1989

O_2 1989

Baker J.

J. Chem. Phys. 1989. 91,

м. п. N3. 1789–1795.

(См. ● BeH; III)

O_2

От 31431 1989

10 Б1028. Неэмпирическое исследование нейтральных O_2, SO, S_2, C_2H_2 и их моно- и дикатионов. Ab initio study of neutral O_2, SO, S_2, C_2H_2 and their mono- and dications / Balaban A. T., De Maré G. R., Poirier R. A. // J. Mol. Struct. Theochem.— 1989.— **183**, № 1/2.— С. 103—119.— Англ.

Методом ССП в базисах ОСТ-3ГФ, 3-21 ГФ и 6-31 ГФ*(5*d*) оптимизированы структурные параметры и вычислены порядки связей, малликеновские заселенности перекрывания и силовые постоянные молекул O_2, SO, S_2, C_2H_2, а также их моно- и дикатионов. Межъядерные расстояния уменьшаются в двухатомных ионах с ростом формального заряда. Все остальные вычисленные х-ки растут с увеличением заряда двухатомного иона. Анализ порядков связей показал, что остовные состояния двухатомных катионов являются синглетами с эффективными тройными связями. Ос-

М.Л.

411

X

Х.1989, N10

новым состоянием дикатиона ацетилена является триплет с двойной связью C=C. Катион и дикатион ацетилена являются стабильными линейными соединениями с R_e(C—C)=1,247 и R_e(C—H)=1,076 А для катиона и R_e(C—C)=1,326 и R_e(C—H)=1,116 А для дикатиона. При оптимизированных геометриях полные энергии всех соединений вычислены методом конфигурац. взаимодействия. Таким образом определены вторые Пт ионизации: 24,1, 19,1, 16,6 и 19,9 эВ для O_2, SO, S_2 и C_2H_2, соотв. И. А. Тополь

O_2 От 31431 1989

5 Д120. Неэмпирическое исследование нейтралов O_2, SO, S_2, C_2H_2 и их моно- и дикатионов. Ab initio study of neutral O_2, SO, S_2, C_2H_2 and their mono- and dications / Balaban Alexandru T., De Maré George R., Poirier Raymond A. // J. Mol. Struct. Theochem.— 1989. — 183, № 1/2.— C. 103—119.— Англ.

Для 12 молекул и катионов, указанных в заголовке, определены порядки связи по Майеру, перекрывание заселенностей по Малликену и силовые постоянные с использованием базисов: минимального ОСТ—3 ГФ, валентно-расщепленного 21 ГФ и 6—31 ГФ* (5*d*). Показано, что все эти величины возрастают с увеличением зарядов для каждой двухатомной группы. Однако межъядерные расстояния уменьшаются с увеличением зарядов. Эти факты свидетельствуют о том, что внешние электроны в нейтральных двухатомных молекулах находятся на разрыхляющих орбиталях. Удаление этих

М.Л.-

+9

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ф.1989, N5

SO^+, SO^{2+}, S_2^+, S_2^{2+}, $C_2H_2^+$, C_2H_2,

электронов приводит к образованию тройных связей в дикатионах, причем расчет показывает, что они стабильны в их основных состояниях, несмотря на электростатич. отталкивание. Для C_2H_2 при удалении внешних электронов поведение изучаемых величин противоположно наблюдаемому для двухатомных групп: эти величины уменьшаются при возрастании заряда. Как катион, так и дикатион ацетилена являются стабильными. С использованием оптимизированных ССП структур рассчитаны полные энергии молекул и 2-е ионизационные потенциалы.
Н. В. В.

SO, S_2, C_2H_2

O_2

1989

5 Б1225. Полосы поглощения $^{16}O^{18}O$ в системе Шумана—Рунге в области длин волн 175—205 нм и спектроскопические константы изотопно-замещенных молекул кислорода. The Schumann—Runge absorption bands of $^{16}O^{18}O$ in the wavelength region 175—205 nm and spectroscopic constants of isotopic oxygen molecules / Cheung A. S.-C., Yoshino K., Freeman D. E., Friedman R. S., Dalgarno A., Parkinson W. H. // J. Mol. Spectrosc.— 1989.— 134, № 2.— С. 362—389.— Англ.

При температурах 300 и 78 К, в обл. 175—205 нм, сфотографирован с высоким разрешением спектр поглощения молекулы $^{16}O^{18}O$. Спектр зарегистрирован с дисперсией 0,06 нм/мм на 6,65 м вакуумном спектрографе с решеткой 2400 штрихов/мм, работающей в первом порядке. Для полосы (2,0)—(16,0) системы Шумана—Рунге проведен вращат. анализ и определены спектроскопич. константы для $B^3\Sigma_u^-$ состояния молекулы $^{16}O^{18}O$ для $2 \leqslant v' \leqslant 16$. В полосе (16,0) обнаружены локальные

М.Л.

X. 1990, N5

вращат. возмущения. Показано, что величины $\mu^{1/2}\Delta G_{v+1/2}$, μB_v, $\mu^2 D_v$, λ_v, $\mu\gamma_v$ изотопически инвариантны относительно ф-ции $\mu^{-1/2}(v+1/2)$. Величины γ_v и λ_v получены путем интерполяции уровней $v'=2$—8, к-рые соответствуют полосам молекулы $^{16}O^{18}O$ с неразрешенной триплетной структурой. Теоретически рассмотрены вопросы о сдвиге наблюдаемых в эксперименте уровней. Получено прекрасное согласие между рассчитанными и эксперим. значениями сдвигов уровней для всех трех изотопно-замещ. молекул. А. В. Столяров

$^{16}O^{18}O$

1989

110: 182016c The Schumann–Runge absorption bands of oxygen ($^{16}O^{18}O$) in the wavelength region 175–205 nm and spectroscopic constants of isotopic oxygen molecules. Cheung, A. S. C.; Yoshino, K.; Freeman, D. E.; Friedman, R. S.; Dalgarno, A.; Parkinson, W. H. (Harvard-Smithsonian Cent. Astrophys., Cambridge, MA 02138 USA). *J. Mol. Spectrosc.* 1989, 134(2), 362–89 (Eng). High-resoln. absorption spectra of $^{16}O^{18}O$ were photographed, at 300 and 78 K, at 175–205 nm, in the 1st order of a 2400 lines/mm grating in a 6.65-m vacuum spectrograph at a dispersion of 0.06 nm/mm. Precise wavelength measurements and rotational analyses of the Schumann–Runge bands (2, 0)–(16, 0) were completed. Spectroscopic consts. of the $B^3\Sigma_u^-$ state of $^{16}O^{18}O$ for $v = 2$–16 were detd. Rotational perturbations were obsd. in the (16, 0) band. The concept of mass-reduced vibrational quantum nos., $\mu^{-1/2}(v + 1/2)$, was used to combine isotopic mol. consts. from $^{16}O_2$, $^{16}O^{18}O$, and $^{18}O_2$. The functions of the vibrational spacings, $\mu^{1/2}\Delta G_{v+1/2}$, rotational consts. μB_v, and $\mu^2 D_v$, spin-spin consts., λ_v, and spin-rotation consts., $\mu\gamma_v$, are isotopically invariant functions of $\mu^{-1/2}(v + 1/2)$. The isotopic dependence of the spin-spin consts. λ_v is discussed in terms of the unique perturber approxn. Values of γ_v and λ_v were obtained by interpolation for the levels $v = 2$–8, which correspond to bands of $^{16}O^{18}O$ with unresolved triplet structure. In a theor. investigation, the calcns. of level shifts and perturbations were reexamd. Agreement between calcd. and exptl. level shifts were obtained for all 3 isotopic mols.

Спектр поглощен.

C.A.1989, 110, N20

O_2

1989

12 Д150. Ридберговы уровни молекулы кислорода, связанные с возбужденными состояниями ионного остова. Rydberg levels of the oxygen molecule associated with excited states of the ion core / Chung Sunggi, Lin Chun C., Lee Edward T. P. // Phys. Rev. A.— 1989.— 39, № 5.— С. 2367—2373.— Англ.

Рассчитаны ридберговы состояния Σ_g^-,, Σ_u^-, Π_g и Π_u молекулы O_2, сходящиеся к возбужденным состояниям $B^2\Sigma_g^-$, $b^4\Sigma_u^-$ и $c^4\Sigma_u^-$ иона O_2^+. Ридберговы электронные волн. ф-ции получены на основе одноцентровых базисных ф-ций, которые являются решениями для ур-ния электронного движения в сферич. потенциале ионного остова. Ридберговы энергетич. уровни получены путем диагонализации полного гамильтониана, который включает как сферическую, так и несферич. части потенциала. Отмечена быстрая сходимость разложения, поскольку базисные ф-ции являются уже хорошим приближением волн. ф-ций ридбергова состояния. Расчеты

М·Л·

ф. 1989, N12

проведены для (nl) от $(3, 0)$ до $(10, 7)$ и для $m=0$ и 1 с использованием двух межъядерных расстояний: $R=1{,}2$ Å и равновесных межъядерных расстояний возбужденных состояний O_2^+. Получено согласие с экспериментом для серий $ns\sigma_g$, $np\sigma_u$ и $np\pi_u$, однако для серии $nd\sigma_g$ обнаружены существенные расхождения с экспериментом.

Н. В. В.

O_2

1989

111: 45554k **Rydberg levels of the oxygen molecule associated with excited states of the ion core.** Chung, Sunggi; Lin, Chun C.; Lee, Edward T. P. (Dep. Phys., Univ. Wisconsin, Madison, WI 53706 USA). *Phys. Rev. A: Gen. Phys.* 1989, 39(5), 2367–73 (Eng). Rydberg states (Σ_g^-, Σ_u^-, Π_g, and Π_u) of O_2 that converge to the $B^2\Sigma_g^-$, $b^4\Sigma_g^-$, and $c^4\Sigma_u^-$ excited states of the parent O_2^+ ion have been calcd. The Rydberg–electron wave functions are expanded by one-center basis functions that are solns. of an electron moving in a sphericalized potential of the parent–ion core. The Rydberg energy levels are obtained by diagonalizing the full Hamiltonian which includes both the spherical and nonspherical parts of the potential. Rapid convergence of the expansion is assured because the basis functions are already a good approxn. to the Rydberg-state wave functions. The calcns. cover (nl) from (3,0) to (10,7) and $m = 0$ and 1 using two internuclear distances, $R = 1.2$ Å and the equil. distances of the parent excited O_1^+ states. The results are compared with photoabsorption and electron–impact energy–loss expts. Good agreement is seen for the $ns\sigma_g$, $np\sigma_u$, and $np\pi_u$ series, but the $nd\sigma_g$ states exhibit larger discrepancies.

Ридберг.
состоян.

C.A. 1989, <u>111</u>, N6

O_2 om. 32740 1989

Dingle T.W., Huzinaga S., et al.,

$({}^3\Sigma_g^-)$ J. Comput. Chem. 1989, 10, N 6, 753-769.

Contraction of the Well-Tempered Gaussian Basis

Sets: The First-Row
Diatomic Molecules.

O_2

1989

10 Д111. Замечание о предиссоциации O_2 в *B*-состоянии.— Ответ авторов. Comment on predissociation of O_2 in the *B* state by A. M. Wodtke et al. — Authors reply / Freeman D. E., Cheung A. S.-C., Yoshino K., Parkinson W. H. // J. Chem. Phys. — 1989.— 91, № 10. — С. 6538—6540.— Англ.

См. / Wodtke A. M. et al. // J. Chem. Phys.— 1988. — 89.— С. 1929.

М·П.

Ф. 1990, N 10

O_2

1989

21 Б4779. Замечание о предиссоциации O_2 в B-состоянии. Ответ авторов. Comment on predissociation of O_2 in the B state / Freeman D. E., Cheung A. S.-C., Yoshino K., Parkinson W. H., Wodtke A. M., Hüwel L., Authors'Reply // J. Chem. Phys.— 1989.— 91, № 10.— С. 6538—6540.— Англ.

Дискуссия по статье / Wodtke A. M. et al. (// J. Chem. Phys., 1989, 89, С. 1929, касающаяся надежности эксперим. данных, на основе к-рых был сделан вывод о предиссоциации с уровня v'-11 состояния O_2-$(B^3\Sigma^-)$. В ответе авторов на основе уточненных измерений сделан вывод, что такая предиссоциация возможна по орбитально-вращат. механизму, но не вследствие спин-орбитального взаимодействия с отталкиват. состоянием $O_2(^5\Pi_u)$. В. Е. Скурат

предиссоц.

Х. 1990, N 21

O_2

1989

112: 44682j Comment on predissociation of molecular oxygen in the B state. Freeman, D. E.; Cheung, A. S. C.; Yoshino, K.; Parkinson, W. H. (Harvard-Smithsonian Cent. Astrophys., Cambridge, MA 02138 USA). *J. Chem. Phys.* 1989, 91(10), 6538-40 (Eng). The conclusions of A. M. Wodtke et al. (*ibid.*, 89, 1929) concerning the predissocn. of the $v = 11$ level of the $B^3\Sigma_u$ state of O_2 are unjustified. In the case of the R(27) feature of the (11, 2) band, which is partially resolved in the exptl. excitation spectrum, their simulated spectra are excitation spectra and not absorption spectra.

предиссоциация в B состоянии

C.A. 1990, 112, N 6

O_2

1989

2 Д67. **Комментарий к статье: «Предиссоциация ридбергова состояния $d^1\Pi_g$ в O_2. Природа взаимодействий ридберговых и валентных уровней».** Comment on: "Predissociation of the $d^1\Pi_g$ Rydberg state in O_2. Nature of the Rydberg — valence interactions" / Friedman R. S., Dalgarno A. // J. Chem. Phys.— 1989.— 90, № 12.— С. 7606—7607.— Англ.

См. van der Zande W. J. et al. // J. Chem. Phys.— 1988.— 89.— С. 6758.

М.П.

Ф. 1990, N2

O_2

1989

Ридберг·сост

111: 183165k Comment on "Predissociation of the $d^1\Pi_g$ Rydberg state in molecular oxygen: nature of the Rydberg-valence interactions". Friedman, R. S.; Dalgarno, A. (Harvard-Smithsonian Cent. Astrophys., Cambridge, MA 02138 USA). *J. Chem. Phys.* 1989, 90(12), 7606-7 (Eng). A polemic concerning the paper by W. J. van der Zande et al. (*ibid* 1988, 89, 6758). A more accurate procedure was used to det. the eigenvalues and eigenfunctions of the interacting state parameters.

C.A. 1989, 111, N20

O_2 1989

Glushkov A.V.,

расчет D_0 Zh. Fiz. Khim. 1989,
и ω_e 63 (11), 3072-4.

Calculation of the molecular
constants of diatomic mo-

C.A. 1990, 112, N 16, 145943a

lecules in the density-functional quasiparticle approximation.

О$_2$ 1989

Горшенков В.Н.,
Райков Г.М. и др.

Горьк. ун-т. Горький, 1989.
м.п. 18с. Библиогр. 3 назв. Рус.
Деп. в ВИНИТИ 21.03.89,
№1785 — ● В89.
(См. У$_2$; III)

O_2

1989

6 Л205. Спин-вращательные эффекты в спектрах отклонения Штерна—Герлаха молекул $^3\Sigma^-$ и их комплексов с аргоном. Spin-rotation effects in the Stern—Gerlach deflection spectra of $^3\Sigma^-$ molecules and their complexes with argon / Herrick D. R., Robin M. B., Gedanken A. // J. Mol. Spectrosc.— 1989.— **133,** № 1.— С. 61—81.— Англ.

Рассчитаны спектры магн. отклонения Штерна — Герлаха парамагн. молекул $^{16}O_2$, $^{17}O_2$, NH, NCH_3 и HCCN в основном электронном состоянии $^3\Sigma^-$. Проанализированы изменения в спектрах за счет проявления эффекта Пашена — Бака. Показано, что антипересечения в системе зеемановских спин-вращательных состояний $^3\Sigma^-$ и их комплексов с аргоном проявляются в спектрах как резкие изменения знака отклонения при изменении магн. поля. Обсуждены общие проявления процессов комплексообразования в спектрах Штерна — Герлаха парамагн. молекул.

В. С. Иванов

М·П·

☒ ㊸

ф. 1989, N6

O_2

1989

12 Д151. Три формы молекулярного кислорода. The three forms of molecular oxygen / Laing Michael // J. Chem. Educ.— 1989.— 66, № 6.— С. 453—455.— Англ.

Применение простых правил теории молекулярных орбиталей для двухатомных молекул приводит к предсказанию существования трех спиновых изомеров молекулярного кислорода. Одна триплетная форма $^3\Sigma$ имеет два неспаренных электрона и две синглетные формы $^1\Delta$, $^1\Sigma$ со спаренными электронами. Состояние $^1\Delta$ лежит выше основного состояния $^3\Sigma$ на 94,7 кДж, а состояние $^1\Sigma$ — на 158 кДж. Длины связей в молекуле равны 1,2074 Å ($^3\Sigma$), 1,2155 Å ($^1\Delta$) и 1,2268 Å ($^1\Sigma$). В эксперим. химии показано, что реакционная способность синглетной формы $^1\Delta$ сильно отличается от реакционной

М.П.

ф. 1989, № 12

способности обычной триплетной формы. Эта особенность в реакционной способности успешно применяется в органич. синтезе.

Г. К.

O_2

1989

112: 13759k Multiphoton ionization of molecular oxygen $X^3\Sigma_g^-$, $a^1\Delta_g$, and $b^1\Sigma_g^+$ via the two-photon resonant nsσ_g, ndσ_g, and ndπ_g Rydberg levels. Loo, R. Ogorzalek; Marinelli, W. J.; Houston, P. L.; Arepalli, S.; Wiesenfeld, J. R.; Field, R. W. (Dep. Chem., Cornell Univ., Ithaca, NY 14853-1301 USA). *J. Chem. Phys.* 1989, 91(9), 5185-200 (Eng). Multiphoton ionization spectra were obtained and analyzed for excitation in the 215-260 nm region from the $X^3\Sigma_g^-$, $a^1\Delta_g^+$, and $b^1\Sigma^+_g$ states of O_2. The 0-0 band of the $C^3\Pi_g$ state is reported for the 1st time. Measurements of other vibrational bands terminating in the $C^3\Pi_g$ and $d^1\Pi_g$ states are in good agreement with detns. by other groups. Several vibrational levels ($v' = 0-5$) of the 3dπ_g Rydberg complex were assigned on the basis of (*1*) an anal. of the spin-orbit couplings between the (Λ,S) basis-set states, (2) spectral simulation, and (3) the behavior of the states when the excitation radiation is changed from linear to circular polarization.

$X^3\Sigma_g^-$,
$a^1\Delta_g$, $b^1\Sigma_g^+$

C.A. 1990, <u>112</u>, N 2

O_3 1989

Magers D.H., Lipscomb W.N. et al.,

равновесн. структура, гармон. колебат. частоты

J. Chem. Phys., 1989, 91, N 3, 1945–1947

O_2

1989

Millot G., Lavorel B. et al.;

Accurate Spectroscopic Parameters of O_2 and N_2 Determined from SRS Spectra of the Fundamental and Hot Bands.

D25

Eleventh Colloquium On High Resolution Molecular Spectroscopy, Giessen, September 18-22, 1989, A1, D25.

O_2

1989

22 Б4015. Диссоциация O_2 при электронном ударе: распределения высоковозбужденных ридберговских атомов по кинетическим энергиям и углам. Electron-impact dissociation of O_2: kinetic energy and angular distributions of highly excited rydberg atoms / Ohshima S., Kondow T., Fukuyama T., Kuchitsu K. // Chem. Phys.— 1989.— 135, № 2.— С. 267—275.— Англ.

