O_3

1990

ОП 35337

18 Б1257. Спектры поглощения $^{16}O_3$ и $^{18}O_3$ в ближней ИК-области: адиабатическая энергия $^1A_2$ состояния? Near-infrared absorption spectra of $^{16}O_3$ and $^{18}O_3$: Adiabatic energy of the $^1A_2$ state? / Anderson S. M., Morton J., Mauersberger K. // J. Chem. Phys.— 1990.— 93, № 6.— С. 3826—3832.— Англ.

Зарегистрированы новые спектры поглощения $^1A_2(0, v_2, 1) \leftarrow {}^1A_1(0, 0, 0)$ полос $^{16}O_3$ и $^{18}O_3$ вблизи 1 мкм. На основании величин изотопич. сдвигов колебат. полос при низких значениях v_2 определено, что минимум $^1A_2$ состояния лежит на 9990±70 см$^{-1}$ выше минимума основного $^1A_1$ состояния и очень близко к диссоц. пределу O_2+O. Измерены величины симм. вал. и деф. кол.: $\nu_1 \sim 1200$ см$^{-1}$ и $\nu_2 = 528 \pm 15$ см$^{-1}$; рассчитаны величины $\nu_3 \sim 90 \pm 80$ см$^{-1}$ и нулевой колебат. энергии: 910±±50 см$^{-1}$. На основании этих данных установлено, что нижнее квантовое состояние лежит на 980 см$^{-1}$ выше диссоц. предела и, следовательно, $^1A_2$ состояние несвязанное. Обсуждена роль возбужденных электронных состояний ($^1A_2$, $^3B_2$ и $^3A_2$) в фотохимии озона.

Е. А. Пазюк

М·П

Х. 1991, № 18

O_3

(Om 34 928)

1990

114: 12515g Ab initio potential surfaces for ozone dissociation in its ground and various electronically excited states. Banichevich, A.; Peyerimhoff, S. D.; Grein, F. (Univ. Bonn, D-5300 Bonn, Fed. Rep. Ger.). *Chem. Phys. Lett.* 1990, 173(1), 1-6 (Eng). Potential-energy curves for five singlet electronic states of ozone which correlate with the first two fragmentation limits $O_2(^3\Sigma_g^-)$ + $O(^3P)$ and $O_2(^1\Delta_g)$ + $O(^1D)$ are calcd. employing MRD-CI treatments in a Gaussian AO basis. Vertical and adiabatic transition energies as well as dissocn. energies based on a two-dimensional optimized energy surface are presented. The vertical transition moments between the different states are also computed.

D_0, расчет

C.A. 1991, 114, N2

0-0-0 от. 33714 1990

Binnewies M.,
Schnöckel H.,
Chem. Rev. 1990, 90,
N 1, 321-330.

Т, термод.
данные

O_3

1990

23 Б1360. Полосы озона в области 3,3 мкм: положение линий и интенсивности. The 3.3-μm bands of ozone: Line positions and intensities / Camy-Peyret C. Flaud J. M., Smith M. A. H., Rinsland C. P. // J. Mol Spectrosc.— 1990.— **141**, № 1.— С. 134—144.— Англ

С разрешением 0,01 см$^{-1}$ получены ИК-фурье-спектры озона в области 3,3 мкм, связанные с переходами между основным и (003), (102) и (201) колебат. уровнями. Анализ вращат. структуры проводился с учетом Кориолисова вз-вия и вз-вия Дарлинга—Деннисона и включал 465 линий ($J_{max}=47$, $K_{max}=16$ для (003), 330 линий ($J_{max}=50$, $K_{max}=4$) — для (102) и 311 линий ($J_{max}=41$, $K_{max}=14$) — для (201)-состояний. Приведены молек. постоянные обсуждаемых состояний. В частности (в см$^{-1}$): $\nu_0(003)=3046{,}882$, $\nu_0(102)=3083{,}7024$ и $\nu_0(201)=3186{,}4097$. Также приведены абс. интенсивности полос $3\nu_0$, $\nu_1+2\nu_3$ и $2\nu_1+\nu_3$ (в см$^{-1}$/молекул·см$^{-2}$ при 296 К) равные соотв.: $0{,}131\times10^{-18}$, $0{,}127\times10^{-19}$ и $0{,}934\times10^{-20}$.

Г. В. Чертихин

М·П·

Х. 1990, N23.

O_3

1990

112: 225853m **The 3.3-μm bands of ozone: line positions and intensities.** Camy-Peyret, C.; Flaud, J. M.; Smith, M. A. H.; Rinsland, C. P.; Devi, V. Malathy; Plateaux, J. J.; Barbe, A. (Lab. Phys. Mol. Atmospherique, Univ. P. M. Curie, 75252 Paris, 05 Fr.). *J. Mol. Spectrosc.* 1990, 141(1), 134-44 (Eng). The anal. of high-resoln. (0.010 cm^{-1}) Fourier transform spectra of $^{16}O_3$ provided an extensive set of rotational energy levels belonging to the (003), (102), and (201) vibrational states of this mol. These exptl. energy levels were then satisfactorily reproduced with a Hamiltonian taking explicitly into account the various resonances (Coriolis and Darling-Dennison) affecting the levels, and precise vibrational energies and rotational and coupling consts. were detd. In particular, the following band centers were derived: $\nu_0(003) = 3046.0882$, $\nu_0(102) = 3083.7024$, $\nu_0(201) = 3186.4097$ cm^{-1}. Also, line intensities were measured with an accuracy of about 3% for the strongest lines and satisfactorily reproduced with suitable transition moment operators expanded with respect to rotational operators. Finally, an extensive list of line positions, intensities, and lower state energy levels was generated for the $3\nu_3$, $\nu_1 + 2\nu_3$, and $2\nu_1 + \nu_3$ bands of $^{16}O_3$.

Di

C.A.1990, 112, N24

O_3

Dm 33097

1990

/112: 87138d **Line parameters for ozone hot bands in the 4.8-μm spectral region.** Camy-Peyret, Claude; Flaud, Jean Marie; Rinsland, Curtis P.; Smith, Mary Ann H.; Devi, V. Malathy; Goldman, Aaron (Lab. Phys. Mol. Atmos., Univ. Pierre et Marie Curie, 75252 Paris, 05 Fr.). *J. Mol. Spectrosc.* 1990, 139(2), 353-60 (Eng). Line positions, intensities, and lower state energies were calcd. for 9 hot bands of $^{16}O_3$ in the 4.8-μm spectral region using improved spectroscopic parameters deduced in recent high-resoln. lab. studies. The good quality of the hot-band parameters was verified through comparisons of line-by-line simulations with 0.005-cm^{-1}-resoln. lab. spectra of ozone. The present work and the line parameters calcd. previously for the main bands provide a complete update of ozone spectroscopic parameters in the 4.8-μm region.

Спектр

C.A. 1990, 112, N10

$^{16}O_3$ От 34882 1990

113: 200405z Line positions and intensities for the $\nu_2 + 3\nu_3$ band of ozone ($^{16}O_3$) around 2.7 μm. Devi, V. Malathy; Perrin, Agnes; Flaud, Jean Marie; Camy-Peyret, Claude; Rinsland, Curtis P.; Smith, Mary Ann H. (Dep. Phys., Coll. William and Mary, Williamsburg, VA 23185 USA). *J. Mol. Spectrosc.* 1990, 143(2), 381-8. (Eng). The absorption spectrum of ozone, was recorded between 3600 and 3900 cm⁻¹ at 0.01 cm⁻¹ resoln. with a Fourier transform spectrometer. The anal. of the spectra has allowed the first high-resoln. study of the $\nu_2 + 3\nu_3$ band of the $^{16}O_3$ mol. The exptl. rotational energy levels of the (013) vibrational state were measured up to $J = 40$ and $K_a = 13$ allowing an accurate set of rotational consts. to be detd. with a Hamiltonian taking into account the Coriolis resonances with the unobserved (112) vibrational state. Moreover, 71 line intensities measured with a relative uncertainty of about 8% were least-squares fitted leading to the detn. of the main $\nu_2 + 3\nu_3$ transition moment consts. Finally, a complete list of line positions, intensities, and lower state energies was generated for the $\nu_2 + 3\nu_3$ and $\nu_1 + \nu_2 + 2\nu_3$ bands of $^{16}O_3$.

Ик-спектр

М.П.

С.А. 1990, 113, N 22

O_3 1990

Ermakow K.V.,
Butaev B.S. et al.

Силов. J. Mol. Struct. 1990,
пост. <u>240</u>, 295–303.

(CCl_4. H_2O; $\overline{\underline{III}}$)

O_3 1990

Farantos S.C., Gomez J.M.
et al.
Int. J. Quantum. Chem.
м.п. Quantum. Chem. Symp. 1990.
N 24. С. 429–446.

(см. ● Na_3; $\overline{\underline{III}}$)

O_3 1990

Flaud Jean-Marie,
Camy-Peyret C., et al.,

Appl. Opt., 1990, 29, N25,
3667-3671.
Improved ● line parameters

for ozone bands in
the 10-μm spectral region.

O_3

Dm 34660

1990

113: 87319j **The vibrational frequencies of ozone.** Lee, Timothy J.; Scuseria, Gustavo E. (Ames Res. Cent., NASA, Moffett Field, CA 94035 USA). *J. Chem. Phys.* 1990, 93(1), 489-94 (Eng). The equil. structure and harmonic frequencies of ozone were detd. at various levels of coupled-cluster theory using large 1-particle basis sets. The singles and doubles coupled-cluster (CCSD) method, the recently proposed CCSD(T) method, and the CCSDT-1 method were used. The largest 1-particle basis sets utilize the at. natural orbital (ANO) general contraction scheme and contain up through *g*-type functions. It is shown that *f*-type functions are essential for obtaining quant. accuracy in the equil. structure and the harmonic frequencies (i.e. ± 0.003 Å and ± 30 cm^{-1}). The CCSD(T) level of theory in conjunction with a [4s 3p 2d 1f] ANO basis set is found to yield an equil. geometry and harmonic frequencies in excellent agreement with expt. At this level of theory the harmonic frequencies are $\omega_1(a_1)$ = 1152, $\omega_2(a)_1$ = 717, and $\omega_3(b_2)$ = 1057 cm^{-1} to be compared with the exptl. values of 1135, 716, and 1089 cm^{-1}, resp. This success encouraged us to det. the cubic and quartic force consts.

Di расчет

C.A. 1990, 113, N ~~5~~ 10

and evaluate the anharmonic corrections to the fundamental vibrational frequencies. This level of theory is shown to be quite good for the a_1 vibrational modes, but some of the cubic force consts. involving $\omega_3(b_2)$ have large errors leading to an anharmonic correction for the asym. stretch that is about a factor of 2 too large.

O_3

1990

1 Б1041. О разнице энергий открытой и циклической форм озона. On the energy separation between the open and cyclic forms ozone / Lee Timothy J. // Chem. Phys. Lett.— 1990.— **169**, № 6.— С. 529—533.— Англ.

В рамках метода связанных кластеров в расширенном базисе натуральных АО, включающем *f*- и *g*-ф-ции рассчитана энергия циклич. изомера озона симметрии D_{3h}. Учитывали все одно- и двукратные возбуждения, поправку для учета трекратных возбуждений. Рассчитаны гармонич. колебат. частоты. По результатам расчета в базисе [$5s4p3d2f$] разница энергий ΔE циклич. и «открытого» изомера симметрии C_{2v} составляет 29,1 ккал/моль. Отмечено, что найденное значение с точностью ±0,8 ккал/моль совпадает с пределом базисного набора для данного метода. Учет энергии нулевых колебаний приводит к уменьшению ΔE на 0,4 ккал/моль. Полученное значение ΔE соответствует нижней границе действит. значения, т. к. учет высших возбуждений вносит больший вклад в энергию открытого изомера. Отмечено, что разница энергий двух изомеров больше, чем энергия диссоциации открытого изомера (26,1 ккал/ /моль).

Н. В. Харчевникова

М.Л.

Х.1991, N1

O_3

1990

113: 103665b On the energy separation between the open and cyclic forms of ozone. Lee, Timothy J. (Ames Res. Cent., NASA, Moffett Field, CA 94035 USA). *Chem. Phys. Lett.* 1990, 169(6), 529-33 (Eng). The equil. structure of the D_{3h} form of ozone has been detd. using large at. natural orbital (ANO) basis sets in conjunction with the singles and doubles coupled-cluster (CCSD) and CCSD(T) ab initio models of electron correlation. The largest one-particle basis sets include *g0type* functions. In addn., harmonic vibrational frequencies have been detd. The results allow a very accurate detn. of the energy difference (ΔE) between the open and cyclic forms of ozone. The highest energies decrease ΔE of 29.1 kcal/mol, of which triple excitations contribute 5.8 kcal/mol. Zero-point vibrational energies decrease ΔE by 0.4 kcal/mol, yielding a final est. of 28.7 kcal/mol. These results demonstrate that cyclic ozone is above the $O_3(X-A_1) \rightarrow O(^3P) + O_2(X^3\Sigma_g^1)$ dissocn. limit (16.1 kcal/mol.).

расчет T_e, R_0

C. A. 1990, 113, N 12

O_3

1990

1 Д67. **О разнице в энергиях открытой и циклической форм озона.** On the energy separation between the open and cyclic forms of ozone / Lee Timothy J. // Chem. Phys. Lett.— 1990.— **169**, № 6.— С. 529—533.— Англ.

