shell states of ethylenedione, C2O2, 2-thiooxoethen-1-one, C2OS, and ethylenedi C2S2. To treat the singlet and triplet states in an even-handed manner, theory (MCSCF), which included all the important configurations for a qua description of these states, was used as the basis of the investigation. Further correlation effects have been included using a multireference CI approach.

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$CS_2 - CO$

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135: 142504x DFT study on the structures, stabilities and vibrational frequencies of the CS_2–XO^- (X=C, N, O) anions. Shao, L.; Chen, M.; Zhou, M. (Laser Chemistry Institute, Department of Chemistry, Fudan University, Shanghai, Peop. Rep. China 200433). *THEOCHEM* 2001, 542, 57–62 (Eng), Elsevier Science B.V. The structures, binding energies and vibrational frequencies of the CS_2–XO^- anions (X = C, N and O) have been studied using the B3LYP method at the 6–311+G(d) level of theory. Different stable structural isomers were found, including covalently bonded compds. and ion–mol. complexes. The covalently bonded anions are coordinated between the C and X atoms, while the ion–mol. complexes are coordinated between the S and X atoms. The covalently bonded anions were predicted to be more stable than the ion–mol. complexes.

теорет. расчет стр-ра, энергии связи и м.п.

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$CS_2 - NO$

$CS_2 - O_2$