В индуцированной электронный ударом диссоциации O_2 (энергия электронов 50—100 эВ) обнаружены ридберговские атомы O^* ($15 \leqslant n \leqslant 30$), угловое распределение к-рых коррелирует с их кинетич. энергией: для быстрых атомов ($E \approx 8$ эВ) зависимость от угла очень слабая, для медленных атомов ($E < 5$ эВ) рассеяние минимально для угла, близкого к 90°. Существование двух типов атомов объясняется распадом ридберговских молекул, состояния к-рых сходятся к пределам двойной ионизации $^3\Sigma_u^-$, $^1\Pi_g$ (для быстрых атомов) и $^3\Sigma_u^-$ (для медленных атомов). Е. Е. Никитин

Х. 1989, 22

O_2

1989

Ридберовск. состояния

111: 243354h **Observation and analysis of the 3dπ $^1\Sigma_g^+$ Rydberg state of molecular oxygen by (2 + 1) multiphoton ionization.** Park, Haiyoon; Li, Leping; Chupka, William A. (Sterling Chem. Lab., Yale Univ., New Haven, CT 06511 USA). *Chem. Phys. Lett.* 1989, 162(4–5), 317–20 (Eng). (2+1) Multiphoton ionization spectra of the v' = 0–3 levels of the 3d$^1\Sigma_g^+$ Rydberg state were obtained, assigned, and analyzed. Rotational line intensities are accounted for by invoking heterogeneous predissocn. due to the 1 $^1\Pi_g$ valence state.

C.A. 1989, 111, N 26

O_2 От. 33602 1989

Sambe H., Ramaker D.E.;

Phys. Rev. A 1989, <u>40</u>,

N7, 3651-3661.

Forbidden electron attachment in O_2.

O_2 1989

Samson James A. R.,
Yin Lifeng.

сечение
поглощен.

J. Opt. Soc. Am. B: Opt.
Phys. 1989, 6(12), 2326-
-33.

(см. ● H_2; III)

O_2

1989

I;

112: 65897y **Rotationally resolved photoionization of dioxygenyl ion (O_2^+) near threshold.** Tonkyn, Russell G.; Winniczek, Jerry W.; White, Michael G. (Chem. Dep., Brookhaven Natl. Lab., Upton, NY 11973 USA). *Chem. Phys. Lett.* 1989, 164(2-3), 137-42 (Eng). A delayed, pulsed field ionization technique is used in combination with a high-resoln. vacuum-UV radiation source to measure the rotational structure assocd. with the $X^2\Pi_g \leftarrow X^3\Sigma_g^-$ (0,0) ionizing transition in O_2. The data were fit to theor. expressions derived for rotationally resolved 1-photon ionization cross sections. From the fit one obtains the ionization potential for O_2 (97348 ± 2 cm^{-1}), as well as evidence that the outgoing $l = 3$ continuum channel is important in the threshold ionization of O_2.

C.A. 1990, 112, N 8

O_2

1989

112: 65888w **Photoionization and photoelectron spectroscopy of molecular oxygen with coherent vacuum ultraviolet radiation.** Tonkyn, Russell G.; Winniczek, Jerry W.; White, Michael G. (Chem. Dep., Brookhaven Natl. Lab., Upton, NY 11973 USA). *J. Chem. Phys.* 1989, 91(11), 6632-42 (Eng). The photoionization of O_2 near its ionization limit was studied with coherent vacuum-UV radiation produced by 3rd harmonic generation in free jet expansions of the rare gases. High resoln. (~ 2 cm^{-1}) photoionization spectra were obtained in the ionization threshold region at 98-103 nm which includes 3 vibrational levels of the H $^3\Pi_u$ (3sσ) Rydberg state. The H, $v = 0$ photoionization spectrum was assigned by simulating the H $^3\Pi_u \leftarrow X\ ^3\Sigma_g^+$ Rydberg excitation, yielding spectroscopic consts. and the overall autoionization lifetime. The $v = 1$ and 2 levels have distinctly different rotational band contours which reflect perturbations with bound and dissociative levels of nearby dark states. The photoionization dynamics were probed further through measurements of photoelectron angular distributions for the $v^+ = 0$ and 1 vibrational levels of O_2^+. In addn. to strong variations in the asymmetry parameter (β) across the H state autoionization resonances, spectrally narrow variations in β were found in the surrounding continuum. These latter results suggest the presence of weak resonance features imbedded in the background continuum which nonetheless strongly influence the photoelectron ejection dynamics.

I;

[illegible]

C.A. 1990, 112, N8

O_2

1989

14 Б1141. Новые оценки сродства к электрону молекул O_2 и NO. Reinvestigation of the electron affinities of O_2 and NO / Travers M. J., Cowles D. C., Ellison G. B. // Chem. Phys. Lett.— 1989.— **164**, № 5.— С. 449—455.— Англ.

С разрешением ~20 мэВ исследованы фотоэлектронные спектры с возбуждением лазерным излучением с энергией 2,54 эВ для пучка анионов O_2^- (I) и NO^- (II), образующихся при электрич. разряде в атмосфере O_2 и N_2O, соотв. В спектре I идентифицированы колебат. полосы, отвечающие трем конечным состояниям O_2 $^3\Sigma_g^-$, $^1\Delta_g$ и $^1\Sigma_g^-$, а в спектре II найдена лишь одна полоса, соотв-щая $^2\Pi$ состоянию NO. Проведен детальный анализ полученных спектров (учет вращат. уширения, франк-кондоновских факторов) и определены: частота колебаний в основном состоянии O_2^- (1073 ± 50 см$^{-1}$), равновесные межъядерные расстояния $1{,}347+0{,}005$ и $1{,}271+0{,}005$ А для I и II: соотв. Сродство к электрону для молекул O_2 и NO оценены в $0{,}451+0{,}007$ и $0{,}027+0{,}005$ эВ.

О. А. Басченко

М·П; Ae

④ ☒

X·1990, N 14

N_2O

O_2

1989

6 Д325. Новые измерения сродства к электрону O_2 и NO. Reinvestigation of the electron affinities of O_2 and NO // Travers Michael J., Cowles Daniel C., Ellison G. Barney // Chem. Phys. Lett.— 1989.— **164**, № 5.— С. 449—455.— Англ.

Методом фотоэлектронной спектроскопии получены и интерпретированы фотоэлектронные спектры ионов O_2^- и NO^-. Селекция ионов по массам проводилась с помощью фильтра Вина. Фотоотрыв электрона проводился с помощью излучения ионного лазера на Ar II. Анализ фотоэлектронов по энергии проводился с помощью электростатического полусферич. анализатора. Наблюдался фотоотрыв, приводящий к трем электронным состояниям ($^3\Sigma_g^-$, $_1\Delta_g$, $^1\Sigma_g^+$) O_2 и одному ($^2\Pi$) — для NO. Получены следующие величины сродства к электрону СЭ(O_2) = 0,451±0,007 эВ и СЭ (NO) = 0,026±±0,005 эВ. Анализ фотоэлектронных спектров дает величину частоты колебаний O_2^- (1073±50 см$^{-1}$) и длины связей $r(O_2)^- = 1,347\pm0,005$ Å и $r(NO^-) = 1,271\pm\pm0,005$ Å. Г. К.

Ae, м.п.

(74) ☒

ф. 1990, N6

O_2

(Оп 33102)

1989

112: 87090g The collision-induced radiation of oxygen molecule ($a^1\Delta_g$). Wildt, J.; Fink, E. H.; Biggs, P.; Wayne, R. P. (Fachbereich Phys. Chem., Bergische Univ.-GH Wuppertal, 5600 Wuppertal, 1 Fed. Rep. Ger.). *Chem. Phys.* 1989, 139(2-3), 401-7 (Eng). Emissions from the 1st excited state of O_2 ($a\ ^1\Delta_g$) were obsd. at pressures 1-30 torr in a flow system and 5-1000 torr in a static system. The relative intensities of the (0,0) band at $\lambda = 1.27$ μm and of the (0,1) band at $\lambda = 1.58$ μm changed as a function of O_2 pressure. At higher pressures a continuum was obsd. under the discrete lines of the (0,1) mol. emission. Comparison of the intensities of the 2 bands enabled rate consts. for the collision-induced radiative processes to be deduced. These rate consts. for the (0,0) and (0,1) bands, resp., were 4.1×10^{-23} and 1.2×10^{-23}, 3.4×10^{-23} and 9.9×10^{-24}, 2.4×10^{-24} and 7.2×10^{-24} cm³ s⁻¹ at 217, 293, and 336 K.

Спектр

C.A. 1990, 112, N 10

O_2

1989

112: 44683k **Reply to "Comment on predissociation of molecular oxygen in the B state".** Wodtke, A. M.; Huwel, L. (Dep. Chem., Univ. California, Santa Barbara, CA 93106 USA). *J. Chem. Phys.* 1989, 91(10), 6540 (Eng). A reply to the polemic of D. E. Freeman et al. (*ibid.* 6538). The SR 11 ← 2, R(27) triplet and a no. of other triplets ($v' = 10$ and 11, $J' > 15$) were remeasured with much higher signal to noise. The F_1:F_2:F_3 spacings are 1.7 and 1.2 cm^{-1}, resp., in close agreement with calcns. based on F's mol. consts. derived from new high resoln. absorption data. The abs. spin-state dependent predissocn. lifetimes are derived. It is impossible to rationalize these data on the basis of spin-orbit coupling to a repulsive $^5\Pi_u$ surface.

предиссоциация
в B-состоян.

C.A. 1990, 112, N6

O_2

1989

6 Б1342. Кривая потенциальной энергии для $O_2X(^3\Sigma_g^-)$ и дипольный момент перехода полосы Шумана — Рунге вблизи диссоционного предела. The potential energy function for $O_2X(^3\Sigma_g^-)$ and the transition dipole moment of the Schumann — Runge band near X-state dissociation / Yang X., Wodtke A. M. // J. Chem. Phys.— 1989.— 90, № 12.— С. 7114—7117.— Англ.

Зарегистрирован спектр испускания перехода $B^3\Sigma_u^- \rightarrow X^3\Sigma_g^-$ молекулы O_2 вплоть до $v''=35$. Определена ф-ция потенциальной энергии $X^3\Sigma_g^-$ состояния до диссоц. предела, к-рый оценен с точностью ±50 см$^{-1}$. Обсужден построенный Пт в сравнении с имевшимися ab initio расчетами. По интенсивностям полос испускания и значениям абс. момента перехода до 3.2 ат. ед. выведена ф-ция дипольного момента перехода полосы Шумана — Рунге до 4.2 ат. ед. Точность и полнота эксперим. данных позволяет использовать молекулу O_2 в кач-ве тестовой для теорет. расчетов потенциальной Пв и радиац. времен жизни. Е. А. Пазюк

М·Л·

Х·1990, №6

O_2

1989

$(X^3\Sigma_g^-)$

М.П.

3 Д272. **Кривая потенциальной энергии $O_2(X^3\Sigma_g^-)$ и дипольный момент перехода системы Шумана—Рунге вблизи диссоциационного предела *X*-состояния.** The potential energy function for $O_2(X^3\Sigma_g^-)$ and the transition dipole moment of the Schumann—Runge band near *X*-state dissociation / Yang X., Wodtke A. M. // J. Chem. Phys.— 1989.— 90, № 12.— С. 7114—7117.— Англ.

Выполнен анализ полученного недавно с использованием перестраиваемого лазера на ArF эмиссионного спектра (с измеренными абс. интенсивностями испускания) системы полос Шумана—Рунге $B^3\Sigma_u^-, v' \to X^3\Sigma_g^-, v''$ (с индуцированным лазером возбуждением отдельных состояний $v'=10—17$) вплоть до переходов на $v''=35$. По спектру построены кривые по-

мет

ия

ф. 1990, N3

тенц. энергии Ридберга—Клейна—Риса как нижнего состояния $v_X(r)$ вблизи диссоциационного предела с точностью ±50 см$^{-1}$, так и верхнего состояния, по которым рассчитаны факторы Франка—Кондона и $v'v''$-центроиды переходов. С их использованием из эксперим. интенсивностей получена зависимость дипольного момента перехода $\mu_e(r)$ от межъядерного расстояния r. Приведена полученная часть потенц. кривой в области $r=(3—5)\ a_0$ (a_0 — радиус Бора), отмечается хорошее совпадение с имеющимися результатами многоконфигурац. приближения с самосогласованным полем, в котором рассчитанная квантовомеханич. зависимость $V_X(r)$ с точностью до некоторой неопределенности начала отсчета (совмещение в минимуме потенц. энергии либо по энергии, соответствующей свободным атомам $O(^3P)$) совмещается с экспериментальной. Выведена зависимость, вплоть до $r=4{,}2$ ат. ед., $\mu_e(r)=66{,}44\cdot\exp(-1{,}528\cdot r)$. В. Н. Сошников

O_2

1989

(потенц. ф-ия)

$X^3\Sigma_g^-$

111: 47472f **The potential energy function for molecular oxygen $X(^3\Sigma_g^-)$ and the transition dipole moment of the Schumann-Runge band near X-state dissociation.** Yang, X.; Wodtke, A. M. (Dep. Chem., Univ. California, Santa Barbara, CA 93106 USA). *J. Chem. Phys.* 1989, 90(12), 7114–17 (Eng). Emission spectra were analyzed for transitions of $O_2(B^3\Sigma_u,v' \rightarrow X^3\Sigma_g^-,v'')$ with v'' as high as 35. The $X^3\Sigma_g^-$ potential energy function, $V_x(r)$, was detd. nearly to the dissocn. limit with an estd. accuracy of ±50 cm^{-1}. $V_x(r)$ Is compared to the highest level ab initio calcn. avalanche. The transition dipole moment function, $\mu(r)$, for the O_2 Schumann–Runge band is also extended almost to the dissocn. limit. The O_2 mol. now provides one of the best testing grounds for ab initio theories of dissocn. and radiation.

C.A. 1989, 111, N6

O_2 (пт. 33950) 1990

Бессонова С. М., Финкельштейн А. И.

оценка
м. п.

Ж. прикл. спектроскопии 1990, 52, №3,
● 451–454.

O_2 От. 36091 1990

Braunstein M., McKoy V.,

фото- et al.,

электр.

спектр J. Chem. Phys. 1990,

<u>93</u>, N 7, 5345–5346

Shape resonance effects in

the rotationally resolved photoelectron spectra of O_2.

O_2 Om. 34643 1990

Carroll T.X., Thomas T.D.,

J. Chem. Phys. 1990,
92, N 12, 7171-7177

Deexitation electron spectroscopy of core-excited O_2.

O_2 от. 35113 1990

Cheung A.S.-C., Yoshino K., et al.,

J. Chem. Phys., 1990,
92, N 2, 842-849

Predissociation linewidths of

the (1,0) – (12,0) Schumann-Runge absorption bands of O_2 in the wavelength region 179 – 202nm.

O_2

1990

113: 218542b Electron-impact excitation of the Rydberg levels of the oxygen molecule. Chung, Snuggi; Lin, Chun C.; Lee, Edward T. P. (Dep. Phys., Univ. Wisconsin, Madison, WI 53706 USA). *Phys. Rev. A* 1990, 42(7), 4391–4 (Eng). Electron-impact cross sections for exciting the O mol. from the ground electronic level to the $ns\sigma_g$, $np\sigma_u$, $nd\sigma_g$, $nf\sigma_u$, $np\pi_u$, $nd\pi_g$, and $nf\pi_u$ Rydberg levels assocd. with the $O_2^+(B\ ^2\Sigma_g^-)$ and $O_2^+(b^4\Sigma_g^-)$ cores are presented. For each Rydberg series of a given l, m, and O_2^+ core state, the cross sections exhibit n dependence of the form n^{-a} with a varying from one series to another in the range of 1.47–4.60 in contrast to the more universal n^{-3} dependence for the H atom. The potential cusps at the 2 nuclear sites of the mol. make the Rydberg orbital d. near the origin quite different from that of the H atom, thereby spoiling the simple n^{-3} dependence.

Сечение ионизации

C.A. 1990, 113, N24.

$^{18}O_2$, $^{18}O^{16}O$

1990

предиссоц.

113: 220530q **Predissociation linewidths of the (3,0)–(11,0) Schumann-Runge absorption bands of molecular oxygen isotopomers ($^{18}O_2$ and ^{16}O ^{18}O) in the wavelength region 180–196 nm.** Chiu, S. S. L.; Cheung, A. S. C.; Yoshino, K.; Esmond, J. R.; Freeman, D. E.; Parkinson, W. H. (Chem. Dep., Univ. Hong Kong, Hong Kong, Hong Kong). *J. Chem. Phys.* 1990, 93(8), 5539–43 (Eng). Predissocn. linewidths of the (3,0)–(11,0) Schumman-Runge bands of $^{18}O_2$ and $^{16}O^{18}O$ in the wavelength region 180–196 nm were obtained from the published measurements of the abs. absorption cross sections of Yoshino et al. (1988), (1989) and spectroscopic consts. of these mols. of Cheung et al. (1988), (1989). The linewidths were detd. as parameters in the nonlinear least-squares fitting of calcd. to measured cross sections. Predissocn. max. were found at upper vibrational levels with $v' = 4, 7,$ and 10 for $^{18}O_2$ and for $^{16}O^{18}O$. The predissocn. linewidths are mostly greater than previous exptl. values for both isotopic mols.

C. A. 1990, 113, N24.

$^{16}O^{18}O$

ОМ 33973

1990

Crownover R.L.;

De Lucia F.C.; et al;

Субмиллиметр-
волнов.
спектр

Astrophys. J. 1990,
349, N1, Pt2, L29-L31

O_2 От 34377 1990

115: 81067v **High resolution Fourier-transform spectra of the $a^1\Delta_{(g)} \rightarrow X^3\Sigma_{(g)}^-$, $b^1\Sigma_{(g)}^+ \rightarrow X^3\Sigma_{(g)}^-$ and $b^1\Sigma_{(g)}^+ \rightarrow a^1\Delta_{(g)}$ systems of oxygen molecule, sulfur monoxide, diatomic sulfur, and isoelectronic molecules in the NIR region.** Fink, E. H.; Kruse, H.; Setzer, K. D.; Ramsay, D. A.; Vervloet, M. (GH Wuppertal, Bergische Univ., D-5600 Wuppertal, Fed. Rep. Ger.). *Acta Phys. Hung.* 1990, 67(1-2), 67-72 (Eng). Emission spectra of the $a^1\Delta(g) \rightarrow X^3\Sigma_{(g)}^-$, $b^1\Sigma_{(g)}^+ \rightarrow X^3\Sigma_{(g)}^- \rightarrow a^1\Delta_{(g)}$ systems of a no. of Group VI-Group VI diatomics were measured at high resoln. with a Fourier-transform spectrometer in the near-IR region. Anal. of the spectra allows a systematic test of different Hamiltonians for the $X^2\Sigma_{(g)}^-(X_10_{(g)}^+, X_21_{(g)}^\pm)$ ground states and of the line strength formulas for the elec. quadrupole, magnetic dipole and elec. dipole transitions involved.

$a^1\Delta_g - X^3\Sigma_g^-$

$b^1\Sigma_g^+ - X^3\Sigma_g^-$

$b^1\Sigma_g^+ - a^1\Delta_g$

м.п.

C.A. 1991, 115, N8

(42) 1☒

SO, S_2

$^{16}O_2$ от. 33753 1990

Friedman R.S.,

сила
осцил-
лятора

J. Quant. Spectrosc. and Radiat. Transfer. 1990, <u>43</u>, N 3, 225-238

Oscillator strengths of the Schumann - Runge bands of isotopic oxygen molecules.

O_2

ОМ 35184 1990

и·п·

Х·1991, N 15

15 Б1186. $C^3\Pi_g$ ридберговое и $1^3\Pi_g$ валентное состояния O_2. The $C^3\Pi_g$ Rydberg and $1^3\Pi_g$ valence states of O_2 / Friedman R. S., Dalgarno A. // J. Chem. Phys.— 1990.— 93, № 4.— С. 2370—2374.— Англ.