С использованием нескольких методов квантовохим. расчетов вычислены энергия, геометрия, гармонич. частоты и силовые постоянные молекулы озона в циклич. D_{3h}-форме и в открытой C_{2v}-форме. Энергия циклич. формы превышает энергию открытой формы на 29,1 ккал/моль. М. В. Т.

М.П.

Ф 1991, N1

O_3

ОМ 34880 1990

11 Б1284. Полосы ν_2 $^{18}O_3$, $^{18}O^{16}O^{18}O$ и $^{16}O^{18}O^{18}O$. Положение и интенсивности линий. The ν_2 bands of $^{18}O_3$, $^{18}O^{16}O^{18}O$, and $^{16}O^{18}O^{18}O$: Line positions and intensities / Perrin A., Vasserot A.-M., Flaud J.-M., Camy-Peyret C., Rinsland C. P., Smith M. A. H., Devi V. M. // J. Mol. Spectrosc.— 1990.— 143, № 2.— С. 311—317. — Англ.

На ИК-фурье-спектрометре в области частот 600—800 $см^{-1}$ с разрешением 0,005 $см^{-1}$ впервые измерены колебательно-вращат. спектры трех изотопомеров озона, $^{18}O_3$ (**I**), $^{18}O^{16}O^{18}O$ (**II**) и $^{16}O^{18}O^{18}O$ (**III**). Анализ ИК-данных выполнен с использованием гамильтониана Уотсона в А-редукции и известных МВ-данных для основного колебательного состояния. Для **I**, **II** и **III**, соотв., определены центры полосы ν_2 661, 492479(57), 668,084958(120) и 677,5038238(810) $см^{-1}$, а также вращат. постоянные, постоянные центробежного искажения в состояниях (000) и (010). Из ИК-данных по абс. интенсивностям линий определены операторы моментов перехода полосы ν_2. Для **I**, **II** и **III**, соотв., полные интенсивности полос ν_2 при т-ре 296 К равны $0{,}593 \cdot 10^{-18}$, $0{,}602 \cdot 10^{-18}$ и $0.600 \cdot 10^{-18}$ $см^{-1}/(моль \cdot см^{-2})$. С. Н. Мурзин

М.П.

Х. 1991, N 11

O_3 ОМ 33096 1990

, 112: 87137c The $2\nu_2 + \nu_3$ and $2\nu_2 + \nu_1$ bands of ozone ($^{16}O_3$) at 4.1 μm: line positions and intensities. Rinsland, Curtis P.; Smith, Mary Ann H.; Devi, V. Malathy; Flaud, Jean Marie; Camy-Peyret, Claude (Langley Res. Cent., NASA, Hampton, VA 23665-5225 USA). *J. Mol. Spectrosc.* 1990, 139(2), 343-52 (Eng). Fourier transform spectra of O_3 was recorded in the 4.1-μm region at a resoln. of 0.010 cm^{-1}, allowing the 1st high-resoln. study of the $2\nu_2 + \nu_3$ and $2\nu_2 + \nu_1$ bands of the $^{16}O_3$ mol. The exptl. rotational energy levels of the (021) and (120) vibrational states were reproduced satisfactorily with a Hamiltonian that takes explicitly into account the Coriolis resonance affecting the levels, and a precise set of vibrational energies and rotational and coupling consts. was detd. In particular, the band centers $\nu_0(021) = 2407.9345$ cm^{-1} and $\nu_0(120) = 2486.5766$ cm^{-1} were obtained. Moreover, the transition moment consts. of the $2\nu_2 + \nu_3$ and $2\nu_2 + \nu_1$ bands were derived from a fit of 46 measured line intensities. From these parameters, a complete list of line positions, intensities, and lower state energies was generated for the 2 bands. In addn., the results for the (021) and (120) states obtained in this work were combined with previous results for the (010) state to generate a complete list of line positions, intensities, and lower state energies for the $2\nu_2 + \nu_3 - \nu_2$ and $2\nu_2 + \nu_1 - \nu_2$ hot bands of $^{16}O_3$ in the 5.7-μm spectral region. The good quality of the new 4.7- and 5.7-μm line lists was verified through comparisons of measured lab. spectra with corresponding simulations.

Спектр, ν_i

C. A. 1990, 112, N10

O_3 От 34933 1990

113: 200496c Emission from ozone excited electronic states. Shi, Jichun; Barker, John R. (Dep. Atmospheric, Oceanic Space Sci., Univ. Michigan, Ann Arbor, MI 48109-2143 USA). *J. Phys. Chem.* 1990, 94(22), 8390-3 (Eng). Time-resolved IR fluorescence was obsd. following the laser photolysis of small amts. of O_3 dild. in up to 1000 torr of O_2. Besides the 9.6- and 4.7-μm bands, which are well-known, three new emissions were obsd. near ~1.9, 2.1-2.7, and ~3.4 μm. The 1.9-μm band originates from an unknown electronic state, $O_3(\beta)$, which is produced through quenching of $O_3(^1B_2)$ by O_2 or Xe during O_3 photolysis in the Hartley band. The other emission bands originate from the O + O_2 recombination reaction, and their kinetics are complex, indicating the formation and subsequent collisional cascade of excited O_3 intermediates.

Электронные переходы, Ti

C.A. 1990, 113, N22

O_3

Om 33117

1990

112: 65674y The 3.6-μm region of ozone: line positions and intensities. Smith, M. A. H.; Rinsland, C. P.; Devi, V. Malathy; Flaud, J. M.; Camy-Peyret, C. (Langley Res. Cent., NASA, Hampton, VA 23665-5225 USA). *J. Mol. Spectrosc.* 1990, 139(1), 171–81 (Eng). Fourier IR spectra of O were recorded ~3.6 μm at a resoln. of 0.01 cm^{-1}. Anal. of the 3 bands $\nu_2 + 2\nu_3$, $\nu_1 + \nu_2 + \nu_3$, and $2\nu_1 + \nu_2$ led to an extensive and precise set of exptl. rotational energy levels for the triad of interacting vibrational states (012), (111), (210). Taking into account explicitly the Coriolis-type interactions between the rotational levels of (012) and (111) and (210) and the Darling–Dennison interaction between the levels of (012) and (210), it was possible to reproduce all of the exptl. energy levels. A precise set of vibrational energies rotational and coupling consts. was obtained. The following band centers (in. cm^{-1}) were derived: $\nu_0(012) = 2726.1066$, $\nu_0(111) = 2785.2391$, $\nu_0(210) = 2886.1781$. There were 190 line intensities measured from which precise transition moment consts. for the 3 bands were detd. A complete list of line positions, intensities, and lower state energy levels were generated for the $\nu_2 + 2\nu_3$, $\nu_1 + \nu_2 + \nu_3$, and $2\nu_1 + \nu_2$ bands of $^{16}O_3$.

М.П.

C.A.1990, 112, N8

O_3 ОМ 36002 1990

114: 30472v **An intersection seam between the ground state of ozone and an excited state of like symmetry.** Xantheas, S.; Elbert, S. T.; Ruedenberg, K. (Dep. Chem., Iowa State Univ., Ames, IA 50011 USA). *J. Chem. Phys.* 1990, 93(10), 7519–21 (Eng). For the O_3 mol., the potential-energy surface (PES) of the ground state in C_{2v} symmetry was found to intersect the PES of an excited state ($^1A_1$) with C_{2v} symmetry at an apex angle of 83.1560° and a bond length (of the 2 identical bonds) of 1.4756 Å. There is a 1-dimensional intersection seam of the 2 PES's extending into C_s symmetry (i.e., for nonisosceles geometries). This seam traverses the coordinate plane assocd. with C_{2v} symmetry in the detd. intersection point. The PES's were obtained from state-averaged MC-SCF calcns. in the full valence space.

потенц.
поверхн.
основн. и
$^1A_1$ сост.,
расчт

C.A. 1991, 114, N 4

O_3

От 36002 1990

11 Д178. Линия пересечения [потенциальных поверхностей] основного и возбужденного состоянии озона той же симметрии. An intersection seam between the ground state of ozone and an excited state of like symmetry / Xantheas S., Elbert S. T., Ruedenberg K. // J. Chem. Phys.— 1990.— **93**, № 10.— С. 7519—7521.— Англ.

Показано, что в молекуле O_3 реализуется ситуация, давно обсуждаемая в литературе, когда имеет место точное пересечение двух потенц. поверхностей одинаковой симметрии. Расчет сделан методом многоконфигурационного самосогласованного поля, усредненного по состояниям. Получено, что в симметрии C_{2v}, соответствующей симметрии основного состояния озона, в плоскости (R, Φ), где R — длина одинаковых связей, а Φ — угол между ними, имеется точечное пересечение потенц. поверхности этого основного состояния X^1A_1 с возбужденным состоянием $^1A_1$, которое переходит в

М.Л.

ф. 1991, N11

одномерную линию пересечения в неравнобедренной геометрии, т. е. в симметрии C_s. Пересечение имеет место в точке $R^+ = 1{,}4756$ Å, $\Phi^+ = 83{,}1860°$ вблизи точки вершины потенц. барьера, соответствующего точке перехода между открытым и кольцевым состоянием озона ($R^* = 1{,}438$ Å, $\Phi^* = 83{,}57°$) на поверхности X^1A_1. Две пересекающихся потенц. поверхности расположены очень близко на некотором расстоянии вдоль вершины барьера открытого и кольцевого озона с энергетич. зазором между точкой пересечения и точкой перехода двух состояний в 0,9 Хартри. И. М. С.

.олне.

O_3 Om. 36114 1991

Anderson S.A., Maeder J.,
спектр et al.,

J. Chem. Phys., 1991,
94, N10, 6351 – 6357

Effect of isotopic substitu

tion on the visible absorption spectrum of Ozone.

O_3

1991

116: 28413z The lowest excited $^1A_2$ and $^1B_1$ states of ozone: two conical intersections and their impact on photodissociation. Braunstein, M.; Hay, P. J.; Martin, R. L.; Pack, R. T. (Theor. Div., Los Alamos Natl. Lab., Los Alamos, NM 87545 USA). *J. Chem. Phys.* 1991, 95(11), 8239–47 (Eng). Results are given of ab initio configuration-interaction calcns. on the lowest excited $^1A_2$ and $^1B_1$ states of ozone near their C_{2v} min. and also at several nearby C_s geometries, where these two states becomes the lowest $^1A''$ states. In C_{2v} symmetry these two states have a seam intersection very near the $^1B_1$ min. which becomes a conical intersection for small distortions to C_s geometries. The influence of this intersection on the Wulf and Chappuis bands of ozone is discussed and a new interpretation of these bands is presented. The existence of a second conical intersection involving these same two states is shown for D_{3h} symmetries, where they become degenerate components of a $^1E''$ state.

($^1A_2$, $^1B_1$ – теор. расчет потенц. крив.)

C.A. 1992, <u>116</u>, N4

O_3

1991

16 Б1039. Низшие возбужденные состояния $^1A_2$ и $^1B_1$ озона: два конических пересечения и их влияние на фотодиссоциацию. The lowest excited $^1A_2$ and $^1B_1$ states of ozone: Two conical intersections and their impact on photodissociation / Braunstein M., Hay P. J., Martin R. L., Pack R. T. // J. Chem. Phys.— 1991.— 95, № 11.— С. 8239—8247.— Англ.

Методом конфигурац. взаимодействия с учетом однократных и двукратных возбуждений по отношению с нескольким исходным конфигурациям рассчитаны потенциальные поверхности состояний $^1A_2$ и $^1B_1$ молекулы O_3 вблизи их минимума симметрии C_{2v}. Использован базис сгруппированных гауссовых ф-ций [3s2p1d]. Орбитали получены многоконфигурац. методом ССП. Найдено, что в рамках симметрии C_{2v} имеет место пересечение рассматриваемых состояний, становящееся коническим при малых искажениях геометрии симметрии C_s. Обсуждено влияние пересечения на полосу Вульфа—Чаппуиса (10 000—22 000 см$^{-1}$); предложено новое отнесение этой полосы. Показано существование также второго конич. пересечения симметрии D_{3h}.

А. А. Сафонов

М.П.

Х. 1992, N 16

$^{16}O_3$

1991

уточнение молекул. постоянных

116: 12604b Tunable far infrared spectroscopy of $^{16}O_3$ ozone. De Natale, P.; Di Lonardo, G.; Fusina, L.; Inguscio, M.; Prevedelli, M. (Eur. Lab. Nonlinear Spectrosc., I-50125 Florence, Italy). *Proc. SPIE Int. Soc. Opt. Eng.* 1991, 1576(Conf. Dig. - Int. Conf. Infrared Millimeter Waves, 1991), 38-9 (Eng). Sixty pure rotational lines of O_3 were obsd. in the spectral region 1.5-4.1 THz with Doppler limited resoln. and very high accuracy (~60 KHz). An improved set of mol. and centrifugal distortion consts. were obtained which reproduce the 1126 transition frequencies within their abs. error. In particular, the observation of high *J* and high K_a transitions allowed to improve the accuracy of the high power centrifugal distortion consts.

C. A. 1992, 116, N2

O_3 1991

Dixit A.N.

M

Indian J. Pure and Appl.
Phys. 1991. <u>29</u>, N 1. C.
41–42.

(см. ● BeH_2; $\overline{\underline{III}}$)

O_3

1991

7 Д145. Не замкнутая и циклическая протонированные формы озона: гиперповерхность потенциальной энергии основного состояния. Open-chain and cyclic protonated ozone: The ground-state potential-energy hypersurface / Meredith Cynthia, Quelch Geoffrey E., Schaefer Henry F. (III) / J. Amer. Chem. Soc.— 1991.— 113, № 4.— С. 1186—1193.— Англ.

С использованием двойного экспоненц. базиса Хузинаги—Даннинга, дополненного поляризующими ф-циями с $\alpha_d(\mathrm{O})=0{,}85$, $\alpha_p(\mathrm{H})=0{,}75$, проведены неэмпирич. расчеты равновесной геометрии и электронного строения протонированных форм озона O_3 с симметрией V_{2v} и D_{3h}. Для стационарных точек в гармонич. приближении вычислены частоты колебаний. Абс. минимум энергии HO_3^+ соответствует протонированию крайнего кислорода озона: (C_v)-трансизомер. Соответствующий цисизомер лежит на 3,6 ккал/моль выше по энергии. Для изучения путей протонирования использована теория граничных орбиталей. Эти данные сопоставлены с данными по изоэлектронным молекулам FNO_4, FON.

Щ. Б. Ф.

М.П.

ф. 1991, N 7

O_3

1991

потенц. поверхность

116: 136605x **Structure of the adiabatic surface of the potential energy of the ground electronic state of ozone molecule.** Minyaev, R. (Inst. Fiz.–Org. Khim., Rostov–on–Don, USSR). *Zh. Strukt. Khim.* 1991, 32(6), 15–20 (Russ). The gradient lines are calcd. of potential surface of O_3 (D_{3h} symmetry). The concept is introduced of the min.–energy gradient line which coincides partially with the min.–energy reaction path. The domain structure is shown of the potential energy surface of O_3.

C. A. 1992, 116, N 14

O_3

1991

5 Д86. Структура адиабатической поверхности потенциальной энергии основного электронного состояния молекулы озона / Миняев Р. М. // Ж. структур. химии.— 1991.— 32, № 6.— С. 15—20

В норм. координатах циклич. формы D_{3h} молекулы озона с помощью метода МЧПДП/3 вычислены и построены градиентные линии на поверхности потенц. энергии O_3. Введено понятие минимально-энергетической градиентной линии, которая на различных участках совпадает с минимально-энергетич. путем реакции.

Показано доменное строение поверхности потенц. энергии O_3.

М.П.

Ф.1992, N5

O_3

1991

8 Б1013. Структура адиабатической поверхности потенциальной энергии основного электронного состояния молекулы озона / Миняев Р. М. // Ж. структур. химии.— 1991.— 32, № 6.— С. 15—200.— Рус.

В нормальных координатах циклич. D_{3h} формы молекулы озона с помощью метода MIND 0/3 вычислены и построены градиентные линии на поверхности потенциальной энергии O_3. Введено понятие минимально-энергетич. градиентной линии (МЭГЛ), к-рая на различных участках совпадает с минимально-энергетич. путем р-ции (МЭПР). Показано доменное строение ППЭ O_3.

М.П.

Х.1992, N 8

O_3

1991

115: 169357a **The 2.5-μm bands of ozone: line positions and intensities.** Perrin, A.; Vasserot, A. M.; Flaud, J. M.; Camy-Peyret, C.; Devi, V. Malathy; Smith, M. A. H.; Rinsland, C. P.; Barbe, A.; Bouazza, S.; Plateaux, J. J. (Lab. Phys. Mol. Appl., Univ. Pierre et Marie Curie, 75252 Paris, Fr.). *J. Mol. Spectrosc.* 1991, 149(2), 519–29 (Eng). A study of high-resoln. (0.010 cm^{-1}) Fourier transform absorption spectra of $^{16}O_3$ around 4020 cm^{-1} was performed leading to the 1st extensive anal. of the $\nu_1 + 3\nu_3$ band of this mol. and the first observation of weaker lines from its $4\nu_3$ and $3\nu_1 + \nu_2$ bands. Then the rotational energy levels of the (103), (004), and (310) vibrational states of ozone were satisfactorily reproduced using a Hamiltonian matrix which takes explicitly into account the ozone classical Coriolis interaction between (103) ↔ (004) together with the unusual Coriolis-type (103) ↔ (310) and Fermi-type (310) ↔ (004) interactions. In these conditions precise vibrational band centers and rotational and coupling consts. were obtained. Also, about 130 line intensities were measured with an accuracy of about 3% and satisfactorily reproduced leading to the detn. of the $\nu_1 + 3\nu_3$ and $3\nu_1 + \nu_2$ vibrational transition moment consts. Finally, a complete list of line positions, intensities, and lower state energies was generated for the $\nu_1 + 3\nu_3$, $4\nu_3$, and $3\nu_1 + \nu_2$ bands of $^{16}O_3$.

М.П.

C.A. 1991, 115, N16

O_3

ОМ 35863

1991

23 Б1068. Расчет методом самосогласованного поля в полном активном пространстве поверхностей потенциальной энергии, функций дипольного момента и спектроскопических постоянных O_3, CF_2, NO_2^- и NF_2^+. Complete active space self-consistent field potential energy surfaces, dipole moment functions, and spectroscopic properties of O_3, CF_2, NO_2^-, and NF_2^+ / K. A. Peterson, R. C. Mayrhofer, E. L. Sibert III, R. C. Woods // J. Chem. Phys.— 1991.— 94, № 1.— С. 414—430.— Англ.

потенц. поверхн.

М

Многоконфигурационным методом ССП в полном активном пространстве рассчитаны полные ПВ потенциальной энергии и дипольного момента изоэлектронных молекул O_3, CF_2, NO_2^- и NF_2^+. Использован базис сгруппир. гауссовских ф-ций (11*s*7*p*2*d*)/[7*s*4*p*2*d*], дополненный в случае NO_2^- набором диффузных ф-ций *s* и *p* типа. Определены ангармонич. спектроскопич. постоянные и колебат. уровни энергии. Предсказан вращат. и колебат. спектр NO_2^- и NF_2^+. Рассчитаны матричные элементы дипольного момента и определены вероятности колебат. переходов. Библ. 96.

А. А. Сафонов

$\boxed{+H}$ +3

Х·1991, N23

O_3

Om 35863

1991

9 Д92. **Расчет поверхностей потенциальной энергии, функций дипольных моментов и спектроскопических характеристик O_3, CF_2, NO_2^- и NF_2^+ методом самосогласованного поля в модели полного активного пространства.** Complete active space self-consistent field potential energy surfaces, dipole moment functions, and spectroscopic properties of O_3, CF_2, NO_2^-, and NF_2^+ / Peterson Kirk A., Mayrhofer Rudolph C., Sibert Edwin L.,

М.П. ☒

+3

ф. 1991, N9

Woods R. Claude // J. Chem. Phys.— 1991.— 94, № 1. — С. 414—430.— Англ.

Неэмпирическим методом ССП МО ЛКАО в базисе гауссовых ф-ций 11*s*7*p*2*d*/7*s*4*p*2*d* с учетом корреляции электронов в модели полного активного пространства исследовано электронное строение O_3 (**I**), CF_2 (**II**), NO_2^- (**III**) и NF_2^+ (**IV**). Рассчитаны ~~поверхности~~ потенц. энергии, ~~ф-ции~~ дипольных моментов, спектроскопич. постоянные. Для **I** и **II** равновесная геометрия согласуется с эксперим. данными. Для **III** и **IV** длины связей и валентные углы найдены равными 1,260 и 1,242 Å и 116,5 и 108,0°. Ангармонич. спектроскопич. постоянные и колебательные уровни энергии рассчитаны на основании построенных аналитич. ф-ций потенц. энергии.

В. Л. Лебедев

O_3

Om 35863 1991

114: 129588z **Complete active space self-consistent field potential energy surfaces, dipole moment functions, and spectroscopic properties of ozone, difluoromethylene, nitrite, and difluoroaminylium.** Peterson, Kirk A.; Mayrhofer, Rudolph C.; Sibert, Edwin L., III; Woods, R. Claude (Dep. Chem., Univ. Wisconsin, Madison, WI 53706 USA). *J. Chem. Phys.* 1991, 94(1), 414-30 (Eng). Three-dimensional potential energy and dipole moment surfaces have been calcd. for the 24 electrons triatomics O_3, CF_2, NO_2^-, and NF_2^+ using complete active space SCF wave functions (CASSCF) and a basis set of 87 (99 for NO_2^-) contracted Gaussian-type orbitals (cGTOs). The anal. potential energy functions (PEFs) have been used in perturbation and variational calcns. of anharmonic spectroscopic consts. and vibrational energy levels. The results for O_3 and CF_2 are compared to the available exptl. data, and predictions of the rotational and vibrational spectra of NO_2^- and NF_2^+ have been made by comparison to these species. The equil. geometries of NO_2^- and NF_2^+ are predicted to be $r_e = 1.260$ Å, $\theta_e = 116.5°$ and $r_e = 1.242$ Å, $\theta_e = 108.0°$, resp. The fundamental vibrational frequencies (ν_1, ν_2, ν_3) and abs. band intensities (at 300 K) of these two ions are predicted to be 1286 cm^{-1}/31 cm^{-2} atm^{-1}, 782 cm^{-1}/13 cm^{-2} atm^{-1}, 1232 cm^{-1}/2900 cm^{-2} atm^{-1} (NO_2^-) and 1272 cm^{-1}/181 cm^{-2} atm^{-1}, 711 cm^{-1}/25 cm^{-2} atm^{-1}, 1210 cm^{-1}/1230 cm^{-2} atm^{-1} (NF_2^+). Band intensities for several low-lying vibrational transitions have been calcd. for all four species from the CASSCF dipole moment functions, and comparisons to expt. have been made for O_3 and CF_2.

расчет
структуры

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C.A. 1991, 114,
N 14

на об.

CF_2, NO_2^-, NF_2^+

O_3

1991

115: 169355y The ν_2 bands of ozone ($^{16}O^{17}O^{16}O$ and $^{16}O^{16}O^{17}O$): line positions and intensities. Rinsland, C. P.; Smith, M. A. H.; Devi, V. Malathy; Perrin, A.; Flaud, J. M.; Camy-Peyret, C. (Langley Res. Cent., NASA, Hampton, VA 23665-5225 USA). *J. Mol. Spectrosc.* 1991, 149(2), 474-80 (Eng). Using a 0.005-cm^{-1} resoln. Fourier transform spectrum of ^{17}O-enriched ozone, the first extensive anal. of the ν_2 bands of the 2 isotopic species $^{16}O^{17}O^{16}O$ and $^{16}O^{16}O^{17}O$ was performed. For each isotopic species, the IR vibration-rotation energies obtained from this anal. together with the available microwave transitions in the ground state were reproduced within their exptl. uncertainties using a Watson A-type Hamiltonian. The band centers $\nu_2(^{16}O^{17}O^{16}O) = 697.07934$ cm^{-1} and $\nu_2(^{16}O^{16}O^{17}O) = 692.43473$ cm^{-1} were obtained as well as precise rotational and centrifugal distortion consts. for both the ground state and the first vibrational state (010) of these 2 isotopic species. In addn., appropriate expansions of the transformed transition moment operators of the 2 ν_2 bands were used to generate a complete list of line positions, intensities, and lower state energy levels for the $^{16}O^{17}O^{16}O$ and $^{16}O^{16}O^{17}O$ isotopic species.

М.п.

C.A. 1991, 115, N16

O_3

1991

спектр
высокого
разрешения

116: 244101p High resolution spectroscopy of ozone. Thiebeaux, C.; Courtois, D.; Delahaigue, A.; Mouanda, J. C. (Lab. Phys. Mol., CNRS, F-51062 Reims, Fr.). *J. Phys. IV* 1991, 1(C7, Int. Conf. Laser M2P, 2nd, 1991), C7/447–C7/449 (Eng). A ten micron laser heterodyne spectrometer was developed for the purpose of investigating the frequency, intensity, and lineshape of some ozone lines. High-resoln. spectra of ozone were recorded and compared with available data.

C. A. 1992, <u>116</u>, N24

O_3

1991

115: 79292w Potential energy surfaces of ozone. I. Xantheas, Sotiris S.; Atchity, Gregory J.; Elbert, Stephen T.; Ruedenberg, Klaus (Ames Lab., USDOE, Ames, IA 50011 USA). *J. Chem. Phys.* **1991,** 94(12, Pt. 1), 8054–69 (Eng). The cross section through the ground-state potential energy surface of ozone which contains the open min., the ring min., and the ring-opening reaction path, including the ring-opening transition state, is detd. through full-valence-space multiconfiguration self-consistent-field calcns. At a point on the ridge sepg. the open-structure basin from the ring-structure basin in C_{2v} symmetry, very close to the transition state, the ground-state surface connects with the lowest excited state surface of the same symmetry ($^1A_1$). This point is part of an intersection seam between these two $^1A'$ surfaces in C_s symmetry. The upper state has its equil. structure very close to the transition state of the lower state. The quant. data of all crit. points are calcd. In addn., a ground-state potential energy surface cross section describing the detachment of an oxygen atom is detd. For several other states, C_{2v} constrained and bond-length-optimized energy curves $E(\phi)$ are also reported.