Представлена интерпретация имеющихся в лит-ре данных о положениях и ширинах колебат. уровней энергии $C^3\Pi_g$ ридбергового состояния O_2. Энергии уровней описаны как резонансы при упругом рассеянии атомов кислорода в несвязанном $1^3\Pi_g$ валентном состоянии, вызываемом вз-вием со связанным $C^3\Pi_g$ ридберговым состоянием. Для расчетов использованы связанные ур-ния рассеяния с эмпирич. кривой потенциальной энергии для валентного состояния и ПТ вз-вия ридбергового валентного состояния. Показано, что эксперим. данные о положениях и ширинах уровней воспроизводятся при величине ПТ вз-вия 63 мэВ и когда кривая потенциальной энергии $1^3\Pi_g$ состояния пересекает потенциальную кривую $C^3\Pi_g$ состояния на внешней части участка, описывающего притяжение атомов.

Е. А. Пазюк

O_2

От 35184.

1990

113: 122863f The $C^3\Pi_g$ Rydberg and $1^3\Pi_g$ valence states of molecular oxygen. Friedman, R. S.; Dalgarno, A. (Harvard–Smithsonian Cent. Astrophys., Cambridge, MA 02138 USA). *J. Chem. Phys.* 1990, 93(4), 2370–4 (Eng). Exptl. data on the positions and widths of the vibrational energy levels of the $C^3\Pi_g$ Rydberg state of mol. oxygen are interpreted. The energy levels are described as resonances in the elastic scattering of oxygen atoms in the open $1^3\Pi_g$ valence state caused by a coupling to the closed $C^3\Pi_g$ Rydberg state. The coupled scattering equations are set up with an empirical valence potential energy curve and Rydberg–valence interaction potential and it is shown that the energy level positions and widths can be reproduced by an interaction of 63 meV and a potential energy curve that crosses the Rydberg curve on the attractive part of its outer limb.

$C^3\Pi_g$, $1^3\Pi_g$

C.A. 1990, 113, N 14.

O_2

От 35184

1990

6 Д90. **Ридберговское $C^3\Pi_g$ и валентное $1\,^3\Pi_g$ состояния молекулы O_2.** The $C^3\Pi_g$ Rydberg and $1\,^3\Pi_g$ valence states of O_2 / Friedman R. S., Dalgarno A. // J. Chem. Phys.— 1990.— 93, № 4.— С. 2370—2374.— Англ.

Проанализированы эксперим. спектры молекулы O_2, относящиеся к колебательным энергетич. уровням ридберговского состояния $C^3\Pi_g$. Рассмотрены положения и ширины спектральных линий; отмечено, что энергетич. уровни описываются как резонансные состояния при упругом рассеянии атомов кислорода в валентном $1\,^3\Pi_g$- и ридберговском $C^3\Pi_g$-состояниях. Построен набор ур-ний, описывающий колебательную структуру полос; ур-ния используют эмпирич. данные о потенц. кривой состояний $1\,^3\Pi_g$ и потенциале взаимодействия между состояниями. Модуль позволяет воспроизводить положения и ширины резонансных колебательных уровней ридбергова состояния с хорошей точностью.

А. Ю. Ермилов

М.П.

ф. 1991, N 6

O_2 ат. 35806 1990

Göthe M.C.,

Acta Univ. Upsal.: Compr.
Summ. Uppsala Diss. Fac. Sci.
1990, N292, 1-80.

Inner Valence studies on
N_2, CO and O_2.

O_α (OM 34369) 1990

Hohm U., Kerl K.,

Mol. Phys. 1990, 69, N5,
819 - 831.

Interferometric measurements of the dipole polarizability α of molecules between 300K and 1100K.

II A new method for measuring the dispersion of the polarizability and its application to Ar, H_2, and O_2.

O_2 (ОМ 34 368) 1990

Hohm U., Kerl K.,

Mol. Phys. 1990, <u>69</u>, N 5,

803-817.

Interferometric measurements of the dipole polarizability α of molecules betwum 300 K and 1100K.

I Monochromatic measurements at $\lambda = 632.99$ nm for the noble gases and H_2, N_2, O_2, and CH_4.

O_2

Om 34442

1990

113: 105476q **Diode laser spectroscopy of the atmospheric oxygen band ($b^1\Sigma_g^+ - X^3\Sigma_g^-$).** Kanamori, Hideto; Momona, Morihisa; Sakurai, Katsumi (Dep. Pure Appl. Sci., Univ. Tokyo, Tokyo, Japan 153). *Can. J. Phys.* 1990, 68(3), 313-16 (Eng). The atm. O_2 band due to magnetic dipole transitions was studied by a diode laser absorption spectroscopy combined with a Zeeman modulation technique. The high-resoln. spectrum of the 0-0 band was obsd. with Doppler-limited resoln. and compared with a previous spectrograph measurement. The Zeeman effect at low magnetic field was investigated by the Zeeman line profiles. The 2nd-order Zeeman effect was observable in the F_2 transition of the $^3\Sigma_g^-$ state with magnetic field as low as 150 G.

$b^1\Sigma_g^+ - X^3\Sigma_g$

М·Л·

C. A. 1990, <u>113</u>, N 12

O_2^-

1990

расчёт
м.п.,
Ti

Klobukowski M.,
Dingle T.W. et al.
Theor. Chim. Acta 1990,
<u>77</u>(3), 191–205.

(см. C_2; III)

O_2 1990

Klobukowski M.,
Dingle T.W. et al.
Theor. Chem. Acta 1990,
<u>77</u>(3), 191-205.

расчёт
м.п.,
Ti

(см. C_2; $\overline{\underline{III}}$)

O_2 Om·34147 1990

Lapiano-Smith D., Lee K., et al.,
J. Electron Spectrosc. and Relat. Phenom. 1990, 51,
Spec. Issue, 221-228
Auger Decay and autoio-

nization of core Hole excited states in molecular oxygen.

O_2 От 34480 1990

Larsson M., Baltzer P., et al.,

спектр

J. Phys. B. 1990, 23, N7, 1175-1195.

X-ray photoelectron, Auger

electron and ion fragment spectra of O_2 and potential curves of O_2^{2+}.

O_2 Om · 34269 1990

Lewis B.R., Gibson S.T., Can. J. Phys., 1990, 68, 231-237.

Rotational line strengths in $^3\Sigma^+ - {}^3\Sigma^-$ electronic transitions.

The $B^3\Sigma_u^+ - X^3\Sigma_g^-$ and $A^3\Sigma_u^+ - X^3\Sigma_g^-$ systems of molecular oxygen.

O_2 от 35977 1990

9 Д130. Замечание к статье: Функция потенциальной энергии для $O_2X(^3\Sigma_g^-)$ и дипольный момент перехода для полосы Шуманна—Рунге вблизи [порога] диссоциации состояния X. — Ответ авторов. Comment on: The potential energy function for $O_2X(^3\Sigma_g^-)$ and the transition dipole moment of the Schumann—Runge band near X state dissociation» — Authors' reply / Lewis B. R., Gibson S. T., Yang X., Wodtke A. M. // J. Chem. Phys.— 1990.— **93**, № 10.— С. 7532—7534.— Англ.

См. / Yang X. et al. // ibid.— 1989.— **90**.— С. 7114.

М.П.

ф. 1991, №9

O_2

Оп 35977

1990

114: 31983z **Comment on "The potential energy function for molecular oxygen (O_2 $X(^3\Sigma_g^-)$) and the transition dipole moment of the Schumann–Runge band near X state dissociation".** Lewis, B. R.; Gibson, S. T. (Res. Sch. Phys. Sci., Aust. Natl. Univ., Canberra, 2600 Australia). *J. Chem. Phys.* **1990,** 93(10), 7532–3 (Eng). A polemic. In studying the emission spectra for the Schumann–Range transition ($B^3\Sigma_u^- \rightarrow X^3\Sigma_g^-$) of O_2, X. Yang and A.M. Wodthe (*ibid.*, 1989, 90, 7114) derived the relative electronic transition moment for internuclear distances of 3.04–4.09 a.u. The normalization of their results fails due to misinterpretations of previous exptl. work, and their anal. representation of the transition moment is erroneous.

$X^3\Sigma_g^-$,
потенц.
кривая

С.А. 1991, <u>114</u>, N 4

O_2 1990

Margreiter D.,
Deutsch H., et al.

сечение
ионизации,
теор.
расчет.

Int. J. Mass Spectrom.
Ion Processes 1990, 100,
157–76.

(см. H_2; III)

O_2 1990

McKoy V., Braunstein M.,
et al.
J. Electron. Spectrosc. and
Relat. Phenom. 1990, 52,
Spec. Issue. 597-612.
Photoelectron Spectroscopy of

Excited Molecular States.

O_2 От 35042 1990

112: 87446c **Identification of the $3d\pi\,^1\Delta_g$ and $^3\Delta_{2g}$ Rydberg state of molecular oxygen by multiphoton ionization and polarization studies.** Park, Haiyoon; Li, Leping; Chupka, William A. (Sterling Chem. Lab., Yale Univ., New Haven, CT 06511 USA). *J. Chem. Phys.* 1990, 92(1), 61–4 (Eng). The $v' = 0$–4 levels of the $3d\pi\,^1\Delta_g$ state and $v' = 0$–3 levels of the $3.d\pi^3\Delta_{2g}$ state of O_2 were identified and studied by multiphoton ionization and polarization techniques. The obsd. levels exhibit no detectable perturbation except for rather large Λ doubling probably due to L uncoupling, and heterogeneous predissocn. probably by a Π_g valence state. The observation of large amts. of O^+ for the higher vibrational levels suggests large non-Franck-Condon effects in the ionization process.

Ридберг. сост.

С.А. 1990, 112, N10

O_2

ОМ 34721 1990

θ) 5 Б1136. **Двухфотонная спектроскопия 3*d*-ридберговских состояний O_2. Состояния $^1\Phi_g$ и $^3\Phi_g$.** Two-photon spectroscopy of the 3*d* Rydberg states of O_2: $^1\Phi_g$ and $^3\Phi_g$ states / Park H., Li L., Chupka W. A., Lefebvre-Brion H. // J. Chem. Phys.— 1990.— 92, № 10.— С. 5835—5840.— Англ.

Методом спектроскопии резонансно усиленной многофотонной (2+1) ионизации $\underline{O_2(a^1\Delta_g)}$ исследованы ридберговские состояния $3d\delta$ $(^1\Phi_g,\ ^3\Phi_g)$ молекулы O_2-$(O_2^+ \xleftarrow{h\gamma} O_2(^1\Phi_g,\ ^3\Phi_g) \xleftarrow{2h\gamma} O_2(a^1\Delta_g))$. Для состояний $^3\Phi_2$, $^3\Phi_3$, $^3\Phi_4$, $^1\Phi_3$ приведены значения T_v, B_v, γ_v $(v'=0-4)$, где γ — параметр описывающий эффективный сдвиг (γJ) уровней энергии вследствие вз-вия компонент $^3\Phi_2$ и $^3\Phi_3$ через оператор разрыва связи S (то же самое имеет место для пары состояний $^3\Phi_4$ и $^1\Phi_3$). В отличие от других ридберговских состояний O_2, состояния $^3\Phi_3$, $^3\Phi_2$, $^3\Phi_4$ не обнаруживают признаков воз-

М.П.

Х. 1991, N5

мущений или предиссоциации каким-либо валентным состоянием. Состояние $^1\Phi_3$ слабо предиссоциировано, вероятно, за счет вз-вия с близколежащим сильно предиссоциир. состоянием $3d\pi^3\Delta_{2g}$. Обсуждены возможные причины, препятствующие обнаружению состояний $3d\pi^1\Sigma_g^-$ и $3d\Pi_g$ (состояния $3d^1\Sigma_g^+$, Δ_g, Φ_g наблюдались). Предположено, что для них низка вероятность двухфотонных переходов в сравнении с наблюдаемыми переходами в ридберговские $3d$-состояния. В. М. Ковба

нм
(13.6)

O_2 Оп 34721 1990

113: 14203g **Two-photon spectroscopy of the 3d Rydberg states of molecular oxygen: $^1\Phi_g$ and $^3\Phi_g$ states.** Park, Haiyoon; Li, Leping; Chupka, William A.; Lefebvre-Brion, Helene (Sterling Chem. Lab., Yale Univ., New Haven, CT 06511 USA). *J. Chem. Phys.* 1990, 92(10), 5835–40 (Eng). The $3d\delta^1\Phi_g$ and $^3\Phi_g$ Rydberg states of O_2 were obsd. by (2 + 1) resonant enhanced multiphoton ionization from the metastable $\alpha^1\Delta_g$ state and the resulting spectra rotationally analyzed. In contrast to all other obsd. Rydberg states of O_2, the $^3\Phi_2$, $^3\Phi_3$, and $^3\Phi_4$ states show no sign of perturbation or predissocn. by valence states. The $^1\Phi_3$ state is apparently weakly predissociated. The energy level structure of those 3d Rydberg states which were reliably assigned is compared with theor. calcns. The reasons for the failure to detect Π_g states in these expts. are discussed.

$^1\Phi_g$, $^3\Phi_g$
Ридберг.
состоян.

C.A. 1990, 113, N2

O_2

1990

Ридберг-состояние

113: 161671m Two-photon spectroscopy of Rydberg states of molecular oxygen. Pratt, S. T.; Dehmer, J. L.; Dehmer, P. M. (Argonne Natl. Lab., Argonne, IL 60139 USA). *J. Chem. Phys.* 1990, 93(5), 3072-84 (Eng). Two-photon resonant, three photon ionization spectrum of $O_2\,X\,^3\Sigma_g^-$, $v'' = 0$ is presented in the energy region between the 5s-4d complex and the $O_2^+\,X\,^2\Pi_{1/2g}$, $v^+ = 0$ ionization threshold. The spectrum exhibits a no. of new transitions to *ns* and *nd* Rydberg states with $n = 5$-9 and $v' = 0$ and 1 as well as transitions to the previously unobserved 5s-4d, $v' = 3$ levels. For a given value of n and v', the obsd. bands split into two groups sepd. by approx. the $O_2^+\,X\,^2\Pi_{1/2g}$ - $^2\Pi_{3/2}$ spin-orbit splitting. All of the bands show at least some sharp rotational structure, although in most cases this structure is limited to a few lines. In addn., the direct 2-photon ionization spectrum of $O_2\,X\,^3\Sigma_g^-$, $v'' = 0$ is presented in the energy region between the $O_2^+\,X\,^2\Pi_{1/2g}$, $v^+ = 0$ and 1 thresholds; the spectrum shows transitions to Rydberg states with $n = 8$-12 and $v' = 1$. These states are analogous to the $v' = 0$ states obsd. below the ionization threshold, and they decay by vibrational autoionization into the $v^+ = 0$ continuum. Taken together, the $v' = 0$ and 1 Rydberg states obsd. here provide a significant addn. to the knowledge of Rydberg series converging to the ground electronic state of O_2^+.

C. A. 1990, 113, N 18

O_2 Om 35112 1990

Shelton D.P.,
Phys. Rev. A 1990, 42,
N5, 2578–2592.
Nonlinear-optical susceptibilities of gases measu-

red at 1064 and 1319 nm.

O_2 От 34477 1990

Stephens J.A., Braunstein M., McKoy V.,

J. Chem. Phys. 1990, 97 N 9, 5319-5327

Multiplet- ● specific shape

resonance and autoionization effects in (2+1) resonance enhanced multiphoton ionization of O_2 via the $d\,^1\Pi_g$ state.

O_2 | от 34851 | 1990

Излучат.
Энергетич.
уровни

Tokuda T., Fujii N.,
et al.,
Chem. Phys. Lett. 1990,
174, N 5, 385–388.

New emission of $CuCl_2$ in chemically produced

$O_2(^1\Delta)$ flow.

O_2

1990

$X^3\Sigma_g^-$,

потенц.
кривая

114: 31984a Reply to "Comment on 'The potential energy function for molecular oxygen (O_2 $X(^3\Sigma_g^-)$) and the transition dipole moment of the Schumann–Runge band near X-state dissociation'". Yang, Xueming; Wodtke, A. M. (Dep. Chem., Univ. California, Santa Barbara, CA 93106 USA). *J. Chem. Phys.* 1990, 93(10), 7534 (Eng). A polemic in response to B.R. Lewis and S.T. Gibson (*ibid.*, 7532). Y. and W. (*ibid.*, 1989, 90, 7114) used data of A. C. Allison et al. (1971) which was erroneous.

C.A.1991, 114, N4

O_2 (ОМ 35346) 1991

Bharate N.S., Behere S.H.,
et al.,

м.п. Nuovo Cim. D. 1991, <u>13</u>, N 1,
15–20.

Estimation of Rotational and
Vibrational Constants for

Diatomic Molecules Using Mattera's Potential Function.

O_2 1991

Boehm R.C., Lohr Lawrence L.,

J. Comput. Chem. 1991, 12,

М.п. N1, c. 119-125.

(См. NO_3^+; III)

O_2 Om. 36452 1991

Cann M.W.P., Nicholls R.W.,

Can. J. Phys. 1991, 69,
N 8/9, 1163–65

Spectral line parameters
for the O_2 Herzberg I band
system.

O_2

1991

5 Д140. Синглет-триплетные разности энергий в гомоядерных двухатомных молекулах. Исследование правила Хунда методом НИК-КВ. Singlet—triplet energy component differences in homonuclear diatomics: a multi-reference configuration interaction study of Hund's rule / Darvesh K. V., Fricker P. D., Boyd R. J. // Chem. Phys.— 1991.— **157**, № 1—2.— С. 99—104.— Англ.

Методом НИК-КВ проведены расчеты низколежащих электронных состояний молекул C_2 ($a^3\Pi_u$ и $A^1\Pi_u$) и O_2 ($X^3\Sigma_g^-$, $a^1\Delta_g$) при различных межъядерных расстояниях. Показано, что синглет-триплетные разности энергий электрон-электронного отталкивания имеют тот же знак, что и синглет-триплетные разности кинетич. энергий. Соответствующие разности энергий электрон-ядерного притяжения имеют противоположный знак в той же геометрии. Адиабатич. приближение для C_2 и O_2 по-

М·Л·

Ⓗ ☒

ф. 1992, N5

C_2

казывает, что электрон-электронное отталкивание и электрон-ядерное притяжение в триплетном состоянии больше, чем в синглетном. Этот результат согласуется с данными для атомных состояний, полученных из тех же конфигураций, но противоречит традиционному объяснению правила Хунда.

O_2 OM·36251 1991

Gibson S.T., Lewis B.R., Baldwin K.G.H., et al.,

J. Chem. Phys. 1991, 94, N 2, 1060 – 1068.

Rotational features in
the fluorescence

excitation spectrum of $O\ (^1D_2)$ from vacuum ultraviolet laser photodissociation of O_2.

O_2

высок. возб.

эл. состоян

(обзор)

1991

Golubkov G.V.,

Ivanov G.K.

Itogi Nauki Tech.

Ser: Kinet Katal.

1991, <u>24</u>, 82-130

●

Ссы. №2 (II)

O_2

1991

115: 217413q E1 transitions of astrophysical interest in neutral oxygen. Hibbert, A.; Biemont, E.; Godefroid, M.; Vaeck, N. (Dep. Appl. Math. Theor. Phys., Queen's Univ., Belfast, UK BT7 1NN). *J. Phys. B: At., Mol. Opt. Phys.* **1991**, 24(18), 3943–58 (Eng). At. transition rates and *f* values were calcd. in the triplet and quintet systems and for some intercombination lines of neutral oxygen. CI was included in the calcns. performed with the CIV3 code of Hibbert for all the transitions connecting the $n = 3$ and $n = 4$ energy levels. In order to reproduce the obsd. energy splittings between the energy states, small empirical adjustments were introduced to the diagonal matrix elements. Comparisons with previously published *f* values and radiative lifetimes are discussed and the subsequent astrophys. applications of the results are briefly mentioned.

и.п.