потенц. поверхности в основном и возбужд. состояниях

C.A. 1991, 115, N 8

O_3

1991

114: 235401t **A benchmark coupled–cluster single, double, and triple excitation (CCSDT) study of the structure and harmonic vibrational frequencies of the ozone molecule.** Watts, John D.; Stanton, John F.; Bartlett, Rodney J. (Dep. Chem., Univ. Florida, Gainesville, FL 32611–2085 USA). *Chem. Phys. Lett.* 1991, 178(5–6), 471–4 (Eng). We report a benchmark calcn. of the structure and harmonic vibrational frequencies of the ozone mol. using the full coupled–cluster single, double, and triple excitation model (CCSDT) with a DZP basis set. The results offer a definitive ref. for assessing the accuracy of methods which approx. the effects of the T_3 cluster operator. For the bending and sym. stretching frequencies, CCSD(T), CCSDT–2, and CCSDT–3 all give results close to CCSDT. For the asym. stretching frequency, however, the values predicted by the CCSD(T) and CCSDT–2 models are resp. about 100 cm^{-1} lower and higher than the CCSDT value, while the CCSDT–3 value exceeds the CCSDT value by 41 cm^{-1}. It is suggested that effects of connected quadruple excitations (T_4) and higher cluster operators may have a significant effect on the asym. stretching frequency.

Vi, расчет

C.A.1991, 114, N24

O_3

1991

17 Б1133. Эталонное исследование структуры и гармонических частот колебаний молекулы озона методом связанных кластеров с учетом одно-, двух- и трехкратных возбуждений (СКОДТ). A benchmark coupled-cluster single, double, and triple excitation (CCSDT) study of the structure and harmonic vibrational frequencies of the ozone molecule / Watts John D., Stanton John F., Bartlett Rodney J. // Chem. Phys. Lett.— 1991.— 178, № 5—6.— С. 471—474.— Англ.

М·Л

В двухэкспонентном базисе с поляризац. АО рассчитаны геометрич. параметры и гармонич. частоты колебаний молекулы O_3 при различных вариантах учета трехкратных возбуждений (в дополнение к одно- и двукратным) в приближении связанных кластеров. Отмечено, что молекула O_3 является достаточно сложным объектом для неэмпирич. корреляц. подходов: в нек-рых вариантах неправильно предсказывается порядок частот симм. и антисим. колебаний или даже получаются

Х.1991, №17

мнимые частоты. Несмотря на очевидную неполноту базиса полученные в варианте полного учета трехкратных возбуждений х-ки молекулы O_3 хорошо согласуются с эксперим. данными (приведены в скобках): $R_e = 1{,}286$ A (1,272), $Q_e = 116{,}7°$ (116,8), $\omega_1 = 1141$ см$^{-1}$ (1135), $\omega_2 = 705$ (716), $\omega_3 = 1077$ (1089). Отмечено, что наибольшее влияние оказывают высшие поправки метода связанных кластеров на частоту антисимм. колебания ω_3. А. В. Немухин

O_3

1991

12 Д86. Поверхности потенциальной энергии озона. I. Potential energy surfaces of ozone. I / Xantheas S. S., Atchity G. J., Elbert S. T., Ruedenberg K. // J. Chem. Phys.— 1991.— 94, № 12, Pt 1.— С. 8054—8064.— Англ.

Неэмпирическим методом МК ССП (полное конфигурац. пространство для валентных орбиталей) в базисе гауссовых ф-ций с включением поляризационных ф-ций исследована поверхность потенц. энергии O_3 в основном состоянии. Найдены и охарактеризованы минимумы, отвечающие циклической и ациклич. структурам, пути размыкания цикла и диссоциации на O_2+O и $O_2+1/2\,O_2$. Обнаружено, что вблизи переходного состояния от циклической к ациклич. структуре поверхность связана с поверхностью возбужденного состояния той же симметрии. Также рассчитаны сечения поверхности для основного состояния, отвечающие прилипанию атома O.

М.П.

ф. 1991, №12

O_3

1992

7 7Д125. Квинтетные электронные состояния в спектроскопии озона. Quintet electronic states in the spectroscopy of ozone / Banichevich A., Peyerimhoff S. D., Grein F. // Chem. Phys. Lett. .— 1992 .— **195** , № 5—6 .— С. 459—468 .— Англ.

Неэмпирическим методом ССП МО ЛКАО в базисе 10s6p1d/6s4p1d с дополнительной s-ф-цией между каждой парой атомов O с учетом конфигурационного взаимодействия исследовано электронное строение O_3 в квинтетных электронных состояниях. Приведены потенциальные кривые, энергии ионизации, обсуждены механизмы диссоциации на O_2+O. Обнаружено, что состояния 1 $^5A''$, 1 $^5A'$ и 2 $^5A'$ являются отталкивательными и диссоциируют на $O(^2P_g)+O_2(X^3\Sigma_g)$, а более высоколежащие $2^5A''$, $3^5A''$ и 3 $^5A'$ являются слабо связанными и диссоциируют на $O(^3P_g)+O_2(A'^3\Delta_u)$. На основании полученных результатов обсуждена фотохимия озона в атмосфере.

М.П.

Ф. 1993, N 7

$^{16}O_3$

1992

5 Б1157. Длинноволновая инфракрасная спектроскопия с перестраиваемым лазером озона $^{16}O_3$. Tunable far infrared spectroscopy of $^{16}O_3$ ozone /Bellini M., De Natale P., De Lonardo G., Fusina L., Inguscio M., Prevedelli M. //J. Mol. Spectrosc. .—1992 .—**152** ,№ 1 .—С. 256—259 .—Англ.

С использованием микроволновой техники, с высокой точностью измерены 63 вращат. линии молекулы озона в области 1,5—4,1 ТГц. Обработка велась на основе гамильтониана уатсоновского типа, получен большой ряд молек. параметров. Л. В. Серебренников

М. П.

Х. 1994, N5

$^{16}O_3$

1992

116: 115927p Tunable far infrared spectroscopoy of $^{16}O_3$ ozone. Bellini, M.; De Natale, P.; Di Lonardo, G.; Fusina, L.; Inguscio, M.; Prevedelli, M. (Eur. Lab. Nonlinear Spectrosc., 50125 Florence, Italy). *J. Mol. Spectrosc.* 1992, 152(1), 256–9 (Eng). An investigation of the far-IR spectra of $^{16}O_3$ gave 63 pure rotational lines in the spectral region 1.5–4.1 THz with Doppler-limited resoln. and ~50 kHz accuracy. Simultaneous anal. of those lines together with all the ground-state transition frequencies reported in the literature gave 2 sets (for *S*- and *A*-reduced Hamiltonians) of rotational and centrifugal distortion consts.

ИК спектр,
м.п.

С. А. 1992, 116, N 12

O_3

1992

7 Б1083. Колебательные частоты озона: многоконфигурационный подход. Vibrational frequencies of ozone: A multiconfigurational approach /Borowski P., Andersson K., Malmqvist P.-Á., Roos B. O. //J. Chem. Phys .—1992 .—**97** № 8 .—С. 5568—5577 .—Англ.

Проведены расчеты основного состояния молекулы озона с использованием ряда одноконфигурац. и многоконфигурац. методов. Исследовано влияние метода учета корреляц. эффектов и выбора базиса на описание равновесной геометрии и колебат. частот. Лучшие результаты достигнуты при использовании метода конфигурац. вз-вия с 27 исходными конфигурациями, а также метода ССП в полном активном пространстве совместно с теорией возмущений Меллера—Плессета второго порядка. Библ. 58.

А. А. Сафонов

М.П.

Х.1993, N 7

O_3

1992

117: 240136b Vibrational frequencies of ozone: a multiconfigurational approach. Borowski, P.; Andersson, K.; Malmqvist, P. A.; Roos, B. O. (Chem. Cent., Univ. Lund, S-221 00 Lund, Swed.). *J. Chem. Phys.* 1992, 97(8), 5568–77 (Eng). The electronic ground state of ozone and, in particular, its equil. geometry and harmonic vibration frequencies were studied by a variety of multiconfiguration and single-configuration methods. The antisym. stretch frequency cannot be correctly obtained by single-ref. methods unless at least triple excitations are included. Basis-set effects must be taken into account since the ω_3 frequency is very sensitive to computational details. The multiconfiguration methods give good results provided that an adequate configuration space is used. The second-order complete active space perturbation method performs very satisfactorily. Traditional multireference CI (MRCI) methods, using a few ref. functions, do not perform so well. A two-ref. CI is able to give reasonable results, but only when the orbitals were prepd. by some properly correlated method. Adding several ref. functions gives small improvements, and the result is dependent on the type of ref. functions included. It is far more important to include a large no. of diverse configurations in the ref. than to treat the remaining dynamical correlation accurately.

структурн-
параметры,
Di, теорет-
расчет

C. A. 1992, 117, N 24

O_3

1992

118: 48220d **Improved spectroscopic line parameters for the ozone molecule.** Flaud, J. M.; Camy-Peyret, C.; Perrin, A.; Rinsland, C. P. (Lab. Phys. Mol. Appl., Univ. Pierre et Marie Curie, 75252 Paris, Fr.). *J. Quant. Spectrosc. Radiat. Transfer* 1992, 48(5-6), 611-15 (Eng). A summary of the O_3 line parameters is presented. The present status is first described, covering line positions, line intensities and linewidths, both for the main isotopic species $^{16}O_3$ and the isotopic variants $^{16}O^{18}O^{16}O$ and $^{16}O^{16}O^{18}O$. The second part of the paper deals with needed future studies.

(спектр)

C.A. 1993, 118, N 6

$^{16}O^{17}O^{16}O$ (Om · 37354) 1992

(ν_1, ν_3)

117: 200803k The ν_1 and ν_3 bands of oxygen-17-labeled ozone $^{16}O^{17}O^{16}O$ line positions and intensities. Heyart, M.; Perrin, A.; Flaud, J. M.; Camy-Peyret, C.; Rinsland, C. P.; Smith, M. A. H.; Devi, V. Malathy (Lab. Phys. Mol. Appl., Univ. Pierre et Marie Curie, 75252 Paris, Fr.). *J. Mol. Spectrosc.* 1992, 156(1), 210–16 (Eng). Using 0.005-cm^{-1} resoln. Fourier transform spectra of ^{17}O-enriched ozone, the ν_1 and ν_3 bands of $^{16}O^{17}O^{18}O$ were extensively analyzed, leading to the detn. of precise vibrational energies and rotational and coupling consts. The following band centers were derived: $\nu_0(\nu_1) = 1087.82895$ cm^{-1}, $\nu_0(\nu_3) = 1024.39553$ cm^{-1}. The line intensities were calcd. by transferring the dipole moment of $^{16}O_3$ to $^{16}O^{17}O^{16}O$, and finally a complete list of line positions and intensities of the ν_1 and ν_3 bands of $^{16}O^{17}O^{16}O$ has been generated.

C.A.-1992, 117, N20

O_3

1992

118: 11363x MC-SCF/MCLR studies of potential energy surfaces, spectra, and properties of the X^1A_1 and a^3B_2 states of ozone. [Erratum to document cited in CA115(18):190249b]. Nordfors, David; Aagren, Hans; Joergen, Hans; Jensen, A. (Inst. Quantum Chem., Univ. Uppsala, S-751 20 Uppsala, Swed.). *Int. J. Quantum Chem.* 1992, 44(3), 413 (Eng). An error in Table VII has been cor. The error was not reflected in the abstr. or the index entries.

(X^1A_1 и a^3B_2,
потенц. ф-ии
и св-ва,
теор. расчет)

C. A. 1993, 118, N2

O_3

1992

116: 161441y **Photoacoustic spectroscopy of ozone with a 450-MHz tunable waveguide carbon dioxide laser.** Sokabe, Noburu; Hammerich, Mads; Pedersen, Thorvald; Olafsson, Ari; Henningsen, Jes (Phys. Lab., H. C. Oersted Inst., Copenhagen, DK-2100 Den.). *J. Mol. Spectrosc.* 1992, 152(2), 420-33 (Eng). Photoacoustic absorption signatures have been obtained for ozone in 450-MHz tuning windows of a waveguide CO_2 laser. Out of 42 obsd. absorption lines, 31 are assigned to the ν_1 and the ν_3 bands, and 7 to various hot bands of $^{16}O^{16}O^{16}O$. Two lines are assigned to the ν_3 band of the isotopomers $^{16}O^{16}O^{18}O$ and $^{16}O^{18}O^{16}O$, which were present in their natural abundance. Precise collision broadening measurements are reported for two lines of the $^{16}O^{16}O^{16}O$ ν_3 band.

(Pi)

C.A. 1992, 116, N 16

O_3

1992

16 Б1155. Полосы ν_3 и ν_1 изотопных модификаций озона $^{17}O^{16}O^{16}O$ и $^{16}O^{17}O^{16}O$. Положение и интенсивности линий. The ν_3 and ν_1 bands of the $^{17}O^{16}O^{16}O$ and $^{16}O^{17}O^{16}O$ isotopic speciems of ozone: line positions and intensities /Perrin A., Heyard M., Flaud J.-M., Camy-Peyret C., Rinsland C. P., Smith M. A. H., Devi V. Malathy //47th Ohio State Univ. Int. Symp. Mol. Spectrosc., Columbus, Ohio, June 15—19, 1992 .—Columbus (Ohio), 1992 .—С. 141 .—Англ.