C:A·1991; 115, N 20

O_2

1991

21 Б1022. Эффективный гамильтониан валентной оболочки и потенциальные кривые молекулы кислорода, полученные с помощью квазивырожденной многочастичной теории возмущений. Effective valence shell Hamiltonian and potential curves of the oxygen molecule from quasidegenerate many-body perturbation theory / Kanzier Alfred W., Freed Karl F. // J. Chem. Phys.— 1991.— 94, № 5.— С. 3778—3789.— Англ.

С помощью квазивырожденной многочастичной теории возмущений получен эффективный гамильтониан валентной оболочки H^v для молекулы O_2 и рассчитаны потенциальные кривые десяти низколежащих электронных состояний O_2. Сопоставлена точность значений спектроскопич. постоянных при использовании различных порядков теории возмущений. Показано, что полученные с H^v 2-го порядка энергии диссоциации и

М.Л.

Х. 1991, № 21

колебат. частоты систематически завышены; переход к 3-му порядку приводит их в соответствие с данными расчетов полным методом конфигурац. вз-вия в том же базисе. Проведены также расчеты H^v с ограниченным набором орбиталей, сводящих молек. валентное пространство к сумме атомных валентных пространств, что позволило использовать значения матричных элементов H^v для проверки полуэмпирич. методов. Зависимости матричных элементов H^v в базисе АО от межъядерного расстояния аппроксимированы простыми функциональными формулами, используемыми в полуэмпирич. методах. Сопоставлены функциональные формы матричных элементов H^v для O_2, S_2 и CH. А. А. Сафонов

O_2

1991

(основн. сост.)

(м.п.)

117: 16141s **Improved fits for the vibrational and rotational constants of many states of nitrogen and oxygen.** Laher, R. R.; Gilmore, F. R. (R and D Assoc., Los Angeles, CA USA). *Report* 1990, RDA-TR-0226129003-001; Order No. AD-A229 996. 90 pp. (Eng). Avail. NTIS. From *Gov. Rep. Announce. Index (U. S.)* 1991, 91(12), Abstr. No. 130,579. All pertinent published measurements of the vibrational intervals and rotational consts. for 17 states of nitrogen, the ground state of O_2 have been assembled and plotted against *v*. These are the states important in modeling the fluorescence produced when air is bombarded by fast electrons. In about 70% of the states considered these tabulated coeffs. do not give optimum fits of the basic spectroscopic data, usually because of new data published since 1979. In these cases new improved coeffs. have been derived by least-squares fitting. The results are tabulated and plotted.

(+1) ☑ ● N_2 (17 нижних сост.)

(м.п.)

C. A. 1992, <u>117</u>, N2

O_2

1991

Основное состояние расчёт

115: 99696j Ab initio electronic structure calculations of oxygen using coupled cluster approaches and many-body perturbation theory. Lee, Yoon Sup; Lee, Sang Yeon (Dep. Chem., Korea Adv. Inst. Sci. Technol., Seoul, 130-650 S. Korea). *Bull. Korean Chem. Soc.* 1991, 12(2), 211-13 (Eng). The ground state of the O_2 is calcd. by various methods of CC approaches and MBPT using a double zeta plus polarization basis set ant the UHF ref. state. All the methods employed are capable of describing O_2 near the equil. bond length and the sepd. atom, but do not correctly depict the breaking of the multiple bond. For this basis set, including more correlations does not necessarily improve the agreement with expt. for mol. properties such as bond lengths and dissocn. energies.

C.A. 1991, 115, №10

O_2 OM·35815 1991

O_2^+ Lee Soo-Y, Lee S.C.,

J. Chem. Phys. 1991, 94,

r_e, D_e, N 8, 5313–5323.

d_e Spectral moment method versus least-squares Franck–Condon

analysis for vibrationally
resolved absorption spectra.

O_2

1991

10 Д110. Три формы молекулярного кислорода / Лэйнг М. // Ж. неорган. химии.— 1991.— 36, № 6.— С. 1618—1622

Описание трех электронных форм молекулярного кислорода: триплетной формы (основное состояние) с двумя неспаренными электронами и двух синглетных форм со спаренными электронами. Резюме

М.Л.

ср. 1991, №10

O_2 1991

Liu Lei, Li Jia-Ming.

J. Phys. B. 1991. 24,
N 8. C. 1893–1898.

м.п.

(см. C_2; III)

O_2

1991

10 Д111. Природа двойной связи кислорода. On the nature of the oxygen double bond / McWeeny R. // J. Mol. Struct. Theochem.— 1991.— 229.— С. 29—38.— Англ.

В рамках бесспинового варианта неэмпирич. метода валентных связей (ВС) исследовано электронное строение O_2. Показано, что метод ВС описывает триплетное основное состояние не менее «естественным» путем, чем метод ССП МО, и является более точным (если не учитывать конфигурац. взаимодействие). Он дает описание специфич. природы двойной связи, образующейся вследствие резонанса двух преобладающих ионных структур. В. Л.

М. Л.

сф. 1991, N10

O_2

1991

21 Б1025. О природе двойной связи в молекуле кислорода. On the nature of the oxygen double bond / McWeeny R. // J. Mol. Struct. Theochem.— 1991.— 229.— С. 29—38.— Англ.

М.Л.

Рассмотрено описание двойной связи в триплетном основном состоянии молекулы O_2 в рамках теории валентных связей. Проведены расчеты энергии O_2 с помощью неэмпирич. метода валентных связей. Показано, что по сравнению с методом МО—ССП метод валентных связей обеспечивает бо́льшую точность и позволяет интерпретировать двойную связь в O_2 как резонанс двух ведущих ионных структур. А. А. Сафонов

Х.1991, N21

$^{16}O^{18}O$

1991

115: 101778h **Microwave absorption lines of oxygen ($^{16}O^{18}O$) in its ($X^3\Sigma_g^-$, v = 0) state.** Mizushima, Masataka; Yamamoto, Satoshi (Dep. Phys., Univ. Colorado, Boulder, CO 80309 USA). *J. Mol. Spectrosc.* 1991, 148(2), 447–52 (Eng). The microwave spectrum of ^{16}O ^{18}O in the X $^3\Sigma_g^-$ ground state is obsd. in the 50–400 GHz region. The rotational and centrifugal distortion consts. and the spin-rotation and spin-spin interaction consts. with their centrifugal distortion terms were detd. The obtained consts. are consistent with those predicted by the theory of the isotope effect of O_2.

$X^3\Sigma_g^-$ (v=0)

Мв спектр,

М.П.

С.А. 1991, <u>115</u>, N10

O_2

1991

116: 28415b Theoretical study of the low-lying bound states of molecular oxygen. Partridge, Harry; Bauschlicher, Charles W., Jr.; Langhoff, Stephen R.; Taylor, Peter R. (Ames Res. Cent., NASA, Moffett Field, CA 94035 USA). *J. Chem. Phys.* **1991**, 95(11), 8292-300 (Eng). Ab initio results are presented for the low-lying bound states of O_2 that dissoc. to ground-state atoms. Spectroscopic consts. and dissocn. energies (D_e) are reported for the $X^3\Sigma_g^-$, $a^1\Delta_g$, $b^1\Sigma_g^+$, $c^1\Sigma_u^-$, $A'^3\Delta_u$, $A^3\Sigma_u^+$, $^3\Pi_u$, $^5\Pi_u$, and $^5\Pi_g$ states. For the first six states, which have been exptl. characterized, authors obtain accurate results at the multireference configuration-interaction level after correction for higher excitations. For example, our computed D_e value for the $X^3\Sigma_g^-$ state cor. for basis-set superposition error in only 0.7 kcal/mol less than the exptl. value.the $^5\Pi_g$ state is estd. to have a D_e of 0.16 ± 0.03 eV, suggesting that the importance of this state in the nightglow should perhaps be reconsidered.

теор. расчет
низших возб.
сост., De

C.A. 1992, 116, N4

O_2

1991

17 Б1034. Теоретическое изучение низколежащих связанных состояний O_2. Theoretical study of the low-lying bound states of O_2 / Partridge Harry, Bauschlicher Charles W. (Jr.), Langhoff Stephen R., Taylor Peter R. // J. Chem. Phys.— 1991.— 95, № 11.— С. 8292—8300.— Англ.

Методом функционала связанных пар рассчитаны потенциальные кривые электронных состояний O_2, отвечающих диссоциации на атомы в основных состояниях ^3P. Использован базис сгруппированных гауссовых ф-ций $(13s8p6d4f2g1h)/[6s5p4d3f2g1h]$. Орбитали получены многоконфигурац. методом ССП в полном активном пространстве. Определены спектроскопич. постоянные для состояний $X^3\Sigma_g^-$, $a^1\Delta_g$, $b^1\Sigma_g^+$, $c^1\Sigma_u^-$, $A'^3\Delta_u$, $A^3\Sigma_u^+$, $^3\Pi_u$, $^5\Sigma_u^-$, $^5\Pi_u$ и $^5\Pi_g$. Для основного состояния энергия диссоциации с учетом поправки на базисную суперпозиц. ошибку отличается от эксперим. значения лишь на 0,7 ккал/моль. Для состояния $^5\Pi_g$ получена оценка энергии диссоциации 0,16±0,03 эВ. Библ. 39.

А. А. Сафонов

М·Л·

Х. 1992, N 17

O_2

1991

8 Д88. Теоретическое изучение низколежащих связанных состояний O_2. Theoretical study of the low-lying bound states of O_2 / Partridge H., Bauschlicher C. W., (Jr), Langhoff S. R., Taylor P. R. // J. Chem. Phys.— 1991.— **95**, № 11.— С. 8292—8300.— Англ.

Методом НИК-КВ проведены расчеты низколежащих связанных состояний O_2, диссоциирующих на атомы в основных состояниях. Представлены спектроскопич. постоянные и энергии диссоциации D_e для состояний $X^3\Sigma_g^-$, $a^1\Delta_g$, $b^1\Sigma_g^+$, $c^1\Sigma_u^-$, $A^1\,{}^3\Delta_u$, $A^3\Sigma_u^+$, ${}^3\Pi_u$, ${}^5\Sigma_u^-$, ${}^5\Pi_u$ и ${}^5\Pi_g$. Для первых 6 состояний при включении поправок на возбуждения более высоких порядков получены точные результаты. Для состояния $X^3\Sigma_g^-$ значение D_e с поправкой на ошибку, обусловленную суперпозицией базисов, лишь на 0,7 ккал/моль отличается от эксперим. значения. Состояние ${}^5\Pi_g$ имеет значение $D_e = 0{,}16 \pm 0{,}03$ эВ.

И.Л.

Ф. 1992, N 8

O_2

1991

114: 134917v Franck-Condon factors and relative strength of the electronic transitions $c^1\Sigma_u$-$X^1\Delta_g$, $c^1\Sigma_u$-$X^3\Sigma_g$ in oxygen molecule. Smirnov, A. D. (Mosk. Gos. Tekh. Univ., Moscow, USSR). *Zh. Prikl. Spektrosk.* 1991, 54(1), 46-50 (Russ). The numerical method for evaluating the Franck-Condon factors (FCF) on the basis of the Mores potential is considered and was applied to the $c^1\Sigma_u$-$a^1\Delta_g$, $c^1\Sigma_u$-$X^3\Sigma_g$ transitions of O_2 ($0 \le v' \le 10$, $0 \le v'' \le 15$). The FCF were used to calc. relative band strengths of these transitons.

$c^1\Sigma_u - X^1\Delta_g$,

$c^1\Sigma_u - X^3\Sigma_g^-$,

факторы Ф.К.

C.A. 1991, 114, N20

O_2 оттиск 35971 1991

$d\,{}^1\Pi_g(v') \leftarrow$ Sur A., Friedman R. S.,
$X\,{}^3\Sigma_g^-(v'')$ et al,

J. Chem. Phys 1991,
94, N 3, 1705 - 1711.

Rotational dependence ~~of~~

the Rydberg - valence interactions in the $^1\Pi_g$ states of molecular oxygen.

O_2

1991

8 Д51. Построение кривых потенциальной энергии молекул посредством метода оптимизации. Construction of molecular potential energy curves by an optimization method / Wang J., Blake A. J., McCoy D. G., Torop L. // Chem. Phys.— 1991.— **150**, № 1.— С. 13—18.— Англ.

Предложена процедура построения кривых потенц. энергии (КПЭ) двухатомных молекул, исходя из эксперим. спектров в диффузной области и в области непрерывного спектра. Подход основан на алгоритме численной минимизации отклонений расчетных и эксперим. значений ряда спектральных характеристик, в том числе сечений столкновения при поглощении. Процедура применена для получения КПЭ состояний $B^3\Sigma_u^-$ и $E^3\Sigma_u^-$ молекулы O_2. Приведены КПЭ состояний по отношению к КПЭ основного электронного состояния $X^3\Sigma_g^-$. Задача нахождения КПЭ $B^3\Sigma_u^-$- и $E^3\Sigma_u^-$-состояний решена в диабатич. приближении. А. Ю. Е.

М. П.

ф. 1991, № 8

O_2

ОМ 36278 1991

4 Б1189. Лазерное возбуждение $A^3\Sigma_u{}^+$, $A'^3\Delta_u$ и $C^1\Sigma_u{}^-$ состояний молекулярного кислорода. Laser excitation of the $A^3\Sigma_u{}^+$, $A'^3\Delta_u$ and $c^1\Sigma_u{}^-$ states of molecular oxygen / Wildt J., Bednarek G., Fink E. H. // Chem. phys.— 1991.— **156**, № 3.— С. 497—508.— Англ.

Молекулярный кислород селективно возбуждался на колебат. уровни метастабильных $A^3\Sigma_u{}^+$, $A'^3\Delta_u$ и $c^1\Sigma_u{}^-$ состояний при поглощении испускания импульсного лазера на красителях ($\lambda \approx 249$ нм) с последующей регистрацией с разрешением во времени ФЛ в полосе O_2 ($b^1\Sigma_g{}^+ \rightarrow X^3\Sigma_g{}^-$) при $\lambda = 762$ нм. Отмечено, что $O_2(b^1\Sigma_g{}^+)$ является продуктом тушения $O_2(A^3\Sigma_u{}^+)$ либо самим кислородом, либо азотом. По зависимости от времени этого испускания определен нижний предел для константы скорости тушения $O_2(A^3\Sigma_u{}^+)$ кислородом для $v = 7, 8$, к-рый составил 1×10^{-11} см^3 с$^{-1}$. Измерена интенсивность испускания $O_2(b^1\Sigma_g{}^+ \rightarrow X^3\Sigma_g{}^-)$ как ф-ция отношения в смеси O_2/N_2. Показано, что не все элементарные акты тушения приводят к заселению $b^1\Sigma_g{}^+(O_2)$-состояния.

Е. А. Пазюк

(М.П)

X·1992, N4

O_2 Om. 36063 1991

Yang X., Wodtke A.M.,

J. Chem. Phys., 1991, 94, N4, 2469 - 2474

Direct observation of orbit rotation predissociation in the

O_2 Schumann – Runge system.

O_2

1992

(спектр)

117: 79191d High resolution inner valence UV photoelectron spectra of the oxygen molecule and CI calculations of $^2\Pi_u$ states between 20 and 26 eV. Baltzer, P.; Wannberg, B.; Karlsson, L.; Carlsson-Goethe, M.; Larsson, M. (Dep. Phys., Uppsala Univ., S-751 21 Uppsala, Swed.). *Proc. SPIE-Int. Soc. Opt. Eng.* **1992**, 1638(Opt. Methods Time- State-Resolved Chem.), 127-31 (Eng). High resoln. He I and He II excited inner valence photoelectron spectra of the O mol. were recorded between 20 and 26 eV. In this range 3 photoelectron bands are clearly seen; they are assocd. with the B $^2\Sigma_g^-$, 3 $^2\Pi_u$ and c $^4\Sigma_u^-$ states of O_2^+. The state of $^2\Pi_u$ symmetry obsd. around 24 eV shows a long vibrational progression, contrary to earlier work, with spacings that decrease successively towards higher electron binding energies. The assignment is confirmed by ab initio calcns. These calcns. show that if the potential curve is followed along the electron configuration rather than the adiabatic curve, the vibrational structure can be accounted for.

C. A. 1992, 117, N8

O_2

1992

чисто вращат. спектр комбинац. рассеяния

116: 94285k High resolution rotational CARS spectrum of oxygen. Brown, Kirk W.; Rich, Nathan H.; Nibler, Joseph W. (Dep. Chem., Oregon State Univ., Corvallis, OR 97331 USA). *J. Mol. Spectrosc.* 1992, 151(2), 482-92 (Eng). A low frequency, high resoln. CARS spectrometer is described which was used to resolve the closely spaced $\Delta N = 2$, $\Delta J = 2$ triplets of oxygen in the pure rotational Raman spectrum. The transition frequencies and intensities from $N = 1$–19 are extd. from the exptl. data with the aid of spectral simulation routines that account for the $|\chi|^2$ interference effects and the contribution of various line broadening mechanisms to the CARS spectrum. The frequencies match well those predicted using mol. consts. obtained from magnetic dipole microwave studies and a Hamiltonian appropriate to a coupling scheme intermediate between Hund's cases (a) and (b). A small, systematic discrepancy is obsd. between exptl. and theor. intensities which may result from a J dependent linewidth variation within each triplet.

C.A. 1992, <u>116</u>, N10

O_2 1992

$(B^3\Sigma_u^-)$ (D_0)

118: 67282s On the dissociation energy of molecular oxygen and the energy of the dioxygenyl ion O_2^+ b $^4\Sigma_g$ state. Cosby, P. C.; Huestis, D. L. (Mol. Phys. Lab., SRI Int., Menlo Park, CA 94025 USA). *J. Chem. Phys.* 1992, 97(9), 6108–12 (Eng). The authors note that a significant discrepancy exists between the recently detd. dissocn. energy of the O_2 $B^3\Sigma_u^-$ state and the energy of the $O(^1D_2)$ + $O(^3P_2)$ dissocn. limit detd. in a spectroscopic cycle. The major contribution to this discrepancy appears to be the currently accepted value for the energy of the O_2^+ *b* $^4\Sigma_g^-$ state relative to the ground electronic state of mol. oxygen.

☒

⊕ O_2^+ $(b^4\Sigma_g^-)$ ● (D_0)

C.A. 1993, 118, N8

O_2

1992

117: 139766g Predissociation of oxygen in the B $^3\Sigma_u^-$ state. Chiu, S. S. L.; Cheung, A. S. C.; Finch, M.; Jamieson, M. J.; Yoshino, K.; Dalgarno, A.; Parkinson, W. H. (Dep. Chem., Univ. Hong Kong, Hong Kong). *J. Chem. Phys.* 1992, 97(3), 1787-92 (Eng). The predissocn. linewidths and level shifts of vibrational levels of three oxygen isotopic mols. $^{16}O_2$, $^{16}O^{18}O$, and $^{18}O_2$ arising from the interactions of the *B* $^3\Sigma_u^-$ state with the four repulsive states $^5\Pi_u$, $^3\Sigma_u^+$, $^3\Pi_u$, and $^1\Pi_u$, were calcd. A set of parameters characterizing these interactions was detd. Good agreement between calcd. and exptl. predissocn. widths and shifts was obtained for all 3 isotopic mols.

(Предисс. в $B^3\Sigma_u^-$ сост.)

C. A. 1992, 117, N 14

O_2

1992

Fournier R., DePristo A.E.,

Энергии связи, расчет

J. Chem. Phys. 1992, 96, N2, c. 1183 – 1193.

● (см. HS_2; III)

O_2

1992

3 Д91. **Высокоселективное заселение спин-орбитальных уровней в электронной автоионизации O_2.** Highly selective population of spin-orbit levels in electronic autoionization of O_2 / Guyon P.-M., Hepburn J. W., Weng T., Heiser F., Reynolds D. // Phys. Rev. Lett.— 1991.— 67, № 6.— С. 675—678.— Англ.

Динамика электронной автоионизации O_2 изучена с использованием методики, сочетающей свободное истечение из сопла сверхзвукового пучка и синхротронное излучение. Ионы и электроны анализировались с использованием времяпролетного спектрометра. Спин-орбитальные подуровни ридберговых состояний $H^3\Pi_u$ ($v'=0$ и 2) в O_2 возбуждались селективно и приводили к появлению конечных состояний O_2^+, для которых наблюдались сильные вариации отношения заселенностей $^2\Pi_{1/2g}/^2\Pi_{3/2g}$. Эти вариации обусловлены селективностью одной волн. ф-ции континуума в автоионизационном процессе.

М.П.

Ф. 1992, N3

O_2 1992

Kutzler F.W., Painter G.S.,

Phys. Rev. B. 1992, 45, N7,

м.л. с. 3236-3244

(см. Li_2; III)

O_2

1992

Mc Lean A.D., Liu B.,
et al.,

ф-ии
потенц.
энергии,
re, We,
g, De,
расчет

J. Chem. Phys., 1992,
97 (11), 8459–64

(см. B_2^+ ; III)

O_2

1992

Rinsland Curtis P.,
Goldman A. et al.

J. Quant. Spectrosc.
Radiat. Transfer
1992, <u>48</u> (5-6), 693-99.

ИК спектр,
HITRAN
database"

(см. CoF_2; <u>III</u>)

O_2

1992

спектр высокого разрешение (КР)

117: 57897m High-resolution stimulated Raman spectroscopy of molecular oxygen. Rouille, G.; Millot, G.; Saint-Loup, R.; Berger, H. (Lab. Spectron. Mol. Instrum. Laser, Univ. Bourgogne, 21000 Dijon, Fr.). *J. Mol. Spectrosc.* 1992, 154(2), 372-82 (Eng). The ^{S}S and ^{O}O branches of the fundamental vibrational band of mol. oxygen in its electronic ground state have been resolved for the first time in Raman spectroscopy. The spectra were obsd., at room temp. and low pressure, with a stimulated Raman scattering (S.R.S) spectrometer including a multipass cell. From these accurate Raman data combined with microwave data, improved were the values of the vibrational, rotational, spin-spin, and spin-rotation interactions consts. in the $\upsilon = 1$ vibrational state. Moreover, Raman Q branches of the first and second hot-bands were recorded, allowing to det. a set of mol. parameters for the $\upsilon = 2$ and $\upsilon = 3$ states, useful for Coherent Anti-Stokes Raman Spectroscopy (C.A.R.S.) diagnostics in combustion media.

C. A. 1992, 117, N6

O_2

1992

7 Б1192. Интегралы франк-кондоновского перекрывания между ридберговым $3s\sigma\,{}^3\Pi_g$- и валентным $1\,{}^3\Pi_g$-состояниями молекулы O_2. Franck—Condon overlap integrals between the $3s\sigma\,{}^3\Pi_g$ Rydberg and the $1\,{}^3\Pi_g$ valence states of O_2 /Sur Abha, Nguyen Loane, Nikoi Nana //J. Chem. Phys. .—1992 .—96 ,№ 9 .—С. 6791—6795 .—Англ.

Спектр резонансно-усиленной (2+1) многофотонной ионизации O_2 в переходах $3s\sigma\,{}^3\Pi_g \leftarrow {}^3\Sigma_g^-$ обнаруживает диффузную структуру для колебат. полос 0—0, 1—0, 3—0 и 4—0 с ширинами от <50 до >150 $см^{-1}$. Спектр полосы 2—0 вращательно разрешен и имеет ширину на полувысоте 6 $см^{-1}$. Ридбергово состояние $3s\sigma\,{}^3\Pi_g$ предиссоциирует через диссоциативное валентное состояние $1\,{}^3\Pi_g$. Наблюдаемые вариации ширин линий в различных колебат. переходах при двухфотонном возбуждении являются следствием вариаций интегралов франк-кондоновского перекрывания между связанным и диссоциативным состояниями. Получен эмпирич. ПТ валентного состояния $1\,{}^3\Pi_g$ путем подбора его параметров до совпадения расчетных и эксперим. ширин линий для двухфотонных переходов в молекулах ${}^{16}O_2$, ${}^{17}O_2$, ${}^{18}O_2$ и ${}^{18}O{}^{17}O$. В. Е. Скурат

М.П.

Х.1994, N 7

O_2

1992

117: 57764r **Franck–Condon overlap integrals between the 3sσ $^3\Pi_g$ Rydberg and the 1 $^3\Pi_g$ valence states of molecular oxygen.** Sur, Abha; Nguyen, Loane; Nikoi, Nana (Dep. Chem., Mount Holyoke Coll., South Hadley, MA 01075 USA). *J. Chem. Phys.* 1992, 96(9), 6791–5 (Eng). The (2 + 1) resonance–enhanced multiphoton ionization spectrum of the 3sσ $^3\Pi_g \ll {}^3\Sigma_g$ transitions in ...

потенц. кривые,
спектр.

C.A. 1992, 117, N6

O_2 1992

теор. расч. Vi
структуры
параметры
f

Takai Y.,
Johnson K.H.
Chem. Phys. Lett.
1992, 189 (6), 578-23

сер. № 2 (III)

O2

1992

пост. спин-
орбит. взаим.
теор. рас.

Vahtras O.;
Ågren H. et al
J. Chem. Phys.
1992, 96 (3), 2118-26

см. CH2 (II)

O_2

1992

16 Б1174. Индуцированное столкновениями испускание $O_2(a^1\Delta_g \rightarrow X^3\Sigma_g^-)$ в газовой фазе. Collision-induced emission of $O_2(a^1\Delta_g \rightarrow X^3\Sigma_g^-)$ in the gas phase / Wildt J., Fink E. H., Biggs P., Wayne R. P., Vilesov A. F. // Chem. Phys.— 1992.— **159**, № 1.— С. 127—140.— Англ.

В области полос 0—0 и 0—1 перехода $a^1\Delta_g \rightarrow X^3\Sigma_g^-$ измерены спектры испускания чистого кислорода и в присутствии др. газов, Ar, Kr, Xe, N_2, NO, CO_2, SF_6. Молекулы O_2 возбуждали в МВ-разряде и после удаления атомарного кислорода (продукты пропускали над нагретой до 50° С ртутью) вводились в проточную трубу большого диаметра (либо вводилась смесь газов). Суммарное давл. в трубе составляло 0,2—25 Торр. Испускание наблюдали вдоль оси трубы, причем на одном конце трубы помещали фурье-спектрометр и спектры измеряли с высоким разрешением (до 0,02 см$^{-1}$), а на др. конце располагали небольшой монохроматор с решеткой и спектры измеряли с низким

М.П.

Х. 1992, N 16.

разрешением (~10 см$^{-1}$). При повышении давл. кислорода или др. газов обнаружен континуум накладывающийся на дискретные линии перехода $a \rightarrow X$, к-рый приписан образованию комплексов $O_2 : M$ при столкновениях, $O_2(a) + M \rightleftarrows O_2(a) : M \rightarrow O_2(X) + M + h\nu$ (континуум) ($K_M{}^c$). В случае Ar, Kr, Xe, N_2, CO_2 и SF_6 континуум в полосе 0—0 оказался боее узким. Из отношения интенсивности континуума и дискретного спектра определены константы скорости излучательного распада бимолек. комплексов (в 10^{-23} см^3 с$^{-1}$): $O_2(a) : O_2$. полоса 0—0—3,4±0,3, полоса 0—1 — 1,4±±0,1; $O_2(a) : NO$, полоса 0—0 — 172±3, полоса 0—1 — 9,2±0,7. Большая величина отношения $K^c(0-0)/$ $/K^c(0-1)$ для $O_2(a) : NO$ связывается с разным энергетич. дефектом процессов $O_2(a, v=0) + NO(X, v=0) \rightarrow$ $\rightarrow O_2(X, v=1) + NO(X, v=0) + h\nu$ или $O_2(X, v=0) +$ $+ NO(X, v=1) + h\nu - \Delta E$. Библ. 46. В. М. Ковба

труе
(С

O_2

1992

7 Б1181. Идентификация состояний $nd\Delta$ **и** Σ **и перехода** $^{1,3}\Phi \leftarrow\leftarrow X^3\Sigma_g^- O_2$ **методом резонансной многофотонной ионизации.** Identification of the nd Δ and Σ states and the $^{1,3}\Phi \leftarrow\leftarrow X^3\Sigma_g^-$ transition of O₂ by resonant multiphoton ionization /Yokelson Robert J., Lipert Robert J., Chupka William A. //J. Chem. Phys. .— 1992 .—97 ,№ 9 .— С. 6144—6152 .— Англ.

М.Л.

Х.1995, N7

O_2

1992

118: 63312a **Identification of the nd Δ and Σ states and the $^{1,3}\Phi \leftarrow X\,^3\Sigma_g^-$ transition of molecular oxygen by resonant multiphoton ionization.** Yokelson, Robert J.; Lipert, Robert J.; Chupka, William A. (Sterling Chem. Lab., Yale Univ., New Haven, CT 06511-8118 USA). *J. Chem. Phys.* 1992, 97(9), 6144-52 (Eng). Spectra of the 3d Rydberg state region of O_2 were obtained by 2-photon resonant ionization of the ground electronic state. By varying the rotational distribution and radiation polarization, all obsd. bands were identified and attributed to excitation of Π, Δ, and Φ states. Earlier assignments were cor. The Δ and Φ assignments are complete while the Σ assignments are so far incomplete.

(Ридберг. сост.)

C.A. 1993, 118, N 8

O_2 1992

(Ридберг. сост)

118: 69313b Identification of the nsσ and ndλ Rydberg states of molecular oxygen for n = 3-5. Yokelson, R. J.; Lipert, R. J.; Chupka, W. A. (Dep. Chem., Yale Univ., New Haven, CT 06511 USA). *J. Chem. Phys.* 1992, 97(9), 6153–67 (Eng). The 4s–3d and 5s–4d Rydberg complexes of diat. O were studied by (2+1) resonance-enhanced multiphoton ionization of the $X^3\Sigma_g^-$ ground state of O_2. The authors have located and identified at least 2 vibrational levels of each of the following states:. Three of 4 expected 4sσ Π states;all 4 expected 5sσΠ states; 18 of 22 expected 3d states(with only the states of the 3dσ orbital remaining unobsd.); and 5 of the 10 predicted 4dπ states. State assignments were assisted by the following: the results of rotational cooling and laser polarization expts. which facilitated the rotational cooling and laser polarization expts. which facilitated the rotational anal., band positions, band intensities, and parameterized calcns. The exptl. detd. state locations are compared with the state locations obtained from ab initio calcns. The authors have carried out isotope expts. and rotational linewidth anal. to study in some detail the mixing between the Rydberg states and the repulsive valence states as well as the mixing between the Rydberg states themselves. Direct predissocn.

C.A.1993, 118, N8

dominates indirect predissocn. as a dissociative mechanism, but there is evidence of $\Delta n = 0$ interactions which perturb the rotational structure of $3d\pi$ Σ and Δ states. The relative intensities of the states detected span a range in excess of 10^4 with the $ns\sigma$ Π states being the weakest and the $nd\pi$ Σ states being the strongest. Photoionization of the $nd\pi$ Σ states appears to be most affected by the shape resonance in the continuum. The measurements confirm the expectation that many of the properties of the Rydberg states in the same series scale as $(n^*)^{-3}$.

O_2

1993

$B^3\Sigma_u^- - X^3\Sigma_g^-$

Высокое разрешение

119: 148783d **High-resolution study of the v = 11 to 18 levels in the ground state of oxygen.** Chen, Ciping; Ramsay, D. A. (Herzberg Inst. Astrophys., Natl. Res. Counc. Canada, Ottawa, ON Can. K1A OR6). *J. Mol. Spectrosc.* 1993, 160(2), 512–6 (Eng). Bands of the $B^3\Sigma_u^-$–$X^3\Sigma_g^-$ system of oxygen have been photographed in absorption at high resoln. following the flash photolysis of ozonized oxygen. The bands have v' = 0 and v'' = 11 to 18. Improved mol. consts. for the ground state levels are obtained from rotational analyses of the bands.

C. A. 1993, 119, N 14

O_2

1993

118: 241273b An ab initio study of the electron affinity of molecular oxygen. Gonzalez-Luque, Remedios; Merchan, Manuela; Fuelscher, Markus P.; Roos, Bjoern O. (Dep. Quim. Fis., Univ. Valencia, Dr. Moliner 50, Burjassot, Valencia, Spain 46100). *Chem. Phys. Lett.* 1993, 204(3-4), 323-32 (Eng). Coupled-pair-functional, multiconfigurational-second-order-perturbation-theory, and MR-CI methods were used to calc. the electron affinity of the oxygen mol. The convergence of the theor. result was checked with respect to a systematic expansion of the one electron basis and the MR CI wave function. The best calcd. value, 0.39 eV, was 0.06 eV smaller than the recent exptl. value 0.45±0.01 eV.

(Ae)

(теор · расчет)

C.A. 1993, 118, N24

O_2

1993

119: 188830y **Experimental and theoretical evidence for a new metastable valence state of oxygen.** Griffith, K. S.; Gellene, Gregory I. (Dep. Chem. Biochem., Texas Tech Univ., Lubbock, TX 79409-1061 USA). *J. Phys. Chem.* **1993**, 97(39), 9882-9 (Eng). A new metastable state of O_2 has been obsd. following the charge exchange of fast beams of O_2^+ with alkali metals. Coupling of the exptl. results with ab initio calcns. provides strong arguments for the identification of the metastable as the previously unknown $1\,^1\Delta_u$ valence state which adiabatically dissocs. to $O(^1D) + O(^1D)$. The primary relaxation pathway is a spin-orbit induced predissocn. by the repulsive $2\,^3\Delta_u$ state for which an $H_{SO} = 9\ (\pm 1)\ cm^{-1}$ matrix element is detd. Due to accidentally small Franck-Condon factors the $v = 2$ level of the $1\,^1\Delta_u$ state is particularly long-lived and evidences extraordinarily large isotope effects with the lifetime for this level being 0.1, 1.8, and 0.5 μs for $^{32}O_2$, $^{34}O_2$, and $^{36}O_2$ resp. The other low vibrational levels of the $1\,^1\Delta_u$ state are predicted to have lifetimes of ~5-10 ns, suggesting that high-quality spectra of these states should be obtainable and that chem. reactions of this new state of O_2 are possible.

новое метастаб. валентное состояние, $1\,^1\Delta_u$.

C.A. 1993, 119, N18

O_2 1993

Hunt R.D., Andrewa L.

ИК спектр в матрице

J. Chem. Phys. 1993, 98 (5), 3690–6.

● (см. ИО; III)

O_2 1993

Peterson K.A., Kendall R.A.,
et al.,

м.п.,
теор. J. Chem. Phys., 1993,
расчет <u>99</u>, N 12, 9790-805

(см. B_2; <u>III</u>)

O_2 (оп. 37773) 1994

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

$^3\Sigma_g^-$, J. Phys. Chem.,
D,
эксперим., 1994, 98, N 40,
теорет.
расчет 9931-44

O_2

1994

120: 119514g **The potential energy curve for the $B^3\Sigma_u^-$ state of oxygen and accurate Franck–Condon factors for the Schumann-Runge bands.** Cheung, A. S. C.; Mok, D. K. W.; Sun, Yan; Freeman, D. E. (Dep. Chem., Univ. Hong Kong, Hong Kong). *J. Mol. Spectrosc.* 1994, 163(1), 9–18 (Eng). A single potential energy curve for the $B^3\Sigma_u^-$ state of O_2 was detd. using the Rydberg–Klein–Rees method with spectroscopic consts. of $^{16}O_2$, $^{16}O^{16}O$, and $^{18}O_2$. Accurate Franck–Condon factors (FCFs) of the Schumann–Runge system ($B^3\Sigma_u^-$–$X^3\Sigma_g^-$) of O_2 were calcd., which cover 16 vibrational levels for the upper $B^3\Sigma_u^-$ state and 19 for the lower $X^3\Sigma_g^-$ state. Agreement between this study and earlier results for the potential energy curve and the FCFs is excellent.

$B\,^2\Sigma_u^+$ – потен

циальн. кривая

C. A. 1994, 120, N10

O_2 Оп. 37648 1994

Minaev B.F., Lunell S.,
Kobzev G.I.,

$b^1\Sigma_g^+ - a^1\Delta_g$ Int. J. Quant. Chem.,
1994, 50, 279-292.

Collision-Induced Intensity
of the $b^1\Sigma_g^+ - a^1\Delta_g$ Transition

in Molecular Oxygen: Model Calculations for the Collision Complex $O_2 + H_2$.

O_2

1994

121: 266942u **Detection of the atmospheric oxygen band $b^1\Sigma_g^+$–$X^3\Sigma_g^-$ by the laser-probed resonant Voigt effect.** Takubo, Yoshitaka; Muroo, Kazuyuki; Miwa, Satoshi; Yamamoto, Kazuhiro; Yamamoto, Manabu (Dep. Appl. Phys., Tokyo Univ. Agric. Technol., Koganei, Japan 184). *Bunko Kenkyu* **1994,** 43(3), 150–5 (Eng). The atm. O band, $b^1\Sigma_d^+(v' = 0)$–$X^3\Sigma_d^-(v'' = 0)$, was detected by the resonant Voigt effect, with a Ta-doped Al_2O_3 laser. Elliptically polarized light was tuned to the rotational lines of the band. The polarization state of light after passing through the air was analyzed with an angle-offset birefringent prism. Adjusting the light ellipticity and the analyzer offset angle, the signal of the $^{P}P(1,1)$ line was obtained with a signal-to-noise ratio of 1 × 10^2 for O_2 in the air of 4 cm optical path under 1 atm. pressure. S. Hoshino

$(b^1\Sigma_d^+(v' = 0)$ — $X^3\Sigma_d^-(v'' = 0)$

лазер. воздух.

C.A. 1994, <u>121</u>, N22

O_2 1994

Tao, Fu-Ming

J. Chem. Phys. 1994,
<u>100</u> (5), 3645-50.

теор.
расчет
D_0, r_e, ω_e

(см. N_2; <u>III</u>)

O_2

1994

122: 145535a **Ab initio investigation of the vibronic structure of the $B^3\Sigma_u^-$, $2^3\Sigma_u^-$ ← $X^3\Sigma_g^-$ spectral system of the oxygen molecule.** Torbica, Vojislava; Peric, Miljenko (Faculty of Physical Chemistry, University of Belgrade, YU-11001 Belgrade, Yugoslavia). *J. Serb. Chem. Soc.* **1994**, 59(7), 473-82 (Eng). A variational method based on representation of the mol. potentials and wave functions by trigonometric series, is developed for ab initio treatment of 2 electronic states exhibiting avoided crossing. The approach is applied for study of the vibronic structure of the $B^3\Sigma_u^-$, $2^3\Sigma_g^-$ transition in O_2.

теор. расчет

$B^3\Sigma_u^-$, $2^3\Sigma_g^-$

C.A. 1995, 122, N 12

O_2

1994

122: 91866p Fourier transform spectroscopy of the Herzberg I bands of O_2. Yoshino, K.; Murray, J. E.; Esmond, J. R.; Sun, Y.; Parkinson, W. H.; Thorne, A. P.; Learner, R. C. M.; Cox, G. (Harvard-Smithsonian Cent. Astrophys., Cambridge, MA 02138 USA). *Can. J. Phys.* 1994, 72(11&12), 1101-8 (Eng). Fourier transform spectroscopic measurements of the adsorption bands of the Herzberg I system ($A^3\Sigma_u^+ - X^3\Sigma_g^-$) of O_2 were made in the wavelength region 240–270 nm. Rotational line positions are detd. with an accuracy of 0.005 cm^{-1}, and rotational term values are presented for the vibrational levels, ν = 4–11. Mol. consts. of these levels are also presented. Interactions with the $c^1\Sigma_u^-$ state are obsd. at J = 13 of the ν = 4 level, at J = 16 of the ν =7 level, and at J = 15 and 24 of the ν = 9 level of the $A^3\Sigma_u^+$ state. Another interaction around J = 10 of the ν = 11 level might result from the weakly bound $^3\Pi_u$ state.