При комнатной т-ре, в области 10 мкм с высоким разрешением (0,005 см$^{-1}$, фурье-спектрометр) измерена вращат. структура полос ν_3 и ν_1 в ИК-спектре поглощения озона частично замещенного по изотопу ^{17}O. Положение начал полос (в см$^{-1}$): $^{16}O^{17}O^{16}O$ — $\nu_0(\nu_1 = 1095,69309$ (полоса B-типа), $\nu_0(\nu_3) = 1035,35869$ (полоса A-типа); $^{17}O^{16}O$-^{16}O — $\nu_0(\nu_1 = 1087,82895$, $\nu_0(\nu_3) = 1024,39553$ (гибридные полосы A- и B-типа). Эксперим. данные по положению

М.Л.

Х. 1993, N16

вращат. подуровней вз-вующих колебат. состояний ($\nu_1=1,0,0$) и ($0,0,\nu_3=1$) удовлетворительно описываются с учетом кориолисовых вз-вий для $^{16}O^{17}O^{16}O$ (симметрия молекулы C_{2v}), кориолисовых вз-вий и вз-вия Ферми для $^{17}O^{16}O^{16}O$ (симметрия молекулы C_s). С использованием ф-ции дипольного момента молекулы $^{16}O_3$ рассчитаны интенсивности линий для $^{16}O^{17}O^{16}O$, к-рые затем использованы для оценки содержания этого изотопомера в смеси и определения интенсивностей 70 линий полос ν_1 и ν_3 изотопомера $^{17}O^{16}O^{16}O$. В. М. Ковба

O_3 1992

Rinsland C.P., Goldman A., et al.,

47th Ohio State Univ. Int. Symp. Mol. Spectrosc., Columbus, Ohio, June 15-19, 1992. — Columbus (Ohio) 1992. — С 142

М.Л.

Р.Ж.Х. № 12, 1993, 12 Б 1183

O_3 1992

Braunstein M., Pack R.T.,

J. Chem. Phys., 1992, 96, N9,
м.л. 6378-6388.

р.ж.Х.N 12, 1993, 12Б1021

O_3

1992

Yu Dake, Rauk Arvi, et al.

(Ab, теор. расчёт) термод. св-ва $C_p^\circ, S^\circ, H^\circ - H^\circ_0$, $\Delta_f H$, $\Delta_f G$

J. Phys. Chem. 1992, <u>96</u> (14), 6031-8.

●

(см. N_3 i $\hat{\underline{III}}$)

O_3

1993

121: 118060q The global potential energy surfaces of the lowest two $^1A'$ states of the ozone molecule: Theoretical determination and analysis. Atchity, G. J. (Ames Lab., Ames, IA USA). *Report* 1993, IS-T-1217; Order No. DE93007537, 264 pp. (Eng). Avail. NTIS. From *Energy Res. Abstr.* 1993, 18(6), Abstr. No. 18168. The two lowest 1A' potential energy surfaces of the ozone mol. are detd. and analyzed using accurate ab-initio MCSCF calcns. The shape-scale perimetric coordinates for triat. mols. are discussed and further developed. Because the previously detd. intersection between these two surfaces of like symmetry is unusual, much of the present work involves this intersection. The relevant theory of intersections is reviewed, and a method for characterizing intersections according to the topol. of the surfaces in their vicinity is developed. The reasons for this particular crossing in ozone are investigated. The intersection point in C_{2v} symmetry is part of a larger, 1-dimensional intersection seam in C_s symmetry. This seam is shown to consist of four branches. A new method for detg. an intersection point in a two-dimensional coordinate space, based on

потенц. поверх-
ности двух
$^1A'$ состоян.,
теорет. расч

C.A. 1994, <u>121</u>, N10

the wavefunction phase–charge theorem of Herzberg–Longuet–Higgins, is also developed. Finally, global mappings of the two potential energy surfaces in the scale–shape perimetric coordinates are detd. The min. of the two surfaces, their dissocn. and rearrangement paths,and the map of the energy difference between them are all discussed. It is shown that direct formation of the ring structure of ozone from O_2 and O is improbable, and that there is no rearrangement pathway on the ground state representing the inter–change of two atoms.

O_3

1993

119: 105061z **Theoretical study of the ground and excited states of ozone in its symmetric nuclear arrangement.** Banichevich, Antonio; Peyerimhoff, Sigrid D. (Institut fuer Physikalische und Theoretische Chemie, Universitaet Bonn, Wegelerstrasse 12, W-5300 Bonn, 1 Germany). *Chem. Phys.* 1993, 174(1), 93-109 (Eng). Potential energy surfaces for the ground state X^1A_1 and the first twelve states of the ozone mol. have been detd. for the sym. arrangement of nuclei employing the multireference CI (MRD-CI) treatment in a [6s, 4p, 1d]+[1s$_b$, 1p$_b$] contracted Gaussian basis. Calcns. were carried out for a two-dimensional grid of points varying the internuclear angle γ and the bond length R to obtain the optimum geometrical parameters R and γ for all states treated. Special emphasis was placed on the interaction of states. The well-known double min. potential of the X^1A_1 state in the sym. arrangement of nuclei is computed. The 2^1A_1 state, possibly responsible for the weak absorption in the Huggins band (3.44-4.13 eV), is found to exhibit a double min. outside of the Franck-Condon region suggesting that a vertical transition reaches the repulsive branch of the potential. The transition moments from the ground

Осн. X^1A_1 и
возб. 1^3A_2 и 1^3B_2

C.A. 1993, 119, N 10

state to the three lowest electronic states are also presented for many grid points. The lowest 1^3A_2 and 1^3B_2 states are found to have an adiabatic excitation energy (0.86 and 1.10 eV, resp.) below the dissocn. energy (D_e = 1.13 eV). The high-lying triplet state 2^3B_1 also shows a double min., whereby the abs. min. occurs at linear geometry. The min. energy paths for C_{2v} dissocn. in the X^1A_1 state in higher states (at the X^1A_1 optimized geometrical values) are calcd.; their correlation to the C_{2v} dissocn. channels is discussed.

O_3

1993

120: 62941n Potential energy surfaces of ozone in its ground state and in the lowest-lying eight excited states. Banichevich, Antonio; Peyerimhoff, Sigrid D.; Grein, Friedrich (Institut fuer Physikalische und Theoretische Chemie, Universitaet Bonn, Wegelerstrasse 12, 53115 Bonn, Germany). *Chem. Phys.* 1993, 178(1-3), 155-88 (Eng). Potential energy surfaces of the ground state and the lowest eight excited states of ozone which correlate with the three fragmentation limits $O(^3P_g)+O_2(X^3\Sigma^-_g)$, $O(^3P_g)+O_2(a^1\Delta_g)$ and $O(^1D_g)+O_2(a^1\Delta_g)$ are calcd. employing multireference CI (MRD-CI) treatments in a Gaussian AO basis. Vertical and adiabatic transition energies as well as dissocn. energies based on the optimized energy surface are presented. The transition moments between the ground state and the excited singlet states are also computed as a function of geometry and are employed to simulate Wulf, Chappuis and Huggins absorption bands. Some aspects about ozone predissocn. and photodissocn. and its formation are discussed.

поверхность
потенц.
энергии

C.A. 1994, 120, N6

O_3

1993

120: 89632z **The $3\nu_3 + 2\nu_2$ band of ozone: line positions and intensities.** Barbe, A.; Bouazza, S.; Plateaux, J. J.; Jacon, M. (GSMA, Fac. Sci., 51062 Reims, Fr.). *J. Mol. Spectrosc.* 1993, 162(2), 335–41 (Eng). The $3\nu_3 + 2\nu_2$ band of O_3 appearing in the 4325 cm^{-1} region has been obsd. for the first time using the FTS of Reims (resoln., 0.004 cm^{-1}) and a very large pl (pressure × pathlength) product: 50 Torr × 36 m. This band has been analyzed using the Watson-type Hamiltonian, including the Coriolis resonance with the $\nu_1 + 2\nu_2 + 2\nu_3$ band. Transitions have been obsd. up to $J = 35$ and $K_a = 11$, the max. absorption being 10% for the most intense line (5×10^{-25} cm^{-1}/mol.-cm^{-2}). A few levels have been found to be slightly perturbed. The perturbing levels have been identified: they belong to the 400 vibrational level, the $4\nu_1$ being much too weak to be obsd. without this perturbation. Furthermore, 64 line intensities have been used and led to the transformation transition moment. Fits for both energy levels and intensities are satisfactory. Finally, a complete list of line positions, intensities, and lower state energies has been generated for the $3\nu_3 + 2\nu_2$ band of $^{16}O_3$.

$(2\nu_3 + 2\nu_2)$

C.A.1994, <u>120</u>, N8

$^{16}O_3$

1993

119: 148735q The $3\nu_1$ and $\nu_1 + 3\nu_3 - \nu_2$ absorption bands of ozone oxygen-16. Bouazza, S.; Barbe, A.; Plateaux, J. J.; Flaud, J. M.; Camy-Peyret, C. (Groupe Spectrosc. Mol. Atmos., Univ. Reims, 51062 Reims, Fr.). *J. Mol. Spectrosc.* **1993,** 160(2), 371–7 (Eng). Using a high-pressure × path length sample of ozone it has been possible to record at high resoln. (0.006 cm^{-1}) the 3-μm absorption region of this mol. A thorough anal. of the spectra has been performed allowing one to assign for the first time the $3\nu_1$ band of $^{16}O_3$. Also, during the course of the anal. it became clear that, in this spectral region, another band almost as strong as $3\nu_1$ was absorbing: it is the $\nu_1 + 3\nu_3 - \nu_2$ hot band. The (300) rotational levels were reproduced together with the (003), (102), and (201) ones [J. Mol. Spectrosc. 141, 134–144 (1990)] using a Hamiltonian matrix which takes explicitly into account the Darling-Dennison and the Coriolis interaction terms affecting the levels. The band centers $\nu_0(3\nu_3) = 3046.0878$, $\nu_0(\nu_1 + 2\nu_3) = 3083.7030$, $\nu_0(2\nu_1 + \nu_3) = 3186.4110$, and $\nu_0(3\nu_1) = 3289.9297$ cm^{-1} were derived as well as precise rotational and coupling consts. Line intensities were also measured for $3\nu_1$ as well as for $\nu_1 + 3\nu_3 = \nu_2$ and were reproduced with suitable transition moment operators. Finally a complete line list of the bands of $^{16}O_3$ absorbing around 3 μm has been generated.

$(3\nu_1, \nu_1+3\nu_3-\nu_2$

C.A.1993, <u>119</u>, N14

O_3 (г, матриц)

1993

118: 263000n Analysis of IR absorption spectrum of ozone in inert matrixes: spectroscopic evidence for two trapping sites. Brosset, P.; Dahoo, R.; Gauthier-Roy, B.; Abouaf-Marguin, L.; Lakhlifi, A. (Laboratoire de Physique Moleculaire et Applications du CNRS, Universite P. et M. Curie, Tour 13, Boite 76, 4 place Jussieu, 75252 Paris, 05 Fr.). *Chem. Phys.* 1993, 172(2–3), 315–24 (Eng). The IR spectra of solid O_3 and of O_3 trapped in rare gas and nitrogen matrixes are analyzed, mainly with $^{16}O_3$, a few expts. being performed with ^{18}O-substituted species. The ν_3 mode appears as a doublet except in solid nitrogen. The intensity ratio between the two components is dependent upon the deposition temp. This gives evidence for two trapping sites. In the ν_2 region, the spectrum exhibits a narrow line and a structure of two weaker lines which can be assigned to monomeric O_3. The two ν_3 components show a very different temp. dependence: one broadens as soon as 15 K, while the effect is significant for the second one only at 25 K. The different hypotheses for the trapping sites are discussed, and the reversible temp. broadening of the ν_3 lines is tentatively explained through a phonon-assisted vibrational energy transfer from the ν_3 mode to the lowest one ν_2.

ИК спектр поглощен.

C.A. 1993, 118, N26

O_3

1993

Farantos Stavros C.

Laser. Chem. 1993,
<u>13</u>(2), 87-99.

теор.
расчёт
потенц.
ф-ций

(см. SO_2 ; $\underline{III}$)

O_3

1993

119: 148736r Line parameters for ozone hot bands in the 3.3-μm spectral region. Flaud, J. M.; Camy-Peyret, C.; Perrin, A.; Devi, V. Malathy; Barbe, A.; Bouazza, S.; Plateaux, J. J.; Rinsland, C. P.; Smith, M. A. H.; Goldman, A. (Lab. Phys. Mol. Appl., Univ. Pierre et Marie Curie, 75252 Paris, Fr.). *J. Mol. Spectrosc.* **1993**, 160(2), 378–86 (Eng). Line positions, intensities, and lower state energies were calcd. for 8 hot bands of $^{16}O_3$ in the 3.3-μm spectral region. The results are based on spectroscopic parameters deduced in recent high-resoln. lab. studies and improved rotational energy levels of the (103), (004), and (310) vibrational states derived by refitting earlier data and exptl. (004) energy levels from measurements of the $4\nu_3 - \nu_3$ hot band. The good quality of the new parameters was verified through comparisons of line-by-line simulations with high-resoln. lab. spectra. The present work and the results of the analyses of the main bands at 3.6 μm [Smith et al., J. Mol. Spectrosc. 139, 171–181(1990)] and 3.3 μm [Camy-Peyret et al., J. Mol. Spectrosc. 141, 134–144(1990)] provide a complete set of ozone spectroscopic line parameters covering the 3-μm region.