$(A\,^3\Sigma_u{}^+ X^3\Sigma_g{}^-)$

C. A. 1995, 122, N8

O_2

1994

21 Б1191. Фурье-спектроскопия полос первой системы Герцберга O_2. Fourier transform spectroscopy of the Herzberg I bands of O_2 / Yoshino K., Murray J. E., Esmond J. R., Sun Y., Parkinson W. H., Thorne A. P., Learner R. C. M., Cox G. // Can. J. Phys. .— 1994 .— **72** , № 11 - 12 .— С. 1101—1108 .— Англ. ; рез. фр.

С высоким разрешением и точностью (0,06 и 0,005 $см^{-1}$) измерена вращательная структура полос $v'=4—11 \leftarrow v''=0$ перехода $A^3\Sigma_u{}^+—X^3\Sigma_g{}^-$ молекулы O_2 (первая система Герцберга). Рассчитаны и приводятся значения молекулярных постоянных T_0, T_v, B_v, D_v, λ_v, γ_v и λ_{dv} для уровней $v_A=4—11$. В спектре наблюдали локальные возмущения, связанные с взаимодействием уровней $v=4$, $j=13$; $v=7$, $j=16$; $v=9$, $j=15$ и 19, состояния $A^3\Sigma_u{}^+$ с уровнями состояния $c^1\Sigma_u{}^-$.

В. М. Ковба

М.П.

X. 1995, N21

O_2

1995

123: 126103n Identification of the 4 $p\sigma_u{}^1\Pi_u$ Rydberg state of O_2. England, J. P.; Lewis, B. R.; Ginter, M. L. (Res. Sch. Phys. Sci. Eng., Australian Natl. Univ., Canberra, ACT 0200 Australia). *J. Chem. Phys.* **1995,** 103(5), 1727–31 (Eng). New high-resoln. measurements of the O_2 photoabsorption cross section in the 1147–1155 Å region are presented. The observation of three previously-unreported narrow lines in a band near 1148 Å has enabled unambiguous assignment of the band to a ${}^1\Pi_u \leftarrow X^3\Sigma_g^-$ transition which gains strength through a spin–orbit interaction with the upper state of a ${}^3\Pi_u \leftarrow X^3\Sigma_g^-$ transition appearing at 1153 Å. Other lines in the 1148 Å band are broadened by predissocn. through a heterogeneous interaction with a nearly energetically coincident ${}^1\Delta_u$ level. The states, labeled $h^1\Pi_u$, $F^3\Pi_u$ and $i^1\Delta_u$, are predominantly of $4p\lambda$ Rydberg MO configurations although there are indications that the Π_u states interact strongly with valence states of the same symmetry.

$4p\sigma_u{}^1\Pi_u$

Ридберг·сост

C.A. 1995, 123, N10

1995

F: O2
P: 3

14Б1246. Пересмотр полос Шумана-Рунге O[2] в Ar-, Kr- и Xe-матрицах. Потенциальные кривые состояния B{3}'СИГМА'[u]{-}. Schumann-Runge bands of O[2] in Ar, Kr and Xe matrices revisited: potential curves of the B{3}'СИГМА'[u]{-} state / Gudipati Murthy S. [Chemical Physics] // Chem. Phys. - 1995. - 201, N 2 - 3. - C. 451-462. - Англ.

Представлены спектры поглощения и возбуждения {16}O[2] в Ar- и Kr- и {18}O[2] в Ar-матрицах при 15K в области перехода B{3}'СИГМА'[u]{-}(v) X{3}'СИГМА'[g]{-}. Анализируется влияние окружения на потенциальную кривую верхнего состояния при различной симметрии клетки. Показано, что для согласования с экспериментом необходим учет электронного взаимодействия атомов решетки с возбужденным состоянием молекулы O[2]. Библ. 38.

РЖХ 1997

O_2

1995

124: 70212y **Schumann–Runge bands of O_2 in Ar, Kr and Xe matrixes revisited: potential curves of the B $^3\Sigma_u^-$ state.** Gudipati Murthy S. (Institut fuer Physikalische Chemie, Universitaet zu Koeln Luxemburger Strasse 116, D–50939 Koln, Germany). *Chem. Phys.* 1995 201(2,3), 451–62 (Eng). Absorption/excitation spectra of $^{16}O_2$ isolated in Ar and Kr matrixes and $^{18}O_2$ isolated in Ar matrixes at 15 K for the B $^3\Sigma_u^-(\nu')$—X $^3\Sigma_g^-(\nu'' = 0)$ transitions (Schumann–Runge bands) of O_2 are presented. The spectra in rare–gas matrixes differ considerably from the gas–phase spectrum. The cage effect caused by the host lattice was analyzed using van der Waals interactions between the O atom and rare–gas atoms. Potential curves of the B $^3\Sigma_u^-$ state were derived for D_{3d} and D_{4h} orientations of O_2 in a substitutional site in rare–gas lattices. When O_2 occupies D_{4h} orientation, these potential curves compare closest with the potential curves obtained independently by using the exptl. vibronic energies and the method of Oldenberg [O. Oldenberg, Z. Physik 56(1929) 563]. An anal. of the potential curves indicates that at larger O–O sepn. (>3.2 Å) in the B $^3\Sigma_u^-$ state, the rare–gas atoms start interacting electronically with the O_2 mol.

$B^3\Sigma_u^-$, потенц., кривые

C. A.- 1996, 124, N 6.

1995

F: O2
P: 3

5Б1216. Об испускании {1}S'->'{1}D O при возбуждении O[2] в континуум и за континуум Шумана-Рунге в Ar-матрицах при 15K. On the {1}S'->'{1}D emission of O by exciting O[2] into and beyond the Schumann-Runge continuum in Ar matrices at 15K / Gudipati M. S. // Chem. Phys. Lett. - 1995. - 242, N 1 - 2. - С. 132-138. - Англ.

РЖХ 1997

O_2

1995

23 Б1170. **Идентификация двух переходов $^3\Pi_u$—$X^3\Sigma_g^-$ $^{16}O_2$ вблизи 93850 и 95360 см$^{-1}$.** Identification of two $^3\Pi_u \leftarrow X^3\Sigma_g^-$ transitions of $^{16}O_2$ near 93850 and 95360 cm^{-1} / Ito K., Huber K. P., Yoshino K., Ogawa M., Morioka Y. // J. Mol. Spectrosc. .— 1995 .— **171** , № 1 .— С. 1—12 .— Англ.

В однофотонном спектре поглощения $^{16}O_2$ высокого разрешения $((\lambda/\Delta\lambda)=2\cdot10^5)$ идентифицированы два перехода на вибронные уровни при 93850 и 95360 см$^{-1}$. Выполнен анализ структуры переходов. Рассчитаны значения вращательных постоянных и параметров Λ-удвоения. Обсуждено отнесение и электронная конфигурация возбужденных состояний, а также тип и природа верхнего электронного состояния в интенсивной полосе $^{16}O_2$ при 86733 см$^{-1}$, наблюдавшейся ранее. Библ. 36.

В. М. Ковба

М.Л.

Х. 1995, N 23

O_2

1995

124: 70271s Determination of molecular constants of the $X^3\Sigma_g^-$ state of O_2. Shimauchi, Midori; Miura, Tokiwa; Takuma, Hiroshi (Institute for Laser Science, Univ. of Electro-Communications, Tokyo, Japan 182). *Jpn. J. Appl. Phys., Part 2* **1995**, 34(12B), L1689–L1691 (Eng). From the absorption lines assigned to the B – X, 2–7 band of O_2 in the KrF laser spectrum, new mol. consts. of v = 7(X) are obtained. The term values, T_v, for v = 0–3 recently detd. by Raman spectroscopy are modified to render them consistent with those obtained by UV spectroscopy for v = 11–18, 4 and 7. This modification, based on the theor. energy formulas of fine structure levels of $^3\Sigma$, is numerically justified by the new T_7 values and also by the set of spectroscopic consts. of $X^3\Sigma_g^-$ obtained.

$(X^3\Sigma_g^-)$

М·Л.

С.А. 1996, <u>124</u>, N6.

1995.

F: O2
P: 3

11Б129. Радикал FO[2]. овый успех теории функционала плотности. The FO[2] radical: A new success of density functional theory / Ventura Oscar N., Kieninger Martina // Chem. Phys. Lett. - 1995. - 245, N 4 5. - С. 488-497. - Англ.

Методом функционала плотности (B3LVP в базисе 6-311++ГФ (3df, 3pd) рассчитаны геометрич. параметры, частоты и энергии нулевых колебаний молекул FO[2] ({2}A"), O[2], OH, FO, H[2]O, FOH, HO[2], F[2]O[2], а также теплоты большого числа р-ций, включающих гомолитич. разрыв связей FO и O, и теплота образования FO[2]. По мнению авторов, используемый подход обладает определенными преимуществами в описании энергетики связей FO по сравнению с другими современными неэмпирич. "термохимическими" процедурами..DHf(FO[2])

X. 1996, N11.

1996

F: O2
P: 3

21Б113. Порядок химической связи и фотоэлектронная спектроскопия. The bond order and the photoelectron spectroscopy / Chang T.-C. // WATOC"96: 4{th} Word Congr. Theor. Orient. Chem., Jerusalem, July 7-12, 1996: Program and Abstr. - [Tel Aviv], 1996. - С. 119. - Англ.
Обсуждены результаты расчета потенциалов ионизации и колебательных прогрессий в фотоэлектронных спектрах простых двухатомных молекул (N[2], O[2], F[2], P[2], S[2], CS, NO, SO) с использованием нового метода, позволяющего связать теор. предпосылки методов МО и валентных схем.

РЖХ, 1998, N21.

O_2

1996

125: 207242a The Schumann–Runge absorption bands of O_2 at 670 K and the spectroscopic constants of the ground state, X $^3\Sigma_g^-$. Cheung, A. S.-C.; Yoshino, K.; Esmond, J. R.; Parkinson, W. H. (Dep. Chem., Univ. Hong Kong, Hong Kong, Hong Kong). *J. Mol. Spectrosc.* **1996**, 178(1), 66–77 (Eng). High-resoln. absorption spectra of O_2 were photographed at 670 K throughout the wavelength region 179 to 212 nm. Precise wavelength measurements and rotational analyses of the Schumann–Runge (ν', ν) bands with $\nu' = 12-17$ and $\nu = 1-4$ were completed. The term values for the B $^3\Sigma_u^-$ and the X $^3\Sigma_g^-$ states are presented. Spectroscopic consts. of the X $^3\Sigma_g^-$ state of O_2 for $\nu = 1-4$ were detd. Good agreement was obtained between the detd. mol. consts. and those reported earlier.

М.п. $X^3\Sigma_g^-$

C.A.1996, 125, N16

O_2 1996

Csaszar, Attila G.
et al.,

re, we, De,
корреляции

J. Chem. Phys. 1996, 104 (7),
2746-48.

(См. №2; III ●)

1996

F: O2
P: 3

16Б1225. Идентификация двух переходов {3}'СИГМА'[u]{-} X{3}'СИГМА'[g]{-} в молекуле {16}O[2] в близи 88 930 и 90 780 см{-1}. Identification of two {3}'СИГМА'[u]{-} X{3}'СИГМА'[g]{-} transitions of {16}O[2] near 88930 and 90780 cm{-1} / England J. P., Lewis B. R., Ginter M. L. [Journal of Chemical Physics] // J. Chem. Phys. - 1996. - 105, N 5. - С. 1754-1763. - Англ.

РЖХ 1997

При температуре 79°К в областях 88 850-89 050 и 90 700-91 000 см{-1} измерены частоты 46 и 25 линий вращат. структуры двух полос E'{3}'СИГМА'[u]{-} X{3}'СИГМА'[g]{-} спектра поглощения {16}O[2]. Определены значения термов при J'=1-17 и J'=1-11, вращат. постоянная, постоянные спин-спинового, спин-орбитального и спин-вращат. взаимодействий. Построены потенциальные кривые. Библ. 41.

O_2

1996

$({}^3\Pi_u \leftarrow X\,{}^2\Sigma_g^-)$

124: 188310g **Assignment of the $^3\Pi_u$—X $^2\Sigma_g^-$ bands of O_2 observed in the region 1040–1200 Å.** England, J. P.; Lewis, B. R.; Gibson, S. T.; Ginter, M. L. (Res. Sch. Phys. Sci. Eng., Australian Natl. Univ., Canberra, ACT 0200 Australia). *J. Chem: Phys.* **1996**, 104(8), 2765–72 (Eng). A comprehensive vibronic assignment of the $^3\Pi_u$ states in the energy region approaching the first ionization threshold of O_2 is presented for the first time. Measurements of seventeen $^3\Pi_u$—X $^3\Sigma_g^-$ bands in the 85,800–93,000 cm^{-1} region of the ground-state photoabsorption spectra of $^{16}O_2$ and $^{18}O_2$ at 79 K are reported, including six bands in the spectrum of $^{18}O_2$ for the first time. Irregularities in vibrational spacings and in the extent of broadening by predissocn. are shown to result from Rydberg-valence interactions. The obsd. transitions have been assigned, using semiempirical modeling of the $^3\Pi_u$ Rydberg–valence interactions based on the coupled-channel Schroedinger equations technique, to two vibrational progressions with upper states which we call F $^3\Pi_u$ and F' $^3\Pi_u$. The F and F' states are formed from the avoided crossings of the npσ_u (n=3–5) Rydberg potential-energy curves by the lowest repulsive $^3\Pi_u$ valence potential-energy curve.

C. A. 1996, 124, N 14

O_2

$^3\Sigma_u^- - X^3\Sigma_g^-$

1996

V

125: 233277k **Identification of two $^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$ transitions of $^{16}O_2$ near 88930 and 90780 cm^{-1}.** England, J. P.; Lewis, B. R.; Ginter, M. L. (Res. Sch. Phys. Sci. Eng., Australian Natl. Univ., Canberra, 0200 Australia). *J. Chem. Phys.* **1996**, 105(5), 1754–1763 (Eng). New $^{16}O_2$ photoabsorption cross-section measurements are presented for 2 bands near 88930 cm^{-1} and 90780 cm^{-1}. The authors have assigned these bands as the (0,0) and (1,0) bands of the $E'^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$ system, where the E' state is a mixed state resulting from the coupling of 4p π_u and 5p π_u $^3\Sigma_u^-$ Rydberg states with the lowest $^3\Sigma_u^-$ valence state. In contrast to the $E^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$ bands seen at lower energies, these bands show resolved rotational structure. Spectroscopic parameters for the upper levels were derived using an effective Hamiltonian and cross-section band models. The obsd. levels are perturbed by spin-orbit interactions with nearby levels (v = 1 and 2) of the 4p π_u $D'^3\Sigma_u^+$ Rydberg state. Transitions to the v = 2 level of the perturbed state were obsd. near 90920 cm^{-1}.

CA 1996, 125, W18

O_2

1996

126: 284501g PFI−ZEKE spectroscopy using coherent vacuum UV: $O_2^+(a^4\Pi_u) \leftarrow O_2(X^3\Sigma_g^-)$. Kong, W.; Hepburn, J. W. (Department of Chemistry, University of Waterloo, Waterloo, Can.). *Int. J. Mass Spectrom. Ion Processes* 1996, 159, 27−35 (Eng), Elsevier. The PFI−ZEKE spectra of the 1st four vibrational levels of $O_2^+(a^4\Pi_u)$ are reported. The rotationally resolved photoelectron spectra were assigned by diagonalizing the appropriate Hamiltonian in a Hund's case a basis set. An extension of a previous model for rotational line strengths (the BOS model) to the intermediate coupling case was applied to the three vibrational bands with $v^+ = 1-3$. As was obsd. with several $^2\Pi$ states in previous ZEKE studies, the intensities of the spin−orbit sub−levels were not in accord with calcd. line strengths. The $a^4\Pi_u$ vibrational levels $v^+ = 0$ and 1 were overlapped by the Franck−Condon forbidden $v^+ = 21$ and 22 levels of the $X^2\Pi_g$ state, allowing for a direct comparison between the intensities of the Franck−Condon allowed and forbidden bands in the ZEKE spectra. These data allowed the authors to det. an accurate ionization energy for the $a^4\Pi_u$ state: 129,892 ± 2cm^{-1} (16.1046 eV).

a_4Пu,
потенц.
ионизац.

С. А. 1997, 126, N21

O_2 1996

126: 66708p **Observation of the second $^3\Pi_u$** [illegible]
Lewis, B. R.; Dooley, P. M.; England, J. P.; Wang [illegible]
Baldwin, K. G. H.; Partridge, H. (Res. Sch. Phys. Sc. [illegible]
Natl. Univ., Canberra, 0200 Australia). *Phys. Rev. A* [illegible]
Phys. 1996, 54(5), 3923–3938 (Eng), American Phys. [illegible]
tional perturbations in the B $^3E_u^-$ state of O_2 were [illegible]
ing high-resoln. vacuum UV laser photoabsorption [illegible]
(16,0)–(18,0) B $^3E_3^-$ ← X $^3E_g^-$ Schumann-Runge [illegible]
observation of numerous extra lines in the spectra [illegible]
initio calcns. of relevant potential-energy curves, [illegible]
state to be assigned as the 2nd valence state of $^3\Pi_u$ [illegible]
weakly bound state, which the authors name $C'^3\Pi_u$ [illegible]
principally responsible for the known rapid increase [illegible]
of the B-state triplet-splitting consts. λ_v and γ_v as [illegible]
approached.

второе $^3\Pi_u$ вал. сост., спектр.

Quadrupole rad
rosphere. Kli
., Russian Acad
., *Opt. Phys.* 19
The process of
re. sphere is co
and classical ap
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quadrupole trans
of magnitude i
parable with th
aled. in the cla
ole transitions
Correlation-in
Agarwal, Giri

C.A. 1997, 126, N5

~1996?

F: O2
P: 3
18Б134. Профили угловых моментов электронов для молекул с открытыми оболочками. Изучение ВЗМО NO, O[2] и NO[2] методами спектроскопии углового момента электрона и квантово-химического расчета в приближениях ССП, функционала плотности и в вариантах ССП, выходящих за пределы метода Хартри-Фока. Momentum profiles for open shell molecules: Studies of the HOMOs of NO, O[2] and NO[2] by electron momentum spectroscopy and SCF, post-Hartree-Fock and DFT calculations / Rolke J., Cann N., Zheng Y., Hollebone B. P., Brion C. E., Wang Y. A., Davidson E. R. // Chem. Phys. - 201, 1. - С. 1-21. - Англ.

O_2 1996

Slanger T.G., Huestis D.L., Cosby P.C. et al.;

J. Chem. Phys., 1996, 105 (21), 9393 – (1стр)

O_2 photoabsor[illegible]ption in the 40 950 – 41 300 cm^{-1} region:

New Herzberg bands, new absorption lines, and improved spectroscopic data.

O_2

1996

(22 валентных сост., теор. расчет)

126: 162534z **Valence states of O_2 Feynman's way.** Sorensen, Thomas E.; England, Walter B. (Dep. Chem. Lab. Surface Studies, Univ. Wisconsin–Milwaukee, Milwaukee, WI 53201 USA). *Mol. Phys.* **1996**, 89(5), 1577–1602 (Eng), Taylor & Francis. Potential energy curves for twelve valence states of O_2 are calcd. with fully linked renormalized Feynman diagrams which dissoc. properly. Compared with expt., av. errors of spectroscopic consts. are: 18 kJ mol^{-1} for D_e, 2.1 pm for R_e, 81 cm^{-1} for ω_e, 15 kJ mol^{-1} for T_e, and 16 kJ mol^{-1} for the sum of asymptotic at. excitation energies.

C. A. 1997, 126, N 12

O_2

1996

24Б1530. Резонансные магнито-оптические спектры перехода $b^1\Sigma_g^+ - X^3\Sigma_g^-$ молекул кислорода. Resonant magneto-optic spectra of the $b^1\Sigma_g^+ - X^3\Sigma_g^-$ transition of oxygen molecules / Takubo Y., Muroo K., Miwa S., Yamamoto K., Suzuki K., Yamamoto M. // J. Mol. Spectrosc.— 1996.— 178, № 1.— С. 31–39.— Англ.

Выполнен анализ профилей отдельных линий различных ветвей вращательной структуры магнитного дипольного перехода $b^1\Sigma_g^+ (v=0) - X^3\Sigma_g^- (v=0)$ в резонансном магнито-оптическом спектре молекулярного кислорода. В качестве источника излучения использовали перестраиваемый Ti-сапфировый лазер. Библ. 33. В. М. Ковба

М-Л·

Х. 1997, N24

O_2

1996

Xi, Xiangzhu,
Paldus, Josef;

теор.
расчет
электрон.
состоян.

J. Chem. Phys., 1996,
<u>104</u>(23), 9555-62.

O_2

1996

129: 195065n **Molecular absorption in the VUV by Fourier transform spectroscopy.** Yoshino, Kouichi; Thorne, Anne P.; Ito, Kenji (Harvard−Smithsonian Center for Astrophysics, Cambridge, MA 02138 USA). *Front. Sci. Ser.* **1996**, 18(Atomic and Molecular Photoionization), 167−176 (Eng), Universal Academy Press, Inc.. Current research on the Earth's upper atm. requires mol. parameters of unprecedented detail and accuracy. State−of−the−art models of the vacuum−UV (VUV) absorbing properties of the atm. call for absorption cross sections with details on the scale of the Doppler linewidths. As a consequence, spectroscopic data at resolving powers of the order of 10^6 are needed. Current particular needs are for ultrahigh resoln. absorption cross section data for some bands of NO and O_2 in the UV to VUV region. To meet these requirements, the authors used a UV Fourier transform (FT) spectrometer at Imperial College (IC) to measure the Herzberg I bands of O_2 and the $\delta(0,0)$ band of NO. To extend measurements to shorter wavelengths, the authors moved the IC VUV FT spectrometer to a synchrotron radiation facility (Photon Factory, KEK, Japan) and measured VUV photoabsorption cross sections of O_2 from 185 to 175 nm and NO from 195 to 160 nm.

Спектр

☒

④ NO

C.A. 1998, 128, N15

O_2

1997

127: 114774b A high resolution pulsed field ionization photoelectron study of O_2 using third generation undulator synchrotron radiation. Hsu, C.–W.; Heimann, P.; Evans, M.; Stimson, S.; Fenn, P. T.; Ng, C. Y. (Chemical Sciences Division and Advanced Light Source, Accelerator and Fusion Research Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 USA). *J. Chem. Phys.* **1997**, 106(21), 8931–8934 (Eng), American Institute of Physics. The authors have improved a newly developed exptl. scheme for high resoln. pulsed field ionization photoelectron (PFI–PE) studies [Hsu et al., Rev. Sci. Instrum. (in press)] using the high resoln. monochromatized multi–bunch undulator synchrotron source of the Chem. Dynamics Beamline at the Advanced Light Source. This improved scheme makes possible PFI–PE measurements with essentially no contamination by background electrons arising from direct photoionization and prompt autoionization processes. The authors present here a preliminary anal. of the rotationally resolved PFI–PE spectrum for O_2 obtained at a resoln. of 0.5 meV (full–width–at–half–max.) in the photon energy range of 18.1–19.4 eV, yielding accurate ionization energies for the transitions $O_2^+(b\ ^4\Sigma_g^-,\ v^+ = 0-9,\ N^+ = 1) \leftarrow O_2(X\Sigma_g^-,\ v = 0,\ N = 1)$.

(У)

C.A. 1997, 127, N8.

O_2

1997

128: 67887z Raman matrix isolation spectroscopy, Part 4. Raman studies of the isotopic effect in solid and matrix-isolated oxygen. Kornath, A.; Koper, I. (Anorganische Chemie, Fachbereich Chemie, Universitat Dortmund, 44221 Dortmund, Germany). *J. Raman Spectrosc.* **1997**, 28(10), 829–831 (Eng), John Wiley & Sons Ltd.. The Raman spectra of oxygen with different isotope compns. were investigated in the solid state and in argon and nitrogen matrixes at 15 K. The fundamental vibration of the isotopomers $^{16}O^{17}O$, $^{16}O^{18}O$ and $^{17}O^{17}O$ reveal a doublet of lines, each sepd. by 2.2 cm^{-1}, in solid oxygen and in nitrogen matrixes. The isotopic effect is independent of isotope compn. and can be annealed by a warm-up cycle.

спектр.
в
матрице

С.А. 1998, 128, N6

O_2

1997

126: 205006y Ab initio configuration interaction calculations of the predissociation of rovibrational levels of the C $^3\Pi_g$ and d $^1\Pi_g$ 3sσ Rydberg states of the oxygen molecule. Li, Yan; Petsalakis, Ioannis D.; Liebermann, Heinz-Peter; Hirsch, Gerhard; Buenker, Robert (Besamthochschule Wuppertal, Bergische Univ., D-42097 Wuppertal, Germany). *J. Chem. Phys.* **1997**, 106(3), 1123-1133 (Eng), American Institute of Physics. Ab initio CI calcns. were carried out for seven low-lying $^{3,1}\Pi_g$ states of the O_2 mol. Three different types of nonadiabatic couplings were considered: spin-orbit, radial, and rotational. The complex scaling method was employed to compute rovibrational level locations and predissocn. linewidths with a basis of 200 Hermite polynomials for each of 13 different Ω electronic states. The calcns. correctly predict that the $\nu = 2$ level has the narrowest linewidth for the $^{16}O_2$ C $^3\Pi_g$ state, while $\nu = 4$ is narrowest for $^{18}O_2$. Marked variations in the linewidths of the different Ω components of the C state are explained by the fact that the $\pi^* \rightarrow 3s\sigma$ Rydberg and $\sigma \rightarrow \pi^*$ valence $^3\Pi_g$ state have different occupations of the π^* orbital, causing opposite orderings of their resp. Ω levels. Rotational coupling is important for high J values of the C state. The d $^1\Pi_g$ 3sσ state shows even more unusual effects by virtue of the fact that there is a sharply avoided crossing between the corresponding Rydberg diabatic state with a bound

предиссоц., ab initio расчет

C. A. 1997, 126, N 15

$\sigma \rightarrow \pi^{*}$ $^1\Pi_g$ valence state. The calcns. find irregular spacings in the d−state vibrational manifold, wide variations in linewidth for different ν,J levels, and a large change in the rotational const. in successive vibrational levels, all of which effects were earlier demonstrated in exptl. work. Satellite lines are indicated for both the $\nu = 2$ and 3 levels as a result of the interaction with the bound $^1\Pi_g$ valence state, whereby exptl. verification exists only for $\nu = 2$. The $\nu = 3$ state has not yet been successfully identified due to the broadness of the d−X spectrum in the energy range of interest. The obsd. temp. dependence of the linewidths of the two features near the expected location of the $\nu = 2$ level can also be understood from these calcns. Finally, the change in the predissocn. mechanism for the d state from spin−orbit to radial as ν changes from 0 to 2 which was deduced exptl. is also verified in the present theor. treatment.

O_2

1997

128: 121125q $b^1\Sigma_g^+ - X^3\Sigma_g^-$ (0,0) **band of oxygen isotopomers in relation to tests of the symmetrization postulate in $^{16}O_2$.** Naus, H.; de Lange, A.; Ubachs, W. (Department of Physics and Astronomy, Laser Centre, Vrije Universiteit, De Boelelaan 1081, 1081 HV Amsterdam, Neth.). *Phys. Rev. A: At., Mol., Opt. Phys.* **1997**, 56(6), 4755–4763 (Eng), American Physical Society. The authors studied the $b^1\Sigma_g^+ - X^3\Sigma_g^-$ (0,0) band of the $^{16}O^{18}O$, $^{16}O^{17}O$, $^{18}O_2$, $^{17}O^{18}O$, and $^{17}O_2$ isotopomers of oxygen. The weak magnetic dipole transitions around 760 nm were obsd. using cavity–ring–down absorption spectroscopy. The positions of over 340 lines are presented together with (re–) analyses of the rotational consts. The authors discuss the importance of these data in view of tests of the symmetrization postulate in $^{16}O_2$ and present a sensitivity scale of 13 orders of magnitude that could be practical for future test expts.

$b^1\Sigma_g^+ - X^3\Sigma_g^-$

(0,0)

C.A. 1998, 128, N10

O_2 1997.

Peterson K.A., Wilson A.K., et al.,

re, ωe, теор. расчет

Theor. Chem. Acc. 1997, 97 (1-4), 257-259

(Cell. B_2; III)

O_2

1997

127: 269681t Precision emission and absorption spectroscopy of the oxygen atmospheric bands ($b^1\Sigma_g^+ - X^3\Sigma_g^-$) from Fourier transform spectroscopy. Phillips, Alexander J.; Peters, Frank; Hamilton, Peter A. (Dep. of Chem., Queen Mary and Westfield Coll., Univ. of London, London, UK E1 4NS). *J. Mol. Spectrosc.* **1997**, 184(1), 162–166 (Eng), Academic. The oxygen $b^1\Sigma_g^+ - X^3\Sigma_g^-$ electronic spectrum (the atm. system) was recorded at high resoln. in both emission and absorption on the same Fourier transform spectrometer but with independent calibration methods used in each case. After correction for the known pressure shift of the transitions, excellent agreement is achieved between the data sets recorded in this work, allowing significant errors to be identified within and between previous data sets. Mol. consts. appropriate to the low pressure limit are detd. from these new data for this important transition.

($b^1\Sigma_g^+ - X^3\Sigma_g^-$)

М.п.

C.A. 1997, 127, N 19

O_2

1998

$A'^3\Delta_u - X^3\Sigma_g^-$
система
2400–2900 A°
ранее отнесена
к $(O_2)_2$

130: **73197g** **The Wulf bands of oxygen.** Bernath, Peter; Carleer, Michel; Fally, Sophie; Jenouvrier, Alain; Vandaele, Ann Carine; Hermans, Christian; Merienne, Marie-France; Colin, Reginald (Service de Chimie Physique Moleculaire, Universite Libre de Bruxelles, B-1050 Brussels, Belg.). *Chem. Phys. Lett.* **1998**, 297(3,4), 293–299 (Eng), Elsevier Science B.V.. The Wulf bands of O in the 240–290 nm spectral region are caused by collision-induced absorption of the Herzberg III ($A'^3\Delta_u-X^3\Sigma^-_\kappa$) system. These bands had been previously attributed to the O dimer, $(O_2)_2$. Under atm. conditions the Wulf bands are thus the long-wavelength extension of the Herzberg continuum. Absorption of solar radiation by the Wulf bands may be an addnl. source of NO in the stratosphere.

C.A. 1999, 130, N6

O_2

1998

(предисс. в Шуман Рунге полосе)

129: 251920b A comparative high-resolution study of predissociation linewidths in the Schumann-Runge bands of O_2. Dooley, P. M.; Lewis, B. R.; Gibson, S. T.; Baldwin, K. G. H.; Cosby, P. C.; Price, J. L.; Copeland, R. A.; Slanger, T. G.; Thorne, A. P.; Murray, J. E.; Yoshino, K. (Research School of Physical Sciences and Engineering, The Australian National University, Canberra, 0200 Australia). *J. Chem. Phys.* **1998**, 109(10), 3856-3867 (Eng), American Institute of Physics. Results are presented of a comparative study in which 3 distinct high-resoln. exptl. techniques (vacuum-UV laser spectroscopy, laser-induced fluorescence spectroscopy and vacuum-UV Fourier-transform spectroscopy) were used to study predissocn. in the Schumann-Runge bands of O_2 B $^3\Sigma_u^-(v')$ X $^3\Sigma_g^-(v'')$ with v' = 13 and 14. Measurements are the 1st to be performed at high resoln. for these levels and represent a significant advance on previous knowledge, characterizing completely the fine-structure and rotation dependencies of the B $^3\Sigma_u^-(v = 13$ and $14)$-state

С. А. 1998, 129, N 19

predissocn. for the 1st time. The measured fine−structurespecific linewidths will result in significant improvements in the parameterization of models describing predissocn. of the B−state and will have an impact on the development of realistic photochem. models of the terrestrial atm. Good agreement was found between linewidths measured using vacuum−UV laser spectroscopy and laser−induced fluorescence spectroscopy, but unexpected difficulties arose in detg. quant. linewidths using vacuum−UV Fourier−transform spectroscopy. For each exptl. technique, the instrumental resoln. had to be carefully controlled and monitored to ensure reliable interpretation of the measured spectra.

O_2 1998

1

129: 142007p High−resolution pulsed field ionization photoelectron study of O_2: Predissociation lifetimes and high−n Rydberg lifetimes converging to O_2^+ ($c^4\Sigma_u^-$, $v^+ = 0,1$). Evans, M.; Stimson, S.; Ng, C. Y.; Hsu, C.−W. (USDOE and Department of Chemistry, Ames Laboratory, Iowa State University, Ames, IA 50011 USA). *J. Chem. Phys.* **1998**, 109(4), 1285−1292 (Eng), American Institute of Physics. The authors measured pulsed field ionization photoelectron (PFI−PE) spectrum of O_2 in the energy range of 24.53−25.0 eV at a PFI−PE resoln. of 11 cm^{-1} (full width at half max., FWHM). The PFI−PE bands for O_2^+ ($c^4\Sigma_u^-$, $v^+ = 0$ and 1) obtained at O_2 rotational temps. of 35 and 298 K have been simulated using the Buckingham−Orr−Sichel model. Only the $\Delta N = -3, -1, +1$, and +3 (or N, P, R, and T) rotational branches are obsd., indicating that the outgoing electron continuum channels with angular momenta l = 0, 2, and 4 dominate in the threshold ionization

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O_2^+

(эл. п. в Δ

нижних эл. сост.)

С.А. 1998, 129, N 11

transitions O_2^+ ($c^4\Sigma_u^-$, $\nu^+ = 0$ to 1, N^+) O_2 ($X\ ^3\Sigma_g^-$, $\nu'' = 0$, N''). The simulation yields natural rotational linewidths of 19.6±2.0 and 77±8 cm^{-1} (FWHM) for the resp. $\nu^+ = 0$ and 1 PFI−PE bands of the O_2^+ ($c^4\Sigma_u^-$) state. These linewidths make possible the detn. of the predissocn. lifetimes for the $\nu^+ = 0$ and 1 levels of O_2^+ ($c\ ^4\Sigma_u^-$) to be $(2.7\pm0.3)\times10^{-13}$ and $(6.9\pm0.7)\times10^{-14}$ s, resp. This expt. also provides accurate ionization energies of $24.5622_7\pm0.0005$ and $24.7544_5\pm0.0005$ eV for transitions to O_2^+ ($c\ ^4\Sigma_u^-$, $\nu^+ = 0$, $N^+ = 0$) and O_2^+ ($c\ ^4\Sigma_u^-$, $\nu^+ = 1$, $N^+ = 0$) from O_2 ($X\ ^3\Sigma_g^-$, ν'', $N'' = 1$), resp. The rotational consts. of 1.58±0.02 and 1.54±0.04 cm^{-1} obtained here for the O_2^+ ($c\ ^4\Sigma_u^-$, $\nu^+ = 0$) and O_2^+ ($c\ ^4\Sigma_u^-$, $\nu^+ = 1$) states allow the calcn. of their corresponding equil. bond distances to be 1.155±0.011 and 1.170±0.015 Å. The (nominal) effective lifetimes for high−n Rydberg states converging to the O_2^+ ($c\ ^4\Sigma_u^-$, $\nu^+ = 0$ and 1) states are measured to be ≈0.33 μs, which are significantly shorter than the values of ≈1.9 μs measured for the O_2^+ ($b\ ^4\Sigma_g^-$, $\nu^+ = 0-5$) states. The shorter (nominal) effective lifetimes for high−n Rydberg states converging to O_2^+ ($c\ ^4\Sigma_g^-$, $\nu^+ = 0$ and 1) obsd. are attributed to the higher kinetic energy releases (or velocities) of O^+ fragments resulting from predissocn. of the O_2^+ ion cores.

1998г

O_2

(спектр, предиссоц)

C.A. 1998, 128, N26

128: 328155v Theoretical treatment of predissociation of the (4pσ) 1,3Π$_u$ rovibrational levels in the spectrum of the oxygen molecule. Li, Yan; Hirsch, Gerhard; Buenker, Robert J. (Fachbereich 9–Theoretische Chemie, Bergische Universitat–Gesamthochschule Wuppertal, Gaussstr. 20, D–42097 Wuppertal, Germany). *J. Chem. Phys.* 1998, 108(19), 8123–8129 (Eng), American Institute of Physics. Ab initio CI calcns. are carried out for 8 low–lying $^{1,3}\Pi_u$ and 4 $^1\Delta_u$ states of the O_2 mol. Three different types of couplings are considered: nonadiabatic, spin–orbit, and rotational, and the complex scaling method was employed to det. rovibrational energies and wave functions. The calcns. correctly predict a large no. of trends in the measured level locations, predissocn. linewidths, rotational consts., and line intensities for the (4pσ) $^{1,3}\Pi_u$ states. The v = 1 level has the lowest frequency and strongest absorption intensity among the 4 obsd. vibrational levels of the (4pσ) $^3\Pi_u$ state, while the v = 2 has the broadest predissocn. linewidth and v = 0, the smallest rotational const., all in agreement with exptl. findings. The linewidth of the v = 0 level of the $^1\Pi_u$ state is computed to be 0.01 cm^{-1}, consistent with the measured value of <0.1 cm^{-1}. The calcns. indicate that the v = 0 level of the (4pσ) $^1\Pi_u$ state borrows intensity from the allowed (4pσ) $^3\Pi_u$–X $^3\Sigma_g^-$ through spin–orbit interaction and that the v = 4 level of the (4pσ) $^3\Pi_{1u}$ component, which has not yet been identified exptl., is strongly perturbed by the v = 3 level of the (4pσ) $^1\Pi_u$ state. The L–uncoupling–type interaction between $^1\Pi_u$ and $^1\Delta_u$ states is studied, and the explanation for the missing lines of the v = 0, J ≥ 2 rovibrational levels of the (4pσ) $^1\Pi_u$ states is sought based on the calcd. results.

1998

O_2 1998

Litorja, Maritoni,
et al.,

(AP) J. Electron Spectrosc.
Relat. Phenom. 1998,
97 (1-2), 131-146.

(см. HO_2; III)

O_2

1998

Moscardo F, et al.,

J. Comput. Chem.
1998, <u>19</u>(16), 1899–1908

теорет.
расчет
структурн.
парамет.,
ω, ν,
$\Delta H_{атом}$

(см. H_2; <u>III</u>)

O_2
изотопомеры

Om. 39566

1998

$(b^1\Sigma_g^+ - X^3\Sigma_g^-)$

130: **73203f** **Cavity-ring-down spectroscopy on the $b^1\Sigma_g^+ - X^3\Sigma_g^-$ (1,0) band of oxygen isotopomers.** Naus, H.; Van der Wiel, S. J.; Ubachs, W. (Laser Cent., Dep. Phys. Astronomy, Vrije Univ., 1081 HV Amsterdam, Neth.). *J. Mol. Spectrosc.* **1998**, 192(1), 162–168 (Eng), Academic Press. The $b^1\Sigma_g^+ - X^3\Sigma_g^-$ (1,0) band of $^{16}O^{17}O$, $^{16}O^{18}O$, $^{18}O_2$, $^{17}O^{18}$, AND $^{17}O_2$ isotopomers was studied employing the technique of cavity-ring-down spectroscopy. More than 400 transition frequencies of magnetic dipole lines were detd. with a typical uncertainty of 0.01 cm^{-1}. This work results in new or improved accurate mol. consts. for the excited $b^1\Sigma_g^+$, $\nu = 1$ state of all isotopomers and for the $X^3\Sigma_g^-$, $\nu = 0$ ground state of $^{17}O_2$. (c) 1998 Academic Press.