(область 3.3мкм)

C.A. 1993, 119, N 14

O_3

1993

F: O3
P: 3

8Б133. О теоретическом определении сродства озона к электрону. On the theoretical determination of the electron affinity of ozone / Gonzalezluque R., Merchan M., Borowski P., Roos B. O. // Theor. chim. acta. - 1993. - 86, N 6. - C. 467-476. - Англ.

Р.Ж.Х. N 8, 1996

ν_3

1993

118: 69217y **The hybrid-type bands ν_1 and ν_3 of ozone $^{16}O^{16}O^{17}O$ line positions and intensities.** Heyart, M.; Perrin, A.; Flaud, J. M.; Camy-Peyret, C.; Rinsland, C. P.; Smith, M. A. H. (Lab. Phys. Mol. Appl., Univ. Pierre et Marie Curie, 75252 Paris, Fr.). *J. Mol. Spectrosc.* 1993, 157(2), 524-31 (Eng). A study of 0.005 cm^{-1} resoln. room temp. absorption spectra of ^{17}O-enriched ozone around 10 μm was performed leading to a thorough anal. for the hybrid ν_1 and ν_3 bands of $^{16}O^{16}O^{17}$. The exptl. rotational levels of the interacting states (001) and (100) were reproduced using a Hamiltonian taking fully into account the rovibrational interactions. Precise vibrational energies and rotational and coupling consts. were deduced and the following band centers were detd.: $\nu_0(\nu_1) = 1095.69309$ cm^{-1} and $\nu_0(\nu_3) = 1035.35869$ cm^{-1}. Using the $^{16}O^{17}O^{16}O$ line intensities calcd. previously and assuming a factor of 2 between the abundances of $^{16}O^{16}O^{17}O$ and $^{16}O^{17}O^{16}O$, the amt. of $^{16}O^{16}O^{17}O$ in the cell was evaluated and used to derive the line intensities for this latter species. Then the exptl. intensities were least squares fitted, leading to the detn. of the transition moment consts. of the ν_1 and ν_3 bands of $^{16}O^{16}O^{17}O$. Finally, a complete spectrum of these bands was computed.

(ν_1, ν_3)

C.A. 1993, 118, N 8

O_3

1993

(ик в матрице)

119: 281163t **Interpretation of the infrared spectrum of ozone trapped in inert matrixes.** Lakhlifi, A.; Girardet, C.; Dahoo, R.; Brosset, P.; Gauthier-Roy, B.; Abouaf-Marguin, L. (Laboratoire de Physique Moleculaire, URA CNRS 772, UFR Sciences, Universite de Franche-Comte, 25030 Besancon, Fr.). *Chem. Phys.* **1993**, 177(1), 31-44 (Eng). The IR spectrum of O_3 trapped in rare gas crystals is interpreted on the basis of 2 trapping sites, the single and double substitutional sites in which the mol. experiences nearly the same total energy, but its orientational motions are different. In the single cage, the direction of the larger dimension of the mol. librates about the C_4 axis of the site, which is the only restriction to the proper rotation; in the double cage, the only motions are librational. The model then explains the occurrence at low temp., for the ν_3 mode in both sites, of 1 sharp signal corresponding to a Q line, whereas the ν_2 mode appears as a weak hindered rotational structure in the single site and as a single sharp Q line in the double site. Calcns. are furthermore performed to det. the width of the ν_2 and ν_3 peaks and to analyze the various processes responsible for the different behavior of the broadening of the 2 ν_3 signals as temp. rises. The one- and two-phonon inelastic collisional processes contribute in a different way to the broadening mechanism of the ν_3 peak profiles.

C.A. 1993, 119, N 26

O_3 1993

Павлюченко А. И.

м.п.,

Де

Ж. прикл. спектроскопии. 1993. 58, №3-4. С. 358-365.

(см. H_2O; III)

O_3

1993

24 Б1118. Поиск узловых структур для C_{2v}- и D_{3h}-изомеров озона с помощью метода МП4(ОДТЧ) и анализа многочастичного разложения. MP4SDTG search for nodal structures combined with multibody expansion analysis for C_{2v}-isomers and D_{3h} isomers of ozone / Shalabi A. S., Elmisiery A. E. M. // J. Mol. Struct. Theochem .— 1993 .— **100** , № 1 .— С. 1—9 .— Англ.

М·П

Х. 1995, N 24

O_3

1993

120: 173867n An SCF–CI study of highly excited vibrational states of bent triatomic molecules and its application to O_3. Xie, Daiqian; Yan, Guosen; Xie, Junkai; Tian, Anmin (Dep. Chem., Sichuan Univ., Chengdu, Peop. Rep. China 610064). *Chin. Chem. Lett.* 1993, 4(2), 175–8 (Eng). An SCF–CI procedure for studying highly excited vibrational states of bent triat. mols. is suggested and applied to the O_3 mol.

высокие возбужд.
колебательн.
состояния,
теор. расчет

C. A. 1994, 120, N 14

O_3

1993

119: 103741x Anion-radical and protonated forms of molecular ozone. Ab initio calculation taking into the electronical correlation. Zakharov, I. I.; Kolbasina, O. I.; Semenyuk, T. N.; Tyupalo, N. F.; Zhidomirov, G. M. (Inst. Katal., Russia). *Zh. Strukt. Khim.* 1993, 34(2), 28–32 (Russ). The MP4 method in a 4-31G(d,p) basis was used to calcd. the electronic states of O_3 ($^1A_1$, $^3B_2$, $^3A_2$, $^3B_1$, and 2^1A_1) as well as the geometry of O_3^- and O_3H^+. The proton affinity of O_3 is 6.8 eV, 1 eV less than that of H_2O.

Структура,
стабильн.,
теор. расчет

O_3^-, O_3H^+

⑫ ☒

C. A. 1993, 119, N 10

O_3

1993

7 Д124. Анион-радикальная и протонированная форма молекулярного озона. Неэмпирический расчет с учетом электронной корреляции / Захаров И. И., Колбасина О. И., Семенюк Т. Н., Тюпало Н. Ф., Жидомиров Г. М. // Ж. структур. химии .— 1993 .— 34 , № 2 .— С. 28—32 .— Рус.

Неэмпирическим методом в базисе 4-31 G(d, p) с учетом электронной корреляции по теории возмущений Меллера — Плессета четвертого порядка рассчитаны электронные состояния озона $^1A_1$, $^3B_2$, $^3A_2$, $^3B_1$ и 2^1A_1. Рассчитана геометрическая структура ионов O_3 и O_3H^+. Оценка сродства к протону для O_3 дает величину 6,8 эВ, что на 1 эВ меньше, чем для H_2O.

М.1.

(Н) △

Ф 1993, N 7

O_3

1994

V **10 Б1228. Высокоточное измерение колебательных полос спектров комбинационного рассеяния озона, возбуждаемых при 266 и 270 нм.** High-accuracy measurement of vibrational Raman bands of ozone at 266 and 270 nm excitations /Chang Bor-Yu, Kung Chung-Yi, Kittrell Carter, Hsiao Chin-Wei, Johnson Bruce R., Glogover Stella G., Kinsey James L. //J. Chem. Phys. .— 1994 .— **101** ,№ 3 .— С. 1914—1922 .— Англ.

Измерены спектры резонансного комбинационного рассеяния озона (Δν до 11 000 см$^{-1}$), возбуждаемые при 266 и 270 нм. Приведено положение и отнесение наблюдаемых в спектрах полос, основная часть которых может быть представлена в рамках двухосцилляторной модели Дарлинга-Деннисона (ДД). Значения полученных спектроскопических параметров (в см$^{-1}$): $\omega_1 = 1107{,}40$, $\omega_3 = 1054{,}43$, $x_{11} = -4{,}99858$, $x_{33} = -10{,}0910$, $x_{13} = -38{,}6340$, $\gamma = -30{,}8666$ (γ — параметр взаимодействия ДД). На базе новых экспериментальных данных построена аналитическая двумерная поверхность потенциальной энергии и приведены ее параметры. Библ. 39. В. М. Ковба

ll·Л-

Х·1995, N10

O_3

1994

121: 216220m **High-accuracy measurements of vibrational Raman bands of ozone at 266 and 270 nm excitations.** Chang, Bor Yu; Kung, Chung Yi; Kittrell, Carter; Hsiao, Chih Wei; Johnson, Bruce R.; Glogover, Stella G.; Kinsey, James L. (Rice Quantum Inst., Rice Univ., Houston, TX 77251 USA). *J. Chem. Phys.* **1994**, 101(3), 1914–22 (Eng). Resonance Raman spectra of ozone at two excitation wavelengths (266 and 270 nm) have been measured up to 11,000 cm^{-1}. Band origins have been measured to high accuracy and detd. to within a few cm^{-1}. Several band beyond the dissocn. limit have been obsd. All prominent bands obsd. in this work fit to a two-oscillator Darling–Dennison model. An anal. two-dimensional potential energy surface has been constructed based on the new exptl. data.

(СКР)

С.А.1994, 121, N18

$^{17}O_3$

1994

122: 172891v Rotational spectrum of the $^{17}O_3$ isotopomer of ozone. Colmont, Jean-Marcel (UA CNRS, Universite de Lille I, Fr.). *J. Mol. Spectrosc.* **1994**, 168(2), 621-3 (Eng). Rotational spectra of $^{17}O_3$ isotopomer of ozone were investigated over the range from 50 to 395 GHz using a millimeter wave spectrometer with super heterodyne detection and a source-modulated submillimeter wave spectrometer. A total of 93 transition with $2 \leq J \leq 46$ and $0 \leq K_a \leq 8$ have been assigned. The transitions were fitted in a least-squares procedure using Watson's A-type Hamiltonian expressed in the I^r representation.

Вращат-
спектр

C.A. 1995, 122, N 14

$^{17}O_3$

1994

121: 310687r The 10-μm bands of the $^{17}O_3$ isotopic species of ozone. Consalvo, D.; Perrin, A.; Flaud, J. M.; Camy-Peyret, C.; Valentin, A.; Chardonnet, Ch. (Lab. Phys. Laser, Univ. Paris XIII, F-94430 Clement, Fr.). *J. Mol. Spectrosc.* 1994, 168(1), 92-8 (Eng). Using high-resoln. (R ~ 0.002 cm^{-1}) Fourier transform spectra of ozone contg. about 20% of $^{17}O_3$ isotopic species, it has been possible to observe and assign the $\{\nu_1,\nu_3\}$ bands of $^{17}O_3$ up to very high rotational quantum nos. For this anal., we used the ground state energy levels calcd. form the (000) rotational consts. obtained for $^{17}O_3$ in a recent microwave study performed by J.-M. Colmont (submitted for publication). Then, from the {(100), (001)} rotational energy levels derived in the present work, a set of mol. parameters (vibrational band centers and rotational and coupling consts.) for the {(100), (001)} interacting states of $^{17}O_3$ has been detd. using a Hamiltonian matrix which explicitly takes into account the (100) ↔ (001) Coriolis interaction. Finally, using transition moments derived theor. from those of $^{16}O_3$, a synthetic spectrum (line positions and intensities) of the ν_1 and ν_3 bands has been generated.

Фурье спектр,
ν_1, ν_3

C.A. 1994, 121, N 26

O_3

1994

$(\nu_1 + \nu_3)$

121: 68382y **The $\nu_1 + \nu_3$ bands of $^{16}O^{18}O^{16}O$ and $^{16}O^{16}O^{18}O$.** Flaud, J. M.; Bourgeois, M. T.; Barbe, A.; Plateaux, J. J.; Camy–Peyret, C. (Lab. Phys. Mol. Appl., Univ. Pierre et Marie Curie, 75252 Paris, Fr.). *J. Mol. Spectrosc.* **1994,** 165(2), 464–9 (Eng). Using 0.003 cm^{-1} resoln. Fourier transform spectra of ^{18}O–enriched ozone around 4.8 μM, the first high–resoln. anal. of the $\nu_1 + \nu_3$ bands of $^{16}O^{18}O^{16}O$ and $^{16}O^{16}O^{18}O$ has been performed. The exptl. rotational energy levels were reproduced satisfactorily with the aid of a Hamiltonian model taking fully into account the vibration–rotation interactions. Indeed, it did not prove possible to fit properly the (101) levels without those of (002) and (200) and the Darling–Dennison interaction coupling the levels of (002) with those of (200). In this way reliable vibrational energies and rotational and coupling consts. were deduced with the following band–centers: $\nu_0(\nu_1 + \nu_3)$ = 2049.3694 cm^{-1} for $^{16}O^{18}O^{16}O$, and $\nu_0(\nu_1 + \nu_3)$ = 2090.3406 cm^{-1} for $^{16}O^{16}O^{18}O$.