C. A. 1999, 130, N6

O_2

1999

ab initio
расчет
триплет –
синглет.
расщеплен.

131: 37010c Ab initio configuration interaction calculations of Rydberg and mixed valence–Rydberg states. Buenker, Robert J.; Hirsch, Gerhard; Li, Yan (Fachbereich 9 – Theoretische Chemie Bergische Universitat – Gesamthochschule Wuppertal, D-42097 Wuppertal, Germany). *Understanding Chem. React.* **1999**, 20(Role of Rydberg States in Spectroscopy and Photochemistry), 57–91 (Eng), Kluwer Academic Publishers. A review with 84 refs. Rydberg states of satd. mols. (water, ammonia, ethane, and silane) are considered. Rydberg–valence predissocn. effects are discussed, including the HeH excimer laser, the O_2 Schumann–Runge interactions, triplet–singlet interactions in O_2, and TlCl and AsO predissocn.

(+2)

C.A., 1999, 131, N3

O_2 От. 40070 - 1999

Darcy S. Peterka,
et al.,

J. Chem. Phys.,
1999, <u>110</u>, N13,
6095–6098

спектр
фотоиониз.,
фотоэлектр.
спектр,
ab initio

O_2 От. 39749 1999

Lewis B.R., Gibson S.T. et al.,

$3s\sigma_g\ {}^{1,3}\Pi_g$

J. Chem. Phys., 1999, 111, N1, 186 – 197

Ридберг. состоян.

Perturbations in the $3s\sigma_g\ {}^{1,3}\Pi_g$ Rydberg states ~~of~~ [illegible] O_2: bound–

bound interactions with the second $^1\Pi_g$ and $^1\Delta_g$ valence states.

F: O2
P: 3

1999

131:220438 The singlet oxygen absorption to the upper state of the Schuma Runge system: the B3.SIGMA.u- .ltwarw. a1.DELTA.g+ and B3.SIGMA.u- .ltwar b1.SIGMA.g+ transitions intensity calculation. Minaev, Boris F. Cherkassy Engineering and Technological Institute Cherkassy, Ukraine Phys. Chem. Chem. Phys., 1(15), 3403-3413 (English) 1999 The singlet-triplet transition dipole moments were calcd. by quadratic response (QR) multi-configuration SCF (MCSCF) method from the two metasta singlet states of O2, a1.DELTA.g and b1.SIGMA.g+, to the upper triplet ex states. The most intense transitions in the near UV region (200-250 nm) connected with the upper state of the

Schumann-Runge (SR) system, B3.SIGM with the 13.PI.u dissociative state. Calcns. of the transition dipöle mo for the spin allowed bands, SR, n1.SIGMA.u+ .ltwarw. b1.SIGMA.g+ and n1.D .ltwarw. a1.DELTA.g, by linear -response (LR) MCSCF method were compared w previous studies and are quite reliable. A similar anal. was performed f spin-orbit coupling matrix elements, calcd. with the full Breit-Pauli ope Spin-orbit coupling between the b1.SIGMA.g+ and X3.SIGMA.g- (MS = 0) stat provides their effective mixing at all internuclear distances (r) and pro strong contribution to the parallel component of the B3.SIGMA.u- .ltwarw. b1.SIGMA.g+ transition dipole moment (Dz) by intensity borrowing from the Schumann-Runge band in a wide range of the r values. The Dz(B-b) integra an averaged value 0.08 ea0 in the most important range, r = 1.18 to 1.45 exhibits some irregular behavior at longer distances. The perpendicular component of the B-b transition is negligible. The B3.SIGMA.u- .ltwarw. a1.DELTA.g transition has only perpendicular dipole moment which is relat non-intense, D(B-a)~0.0004 ea0, to compete with the absorption in the Her continuum (D ~ 0.001 ea0). The transition dipole moments as functions of some oscillations at very short and long distances, connected with level crossings and avoided crossings. The singlet-triplet transitions 13.PI.u .ltwarw. a1.DELTA.g and 13.PI.u .ltwarw. b1.SIGMA.g+ are 30-20 times weak the B-b absorption.

F: O2
P: 3

от. 39750

1999

131:176581 The (x 2.PI.g) ns.sigma.g1,3.PI.g Rydberg states of O2: Spectr structures, and interactions. Morrill, J. S.; Ginter, M. L.; Lewis, B. R. Gibson, S. T. (E. O. Hulburt Center for Space Research, Naval Research Laboratory, Washington, DC 20375-5352, USA). J. Chem. Phys., 111(1), 173 (English) 1999 The results of a crit. reexamn. of previous exptl. observations of the (2.PI.g) ns.sigma.g1,3.PI.g Rydberg states of O2 are employed to optimize coupled-channel Schrodinger-equation (CSE) model describing rovibronic interactions among a no. of 1,3.PI.g Rydberg and valence states. The res calcns. using this CSE model are compared with the exptl. energy-level an predissocn. linewidth data base. As a result of the optimization process relevant potential-energy curves and Rydberg-valence, Rydberg-Rydberg, an valence-valence interactions are characterized for 1,3.PI.g states in the 9.5 eV region above the ground state of O2. The precision of these characterizations and the interpretation of the exptl. observations are l by the quality of the existing data, which exhibit a no. of inconsistenci cannot be reconciled without new, well-characterized exptl. studies. In of these difficulties, the present CSE model, as currently parametrized, represents a significant improvement over previous work, enabling identif of a no. of previously unassigned spectral features assocd. with perturba the 3 s.sigma.gd 1.PI.g state by the || 1.PI.g valence state and an anoma sensitivity in predissocn. branching ratios for the d(.upsilon. = 1) leve electronic structure and predissocn. of the nssg states for n .gtoreq. 4 strongly influenced by ns.sigma.g - (n - 1)d.sigma.g Rydberg-Rydberg interactions.

$^{16}O_2$, $^{18}O_2$

1999

130: 202328b **The $b^1\Sigma_g^+-X^3\Sigma_g^-$ (3, 0) band of $^{16}O_2$ and $^{18}O_2$.** Naus, H.; Ubachs, W. (Dep. Phys. Astronomy, Vrije Univ., 1081 HV Amsterdam, Neth.). *J. Mol. Spectrosc.* **1999**, 193(2), 442–445 (Eng), Academic Press. The authors obtain updated values for the mol. consts. for the $b^1\Sigma_g^+-X^3\Sigma_g^-$ (3,0) band of $^{16}O_2$ and $^{18}O_2$. These values may help to identify emission bands from excited vibrational levels of $O_2(b^1\Sigma_g^+)$, including minority isotopomers, as obsd. in the Earth's atm. (c) 1999 Academic Press.

($b^1\Sigma_g^+ \leftarrow X^3\Sigma_g^-$)

C.A. 1999, 130, N15

O_2

1999

$(b^1\Sigma_g^+ - X^3\Sigma_g^-)$

131: 37180h The γ–band of $^{16}O_2$, $^{16}O^{17}O$, $^{17}O_2$ and $^{18}O_2$. Naus H.; Navaian, K.; Ubachs, W. (Laser Centre, Department of Physics and Astronomy, Vrije Universiteit, 1081 HV Amsterdam, Neth.). *Spectrochim. Acta, Part A* **1999**, 55A(6), 1255–1262 (Eng), Elsevier Science B.V.. The $b^1\Sigma_g^+ - X^3\Sigma_g^-$ (2,0) band of the $^{16}O_2$, $^{16}O^{17}O$, $^{17}O_2$ and $^{18}O_2$ O isotopomers was studied by cavity–ring–down laser spectroscopy. Line positions of the four branches in each band were detd. with an accuracy of 0.01 cm^{-1}. Improved or new mol. consts. are derived for the $b^1\Sigma_g^+$, v = 2 excited state of the four isotopomers.

C.A., 1999, 131, N3

1999

F: O2
P: 3
131:220493 Fourier transform spectroscopy and cross-section measurements Herzberg II bands of O2 at 295 K. Yoshino, K.; Esmond, J. R.; Parkinson, H.; Thorne, A. P.; Learner, R. C. M.; Cox, G. Harvard-Smithsonian Center Astrophysics Cambridge, MA 02138, USA J. Chem. Phys., 111(7), 2960- 2967 (English) 1999

Fourier transform spectroscopic measurements of the absorption bands of the Herzberg II (c 1.SIGMA.u--X 3.SIGMA.g-) of O2 at 295 K have been made resoln. of 0.06 cm-1 in the wavelength region 240-275 nm. Rotational lin positions are detd. with an accuracy of 0.005 cm-1, and rotational term v are presented for the vibrational levels, v'=6-16. Precise band oscillat strengths of the (7,0)-(16,0) bands are obtained for the first time by di measurement by summing the cross sections of individual rotational lines bands. The rotational line strengths and the branching ratios are also presented for the same bands.

2000

F: O2
P: 3
132:114598 Wavenumbers, strengths, widths and shifts with pressure of lin in four bands of gaseous 16O2 in the systems a1.DELTA.g - X3.SIGMA.g- and b1.SIGMA.g+ - X3.SIGMA.g-. Cheah, Swee-Lan; Lee, Yuan-Pern; Ogilvie, J. F Department of Chemistry, National Tsing Hua University Hsinchu 30043, Taiwan J. Quant. Spectrosc. Radiat. Transfer, Volume Date 2000, 64(5), 467-482 (English) 1999 In spectra of gaseous O at 299 K with pressure/bar in the range [0.13,1.06] and lengths of absorbing path up to 107 m, the authors measur the wavenumbers, strengths, widths and shifts with pressure

C. A. 2000, 132

of 118 mostly fully resolved lines of 16O2 due to rotational fine structure in the band a1.DELTA.g(v = 0) - X3.SIGMA.g-(v = 0), 59 lines in the band b1.SIGMA.g+(0) - X3.SIGMA.g-(v = 0), 58 lines in the band b1.SIGMA.g+(v = 1) - X3.SIGMA.g-(v = 0) and 43 lines in the band b1.SIGMA.g+(v = 2) - X3.SIGMA (v = 0); the latter band is measured quant. for the 1st time. Spectral parameters to reproduce wavenumber data are considerably improved over previously existing data. Band strengths, av. widths and shifts of lines with pressure of pure O2 are presented, and extensive comparison of these results is made with corresponding values from the literature.

2000

F: O2
P: 3
132:299111 Spin-orbit coupling in highly vibrationally excited O2(v) and O2(v=0)-O2(v).

Hernandez-Lamoneda, R.; Ramirez-Solis, A.

Centro de Investigaciones Quimicas, Universidad Autonoma del Estado de Morelos Cuernavaca, Mor. 62210, Mex. Chem. Phys. Lett., 321(3,4), 191-196 (English) 2000 Highly correlated ab initio calcns. of the ground and low-lying electron states of O2 and O4 together with a semi-empirical est. of the spin-orbit coupling among them have been performed. For

C.A. 2000, 132

the diat., our calcns. agre with recent spectroscopic measurements. For the O2(v=0)-O2(v) collision avoided crossings allow mixing of the electronic configurations with appr spin-orbit coupling into the lowest-lying excited states. As a consequen spin-orbit transitions can occur at significantly lower vibrational energ the O2(v) moiety induced by collisions with O2(v=0). This mechanism must partially responsible for the obsd. jump in depletion rates of O2(v) detd exptl.

F: O2
P: 3

2000

132:214669 Detection of O(1D) produced in the photodissociation of O2. I. Identification of the 3.SIGMA.u- and 3.PI.u Rydberg states in 113-130 nm. Lee, P. C.; Nee, J. B. Department of Physics, National Central University Taichung 32054, Taiwan J. Chem. Phys., 112(4), 1763-1768 (English) 2000 The metastable O(1D) atom produced in the photodissocn. of O2 in the wavelength region 113-130 nm was detected by measuring the 762 nm fluorescence of the transition O2(b 1.SIGMA.g+ .fwdarw. X 3.SIGMA.g-). T excited states of O2 were

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classified as either the 3.SIGMA.u- state that produces O(1D) + O(3P), or the 3.PI.u state that produces O(3P) + O(3P). authors quantum yield measurements of O(1D) found bands of both pure and overlapped 3.SIGMA.u- and 3.PI.u states. Five bands were found to produc O(1D), including the longest, second, and third bands and two addnl. band ~115.3 and 113.8 nm that were assigned as the E 3.SIGMA.u- (.nu.'=3-4) sta Three bands were assigned to the F 3.PI.u(.nu.'=0-2) state. The authors found a state at 116.2 nm, which did not produce O(1D), but produced weak visible fluorescence. The possibility of attributing the fluorescence to transition D 3.SIGMA.u+-C 3.PI.g was discussed.

F: O2
P: 3

2001

134:345800 **Molecular properties of computationally difficult diatomic systems: O2, F2-, Cl2-, SiF, SiCl, ClO and MgO.** Janoschek, Rudolf; Kalcher, Josef. Institut fur Chemie, Theoretische Chemie, Karl-Franzens-Universitat Graz, Graz, Austria. Z. Phys. Chem. (Muenchen, Ger.) (2001), 215(2), 197-206. in English.

For seven difficult diat. mols., O2, F2-, Cl2-, SiF, SiCl, ClO and MgO, spectroscopic consts., Re, Be, ωe, ωeXe, and D0, have been calcd. by two computational methods, MR-ACPF and CCSD(T). The sequence of aug-cc-pVnZ+ basis sets has been used, and for O2, subsequent extrapolation of the total energies has been performed. In particular, new bond lengths for F2- and Cl2- are presented, and the established exptl. dissocn. energies for SiF and SiCl are cor. The dissocn. energy of the O2 mol. has been calcd. by different methods, overcoming the deficiencies of the aug-cc-pVnZ basis sets, at an accuracy of at least 0.3 kcal mol-1.

O_2

2001

(Ридбер-сост)

135: 144107u Identification of the 3pπ_ue' 3Δ_u Rydberg state of O_2 by (3+1) resonance–enhanced multiphoton–ionization spectroscopy. Lewis, B. R.; Gibson, S. T.; Tucay, Aurea A.; Robertson, Robert; Hwang, Eunsook S.; Bergman, Aaron; Copeland, Richard A. (Research School of Physical Sciences and Engineering, The Australian National University, Canberra, 0200 Australia). *J. Chem. Phys.* 2001, 114(19), 8364–8371 (Eng), American Institute of Physics. The diffuse v = 0 to 4 levels of the 3pπ_u e' $^3\Delta_u$ Rydberg state of O_2 are identified and characterized using (3+1) resonance–enhanced multiphoton–ionization spectroscopy. An exptl. potential–energy curve for the e' state, together with the magnitude of its interaction with the A' $^3\Delta_u$ valence state, are detd. semiempirically by analyzing the predissociated spectra using the coupled–channel Schrodinger–equation method. The exptl. Rydberg–valence coupling (930 cm^{-1}) exceeds significantly the value calcd. ab initio by Buenker and Peyerimhoff [Chem. Phys. Lett. 34, 225-(1975)] (<320 cm^{-1}), but is in good agreement with the single–configuration model prediction of Lewis et al. [J. Chem. Phys. 113, 2214(2000)] (900 cm^{-1}).

C. A. 2001, 135, N10

O_2

2001

теорет.
расчет
возбужд.
состоян.

134: 227586e **MCSCF response calculations of the excited states properties of the O_2 molecule and a part of its spectrum.** Minaev, Boris F.; Minaeva, Valentina A. (Cherkassy State University, Cherkassy, Ukraine 1800). *Phys. Chem. Chem. Phys.* 2001, 3(5), 720–729 (Eng), Royal Society of Chemistry. A no. of transitions including the triplet–singlet band $f^1\Sigma_u^+$ $X^3\Sigma_g^-$, have been studied by ab initio multi-configurational SCF (MCSCF) response methods. Potential energy curves for eight excited states obtained by linear response calcn. are in a good agreement with recent exptl. data and exhibit some new findings. Quadrupole moments for the 12 lowest states have been calcd. which can be used for intermol. interaction anal. and solvent shift estns. The nuclear quadrupole coupling const., magnetizability tensor, nuclear spin–rotation coupling const. and rotational g–factor are also presented. For the three lowest singlet states these parameters are analyzed in detail.

С. А. 2001, 134, N16

2001

F: O2
P: 3
135:37388 **A systematic theoretical investigation of the valence excited states of the diatomic molecules B2, C2, N2 and O2.** Muller, Thomas; Dallos, Michal; Lischka, Hans; Dubrovay, Zsofia; Szalay, Peter G. Institute for Theoretical Chemistry and Structural Biology, University of Vienna, Vienna, Austria. Theor. Chem. Acc. (2001), 105(3), 227-243. in English.

A quant. survey on the performance of multireference (MR), CI with all singles and doubles (CISD), MRCISD with the Davidson correction and MR-av. quadratic coupled cluster (AQCC) methods for a wide range of excited states of the diat. mols. B2, C2, N2 and O2 is presented. The spectroscopic consts. re, ωe, Te and De for a total of 60 states have been evaluated and critically compared with available exptl. data. Basis set extrapolations and size-extensivity corrections are essential for highly accurate results: MR-AQCC mean-errors of 0.001 A, 10 cm-1, 300 cm-1 and 300 cm-1 have been obtained for re, ωe, Te and De, resp. Owing to the very systematic behavior of the results depending on the basis set and the choice of method, shortcomings of the calcns., such as Rydberg state coupling or insufficient configuration spaces, can be identified independently of exptl. data. On the other hand, significant discrepancies with expt. for states which indicate no shortcomings whatsoever in the theor. treatment suggest the re-evaluation of exptl. results. The broad variety of states included in our survey and the uniform quality of the results indicate that the obsd. systematics is a general feature of the methods and, hence, is mol.-independent.

O_2

2001

135: 159473j **Molecular Constants for the v = 0, $b^1\Sigma_g^+$ Excited State of O_2: Improved Values Derived from Measurements of the Oxygen A–Band Using Intracavity Laser Spectroscopy.** O'Brien, Leah C.; Cao, Hong; O'Brien, James J. (Department of Chemistry, Southern Illinois University Edwardsville, Edwardsville, IL 62026–1652 USA). *J. Mol. Spectrosc.* **2001**, 207(1), 99–103 (Eng). Academic Press. High–resoln. intracavity laser spectroscopy (ILS) absorption measurements have been made on the b–X oxygen electronic transition (the A–band) which has bandheads occurring in the region of 13 165 cm^{-1}. The positions of the lines were detd. to an accuracy that is based on calibration with I_2 absorption lines using the Laboratoire Aime Cotton (Orsay) Atlas as ref. Based on the ILS measurements and the more accurately detd. positions given by L. R. Brown and C. Plymate (J. Mol. Spectrosc. 199, 166–179 (2000)) and with the $^3\Sigma_g^-$ ground state mol. consts. fixed at the values detd. by G. Rouille et al. (J. Mol. Spectrosc. 154, 372–382 (1992)), the following values (in cm^{-1}) were found for the mol. consts.: T_0 = 13122.2524(1); B_0 = 1.391244(2); D_0 = 5.352(4)×10^{-6}; and H_0 = −1.2(2)×10^{-11}. These results are compared with values derived from fits of the line positions listed in several other studies of this transition. (c) 2001 Academic Press.

М.П.
(Вращ. коэф.
$b^1\Sigma_g^+$)

O_2
O_2^-

2001

Sordo J.A.,

неэмпир. расчёт D_0 и A_e

J. Chem. Phys. 2001, <u>114</u>(5), 1974–1980

(см. C_2; <u>III</u>)

O_2 Om. 41326 2002

Edward S. Chen and Edward C. M. Chen,

Ae

J. Phys. Chem. A 2002, <u>106</u>, 6665 – 6669.

Semiempirical characterization of Homonuclear Diatomic Ions;

5. The General Classification of Herschbach Ionic Morse Potential Energy Curves.