C. A. 1994, 121, N6

O_3

1994

122: 41018t **Infrared and microwave spectroscopy of ozone: Historical aspect.** Ivanov, S. V.; Panchenko, V. Ya. (Scientific Research Center Technological Lasers (NICTL), Russian Academy Sciences, Troitsk, Russia 142092). *Usp. Fiz. Nauk* **1994,** 164(7), 725–42 (Ger). The evolution of IR and microwave (vibrational–rotational) ozone spectroscopy from the mid–19th century up to the present is reviewed with 254 refs. and the development of both linear and nonlinear spectroscopy is considered. Where necessary the allied fields of ozone physics and chem. (monitoring in the atm., laser stimulation of chem. reactions, study of relaxation processes, etc.) are touched on. The current state of vibrational–rotational ozone spectroscopy is evaluated and the prospect of its future development is discussed.

ИК, МВ
спектр.,
обзор

С.А. 1995, 122, N4

O_3 1994

121: 240874y Comment on "Potential energy surfaces of ozone in its ground state and in the lowest-lying eight excited states". Joens, Jeffrey A. (Department of Chemistry, Florida International University, Miami, FL 33199 USA). *Chem. Phys. Lett.* 1994, 227(6), 688–9 (Eng). A polemic. The suggestion by Banichevich, Peyerimhoff, and Grien (Chem. Phys. 178 (1993) 155) that two weak absorption bands of ozone previously assigned as belonging to the Huggins system might be members of the Chappuis system is shown to be contrary to available evidence. The original assignment of these bands as belonging to the Huggins system is shown to be correct.

Ф-ии потенц. энергии в осн. к возб. сост.

С.А. 1994, <u>121</u>, N20

O_3

1994

120: 283414v An assignment of the structured features in the Hartley band absorption spectrum of ozone. Joens, Jeffrey A. (Dep. Chem., Florida Int. Univ., Miami, FL 33199 USA). *J. Chem. Phys.* 1994, 100(5), 3407–14 (Eng). Using recent exptl. data for the Hartley band absorption spectrum obtained at low temp., a vibrational anal. of the discrete structure in the spectrum is given. It is found that all of the peaks in the range 238–292 cm can be assigned to transitions between the (0,0,0) vibrational state in the ground electronic state and (ν_1',ν_2') vibrational states in the upper electronic state. The obsd. structure in the Hartley band is due to a long progression in the sym. stretching mode, and a shorter progression in the bending mode. Based on the vibrational assignment, the following information is obtained on the vibrational parameters and geometry of ozone in the $^1B_2$ electronic state (all parametes are given for C_{2v} symmetry): $\omega_1' = 1108 \pm 25$ cm^{-1}, $\omega_1'x_1' = 9 \pm 3$ cm^{-1}, $\omega_2' = 298 \pm 12$ cm^{-1}, $\omega_3' = (1650 \pm 300)i$ cm^{-1}, $r_{00} = 0.140 \pm 0.002$ nm, $\varphi = 105 \pm 2°$. The anal. that is presented demonstrates that residual vibrational structure can occur in dissociative transitions, confirming previous suggestions.

Спектр
ω_i, $\omega_i x_i$

C.A. 1994, 120, N 22

$^{16}O_3$

1994

16 Б1171. Переотнесение колебательной структуры полосы поглощения Хаггинса озона. Reassignment of the vibrational structure of the Huggins absorption band of ozone / Joens Jeffrey A. // J. Chem. Phys. .— 1994 .— **101** , № 7 .— С. 5431—5437 .— Англ.

Предложено новое отнесение (прежнее см.//J. Chem Phys.—1979.—71.—С. 815) колебат. структуры полосы Хаггинса озона (область 27 000—33 000 см$^{-1}$), к-рая, согласно теор. расчетам, связана с запрещенным переходом $2^1A_1 \leftarrow \tilde{X}^1A_1$. Значения рассчитанных колебат. постоянных для молекулы $^{16}O_3$ (в см$^{-1}$): $\nu_{eO}=26120{,}6$, $\omega'_1=762{,}2$, $\omega'_2+x'_{22}=409{,}4$, $\omega'_3=798{,}7$, $x'_{11}=-19{,}0$, $x'_{12}=-18{,}8$, $x'_{13}=-37{,}5$, $x'_{23}=-23{,}0$, $x'_{33}=-19{,}5$. Аналогичные данные приведены для молекулы $^{18}O_3$.

В. М. Ковба

М. П.

Х. 1995, N 16

O_3

1994

теор. расчет колебат. спектра

126: 230866m IMRINDO/S−224−CI calculations on the electronic spectra of O_3, CO_2 and C_4H_4O. Joshi, B. A.; Chhaya, V. M.; Chhag, Smita (Department of Physics, Saurashtra University, Rajkot, 360 005 India). *Asian J. Phys.* 1994, 3(2), 81−87 (Eng), Anita Publications. Joshi−Chhaya models were used to evaluate true approx. values for two center repulsion integrals as an improvement to the MRINDO/S method (IMRINDO/S−244). The electronic spectra of ozone (O_3), CO_2 (CO_2) and furan (C_4H_4O) were studied employing IMRINDO/S−224−CI method and the results are found closer to the exptl. results for ionization potentials (IP's) and other spectral properties like lowest energy S → S transitions, Rydberg excitations and valence transitions.

+2 ☒

C. A. 1997, 126, N 17

О3 1994

Иванов С.В., Панченко В.Я.,

Успехи физ. наук. — 1994,
164, N 7, с. 725-742.

(м.п.)

Инфракрасная и микроволновая спектроскопия озона: исторический аспек[illegible]т.

р.ж.Х. N 6, 1995, 6 Б 2276

O_3 1994

Kobayashi Rika,
Amos R. D. et al.

теор. расчёт
ℓ, $\sphericalangle$, ω_e
ν_i

J. Chem. Phys. 1994,
<u>100</u> (2), 1375–9.

(сел. HF; $\underline{III}$)

O_3 1994

120: 176800w **The interpretation of the Wulf absorption band of ozone.** Minaev, Boris; Agren, Hans (Department of Chemistry, Cherkassy Engeneering and Technological Institute, Cherkassy, Ukraine 257006). *Chem. Phys. Lett.* 1994, 217(5–6), 531–8 (Eng). The intensities and energies of the three lowest singlet–triplet transitions of the ozone mol. have been obtained by means of analytic response theory calcns. based on multi-configuration wavefunctions. Contrary to the accepted interpretation of a $^1A_2 \leftarrow X^1A_1$ transition the authors find that the lowest electronic band in the ozone spectrum, the Wulf band, is due to a singlet–triplet $^3A_2 \leftarrow X^1A_1$ transition (oscillator strength 6×10^{-7}). The calcns. also explain the absence of observable absorption to the lowest a^3B_2 state because of negligible oscillator strength (8×10^{-10}).

полоса Вульфа

$a^3A_2 \leftarrow X^1A_1$

a^3B_2-не набл., т.к. низка сила осцил.

С.А. 1994, 120, N14

O_3

1995

122: 199872b **High-resolution infrared spectra of ozone in the 2300–2600 cm^{-1} region.** Barbe, A.; Sulakshina, O.; Plateaux, J. J.; Hamdouni, A.; Bouazza, S. (Fac. Sciences, Equipe Associee au CNRS, 51062 Reims, Fr.). *J. Mol. Spectrosc.* **1995,** 170(1), 244–50 (Eng). The spectra of ozone in the region 2300–2600 cm^{-1} have been recorded with the high-resoln. Fourier transform spectrometer of Reims. A White-type cell with a length of 36 m and pressure of 50 Torr of ozone has been used. This region corresponds mainly to the weak bands $\nu_1 + 2\nu_2$ and $2\nu_2 + \nu_3$, which were previously analyzed with a much lower amt. of ozone. Now high values of J and K_a have been obsd. up to 55 and 11, resp. The final fit on the 615 energy levels is very satisfactory, 0.39×10^{-3} cm^{-1}, equal to exptl. accuracy. Good agreement is also obtained for line intensities. Furthermore, the two difference bands $3\nu_3 = \nu_2$ and $\nu_1 + 2\nu_3 - \nu_2$ have been obsd. for the first time and their transition moments are given.

Обл. 2300—2600 см$^{-1}$, спектр, ν_i

C.A. 1995, 122, N16

O_3

1995

24 Б1605. Инфракрасные спектры высокого разрешения озона в области 2300—2600 см$^{-1}$. High-resolution infrared spectra of ozone in the 2300—2600 cm^{-1} region / Barbe A., Sulakshina O., Plateaux J. J., Hamdouni A., Bouazza S. // J. Mol. Spectrosc. .— 1995 .— **170** , № 1 .— С. 244—250 .— Англ.

На ИК-фурье-спектрометре в области частот 2300—2600 см$^{-1}$ с точностью около $4 \cdot 10^{-4}$ см$^{-1}$ измерен колебательно-вращат. спектр озона. Для полос $\nu_1+2\nu_2$, $2\nu_2+\nu_3$ уточнены, а для полос $3\nu_3-\nu_2$ и $\nu_1+2\nu_3-\nu_2$ впервые определены молекулярные постоянные.

С. Н. Мурзин

М.П.

Х. 1995, N 24

O_3

1995

123: **20559a A theoretical study of the low-lying excited states of ozone.** Borowski, Piotr; Fuelscher, Markus; Malmqvist, Per-Ake; Roos, Bjoern O. (Theoretical Chemistry, Chemical Center, P.O. Box 124, S-221 00 Lund, Swed.). *Chem. Phys. Lett.* **1995**, 237(3,4), 195–203 (Eng). A theor. study has been performed on the five lowest excited states of the ozone mol. using multiconfigurational second-order perturbation theory (CASPT2). The predicted order of states is: $^3A_2$ (T_0 = 1.15 eV), $^3B_2$ (T_0 = 1.33 eV), $^3B_1$ (T_0 = 1.33 eV), $^1A_2$ (T_0 = 1.44 eV) and $^1B_1$ (T_0 = 1.88 eV). Corresponding exptl. data are: 1.18, 1.30, 1.45, 1.58, and 2.05 eV, resp. Equil. geometries, harmonic frequencies of sym. vibrations, and vertical excitation energies are also reported. The dissocn. limit D_e for the ground state of ozone is found to be 1.08 eV, in agreement with the exptl. value (1.13 eV). The calcns. make use of a modified Fock operator in the CASPT2 theory. Relative energies of states with a different no. of open shells are substantially improved. The modified CASPT2 method was checked by calcg. spectroscopic consts. of the oxygen mol.

теор. расчеты
низших
эл. сост.

C. A. 1995, 123, N 2

O_3

1995

22 Б168. Теоретическое исследование низколежащих возбужденных состояний озона. A theoretical study of the low-lying excited states of ozone / Borowski Piotr, Fülscher Markus, Malmqvist Per-Åko, Roos Björn O. // Chem. Phys. Lett. .— 1995 .— **237** , № 3 - 4 .— С. 195—203 .— Англ. м. л

С помощью неэмпирич. многоконфигурац. теории возмущений второго порядка в базисе, включающем поляризац. функции вплоть до функций f-типа, исследованы пять низших возбужденных состояний молекулы озона. Приведены равновесная геометрия, частоты гармонич. симметричных колебаний, адиабатич. и вертикальные энергии возбуждений. Диссоциационный предел для основного состояния найден равным 1,08 эВ (эксперим. значение 1,13). Библ. 36.

Н. Л.

М.Л.

Х, 1995, N 22

1995

F:O$_3$
P: 3

5Б1258. Полосы 'ню'[1]+'ню'[2]+2'ню'[3] и 'ню'[2]+3'ню'[3] {16}O[3]. The 'ню'[1]+'ню'[2]+2'ню'[3] and 'ню'[2]+3'ню'[3] bands of {16}O[3] / Bouazza S., Mikhailenko S., Barbe A., Regalia L., Tyuterev Vl. G., Plateaux J. J. // J. Mol. Spectrosc. - 1995. - 174, N 2. - С. 510-519. - Англ.

С фурье-спектрометром в области 3700 см{-1}, соответствующей полосам 'ню'[1]+'ню'[2]+2'ню'[3] и 'ню'[2]+3'ню'[3], получен ИК-спектр {16}O[3]. Составлен эффективный гамильтониан с членами взаимодействия состояний (112) и (013). По 542 линиям вычислены его параметры, колебательные энергии, постоянные Кориолиса, переходные дипольные моменты и интенсивности полос.

РЖХ 1997

$^{16}O_3$

1995

124: 70193t The $\nu_1 + \nu_2 + 2\nu_3$ and $\nu_2 + 3\nu_3$ bands of $^{16}O_3$. Bouazza, S.; Mikhailenko, S.; Barbe, A.; Regalia, L.; Tyuterev, Vl. G.; Plateaux, J. J. (Groupe Spectrometrie Mol. Atmospherique, Equipe Assoc. au CNRS, 51062 Reims, Fr.). *J. Mol. Spectrosc.* **1995**, 174(2), 510–19 (Eng). The IR spectra of $^{16}O_3$ have been recorded in the 3700 cm^{-1} region, with a Fourier transform spectrometer at 0.008 cm^{-1} resoln. A White-type cell, $l = 32.16$ m, filled with 42.8 Torr O_3 was used. This spectral region corresponds to the $\nu_2 + 3\nu_3$ and $\nu_1 + \nu_2 + 2\nu_3$ bands. The $\nu_2 + 3\nu_3$ band was obsd. and analyzed previously, but the interacting band $\nu_1 + \nu_2 + 2\nu_3$ is obsd. for the first time. The assignments of this band cover the range $J = 58$, $K_a = 12$; observations up to $K_a = 17$ are available for $\nu_2 + 3\nu_3$. The two states (013) and (112) are satisfactorily treated as a dyad, with a std. deviation of 1.5×10^{-3} cm^{-1} for the 861 obsd. energy levels.

($\nu_2 + 3\nu_3$ и др.)

C.A. 1996, 124, N 6.

F: O3
P: 3

1995

6Б1281. Полосы 'ню'[1]+'ню'[3] {16}O{18}O{18}O и {18}O{16}O{18}O. The 'ню'[1]+'ню'[3] bands of {16}O{18}O{18}O and {18}O{16}O{18}O / Bourgeois M. T., Flaud J. M., Barbe A., Regalia L., Camy-Peyret C., Plateaux J. J. // J. Mol. Spectrosc. - 1995. - 172, N 2. - C. 552-558. - Англ.

В области 4,8 мкм измерены ИК-спектры поглощения (полоса 'ню'[1]+'ню'[3], разрешение 0,003 см{-1}, фурье-спектрометр) изотопообогащенных по {18}O молекул озона, {16}O{18}O{18}O и {18}O{16}O{18}O (начала полос соотв. при 2027,5825 и 2060,0720 см{-1}). Для первого несимметрично замещенного изотопомера при анализе учитывались кориолисовы взаимодействия уровней (101), (002) и (030), для второго - кориолисовы взаимодействия между состояниями (101), (002) и (200), а также взаимодействие Дарлинга-Деннисона между (002) и (200). Приведены рассчитанные значения колебат. уровней, вращат. постоянные и параметры центробежного искажения различных порядков указанных изотопомеров в рассматриваемых колебат. состояниях.

РЖХ 1997

O_3

1995

123: 126040q The $\nu_1 + \nu_3$ bands of $^{16}O^{18}O^{18}O$ and $^{18}O^{16}O^{18}O$. Bourgeois, M. T.; Flaud, J. M.; Barbe, A.; Regalia, L.; Camy-Peyret, C.; Plateaux, J. J. (Groupe Spectroscopie Moleculaire et Atmospherique, Univ. Reims, 51062 Reims, Fr.). *J. Mol. Spectrosc.* 1995, 172(2), 552-8 (Eng). Using 0.003-cm^{-1} resoln. Fourier transform spectra of ^{18}O-enriched ozone around 4.8 μm, the first high-resoln. anal. of the $\nu_1 + \nu_3$ bands of $^{16}O^{18}O^{18}O$ and $^{18}O^{16}O^{18}O$ has been performed. The exptl. rotational levels derived from the anal. were very satisfactorily calcd. using a Hamiltonian model which takes into account the necessary interactions. More precisely, for $^{18}O^{16}O^{18}O$, the Coriolis-type interactions coupling the levels of (101) with those of (002) and (200), as well as the Darling-Dennison interaction between (002) and (200), were considered. For the nonsym. species $^{16}O^{18}O^{18}O$, it proves necessary to include Coriolis-type interactions coupling the levels of (101) with those of (002) and (030). In this way, satisfactory fits were obtained, leading to the following band centers: $\nu_0(\nu_1+\nu_3)$ = 2060.0720 cm^{-1} for $^{18}O^{16}O^{18}O$ and $\nu_0(\nu_1+\nu_3)$ = 2027.5825 cm^{-1} for $^{16}O^{18}O^{18}O$.

$\nu_1 + \nu_3$

полосы изотопомеров

C. A. 1995, 123, N10

1995

F: O3
P: 3

4Б175. Исследование вклада триплетных состояний в полосы Вульфа озона. Investigation of the role of triplet states in the Wulf bands of ozone / Braunstein M., Martin R. L., Hay P. J. // J. Chem. Phys. - 1995. 102, N 9. - C. 3662-3666. - Англ.

Методом МК ССП с учетом КВ в базисе 3s2p1d с использованием одноцентрового одноэлектронного приближения для оператора спин-орбитального вз-вия исследованы три низших триплетных состояния озона {3}B[2], {3}A[2] и {3}B[1]. а основании полученных результатов обсуждена природа полос Вульфа, серии слабых диффузных пиков в ближней ИК-области непосредственно над порогом диссоциации O[2]+O. Сделан вывод, что состояния {3}A[2] и {3}B[1], видимо, вносят вклад в эти полосы, но подчеркнута необходимость проведения более строгих расчетов для подтверждения такого заключения.

Р. Ж. Х. N 4, 1996.

O_3

1995

123: 123662h The rotational spectra, hyperfine interactions, and ^{17}O magnetic shieldings of $^{17}O^{16}O^{16}O$, $^{16}O^{17}O^{16}O$, and $^{17}OS^{16}O$. Cohen, E. A.; Hillig, K. W. II; Pickett, H. M. (Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109 USA). *J. Mol. Struct.* 1995, 352/353, 273–82 (Eng). Measurement of the rotational spectra of $^{17}O^{16}O^{16}O$ and $^{16}O^{17}O^{16}O$ have been extended to allow the detn. of a complete set of sextic centrifugal distortion consts. for both mols. A near degeneracy of the 3_{12} and 4_{04} levels of $^{17}O^{16}O^{16}O$ causes strong perturbations of the hyperfine patterns, gives rise to perturbation-allowed $\Delta J = 2$ transitions, and provides an accurate detn. of χ_{ab}. This has allowed the calcn. of the angle between the principal axis of the quadrupole tensor and the O–O bond. The ^{17}O spin-rotation interactions of $^{17}OS^{16}O$ have been measured for comparison with the corresponding values in O_3, and improved values of the quadrupole coupling have been obtained. Paramagnetic shielding and chem. shifts for ^{17}O have been calcd. from the spin-rotation consts. for both compds.

Вращат- спектры изотопомеров и м.л.

Ⓗ

ОЗО ⊠ ●

С.А. 1995, 123, N10

$^{17}O_3$

1995

122: 145673u **Microwave spectra of all ^{17}O-monosubstituted ozones.** Colmont, Jean Marcel; Drean, Pascal (Laboratoire Spectroscopie Hertzienne, Universite Sciences Technologies Lille, 59655 Villeneuve, Fr.). *J. Mol. Spectrosc.* **1995**, 169(1), 190–200 (Eng). The pure rotational spectra of all possible ^{17}O-monosubstituted ozone species have been investigated at selected frequencies in the range from 49 to 393 GHz. Accurate rotational and centrifugal distortion parameters up to the sextic terms have been detd. using the Watson's Hamiltonian in its A-reduced form. Comparisons are made between exptl. values and those obtained from the force field calcns.

враицат.
спектр

C.A. 1995, <u>122</u>, N 12

O_3

1995

123: 182161s Rotational spectra of all ^{17}O-bisubstituted ozones: comparison between different structures. Colmont, Jean-Marcel; Demaison, Jean; Cosleou, Jean (Lab. Spectroscopie Hertzienne, Univ. Lille I, 59655 Villeneuve D'Ascq, Fr.). *J. Mol. Spectrosc.* **1995**, 171(2), 453-67 (Eng). We report here the results of a millimeter-wave study of all four possible bi-^{17}O isotopic species of ozone, carried out in the frequency range from 49 to 393 GHz. Using Watson's Hamiltonian expressed in the A-redn. form, the rotational consts. and centrifugal distortion coeffs. up to the sextic terms are accurately detd. for each form. The structures calcd. by different procedures are compared.

спектр
изотопозаме-
щения

C.A. 1995, 123; N 14

O_3

1995

123: 68621s Fourier transform spectroscopy of asymmetric top molecules. Flaud, J. M.; Perrin, A.; Camy-Peyret, C. (Laboratoire de Physique Moleculaire et Applications, CNRS, 75252 Paris, Fr.). *Spectrochim. Acta, Part A* 1995, 51A(7), 1217–30 (Eng). A review with 32 refs. Because of its numerous advantages: coverage of wide spectral ranges, consistency of wave nos., high resoln., high signal to noise ratio, etc., Fourier transform spectrometry has been and is still widely used in mol. spectroscopy, producing large amts. of new precise spectroscopic data. The analyses of these data have led to a deep understanding of the very fine effects (resonances, centrifugal distortion, etc.) which affect both the line positions and intensities. As an illustration of progress achieved, using Fourier transform spectra, in the spectroscopy of asym. tops, examples concerning ozone, hydrogen peroxide and nitrogen dioxide are described.

Фурье-спектр

обзор

C. A. 1995, <u>123</u>; N 6

O_3

1995

124: 127367j The bonding in the ozone molecule: from a different perspective. Laing, Michael (Department Chemistry, University Natal, Durban, S. Afr.). *Struct. Chem.* **1995**, 6(6), 397–402 (Eng). A new qual. treatment of the bonding in ozone is presented. It is based upon a combination of several simple concepts: the nonparticipation of the pairs of electrons tightly held in the at. 2s orbitals; simple overlap of the 2p orbitals to form sigma bonds; interaction of three 2p orbitals to yield bonding and nonbonding pi MOs that are populated by electron pairs; and van der Waals repulsion between the two terminal oxygen atoms forcing these atoms apart to yield the bond angle of 117° as a compromise. Both the assumptions and the resulting bonding picture are in accord with the photoelectron spectroscopic data, the results from sophisticated MO calcns., and the common phys. properties of ozone.

(связь в мол-ле)

C. A. 1996, 124, N10

O_3

1996

125: 259782w Study of electronically excited states of ozone by electron−energy−loss spectroscopy. Allan, Michael; Mason, Nigel J.; Davies, Julia A. (Institut de Chimie Physique, Universite de Fribourg, CH−1700 Fribourg, Switz.). *J. Chem. Phys.* **1996**, 105(14), 5665−567' (Eng). Electronically excited states of ozone were studied by EELS. Two broad bands without visible vibrational structure are obsd. at 1.8 ± 0.2 eV and 2.05 ± 0.05 eV under scattering conditions favoring singlet excitation, that is a scattering angle of $\theta = 10°$ and residual energy $E_r = 20$ eV. The lower is assigned as $^1A_2$, the higher as $^1B_1$ (Chappuis band). Bands with rich vibrational structure are obsd. under scattering conditions favoring triplet excitation, $\theta = 30°-135°$ and residual energy $E_r = 1-3$ eV. At least two progressions can be discerned. The 1st has an origin at 1.30 eV, the origin of the 2nd cannot be detd. unambiguously, it is either at 1.53 or 1.45 eV. The known Hartley band and a no. of other singlet and triplet excited states are obsd. at higher energy losses. Excitation functions and angular distributions of the triplet band at 1.30 eV and of the Hartley band are presented. The abs. value of the differential cost section for excitation of the Hartley band is given.

Эл.- возб.
сост.

C.A. 1996, 125, N 20

1996

F: O3
P: 3
14Б1283. Положения линий и интенсивности полосы 3'ню'[1]+'ню'[3] озона. Line positions and intensities of the 3'ню'[1]+'ню'[3] band of ozone / Barbe A., Sulakshina O., Plateaux J. J., Tyuterev Vl. G., Bouazza S. [Journal of Molecular Spectroscopy] // J. Mol. Spectrosc. - 1996. - 175, N 2. - C. 296-302. - Англ.

РЖХ 1997

Исследован ИК-фурье-спектр поглощения (в области 4250 см{-1}, с разрешением 0,008 см{-1}) газообразного озона (I) с использованием кюветы Уайта длиной 36,16 м при давлении 42,8 Торр. Идентифицирована полоса составного колебания 3'ню'[1]+'ню'[3] I, для которого верхнее колебат. состояние представляет собой пентаду (400), (301), (202), (103), (104), связанную через кориолисово взаимодействие и взаимодействие Дарлинга-Деннисона. Предложено отнесение наблюдаемых линий до J=43 и K[a]=13. Проведена теор. обработка эксперим. данных с использованием гамильтониана, учитывающего кориолисово взаимодействие состояния (301) с состоянием (230), удовлетворительно воспроизводящая положения линий и их интенсивности в области 4170-4265 см{-1}.

O_3

1996

23Б1481. Характеристика метастабильного состояния озона с помощью фурье-спектрометрии высокого разрешения. Characterization of a metastable state of ozone by high-resolution Fourier transform spectrometry / Bouvier A. J., Bacis R., Bussery B., Churassy S., Inard D., Nota M., Brion J., Malicet J., Anderson S. M. // Chem. Phys. Lett.— 1996.— **255**, № 4-6.— С. 263-266.— Англ.

М-Л.

В области частот 9100–10 200 см$^{-1}$ получен с разрешением 0,05 см$^{-1}$ спектр озона, отнесенный к переходу $^3A_2 \leftarrow X^1A_1$. Измерены полуширины линий и частоты голов полос Вульфа 0←0 и 1←0. Радиационное время жизни уровня $^3A_2$ равно 0,1–0,01 с, что указывает на его метастабильный характер. Нулевой уровень расположен на 1085 см$^{-1}$ выше предела диссоциации основного состояния. Частота деформационного колебания ω_2=530,9±0,4 см$^{-1}$. М. А. Ковнер

Х.1997, №22

O_3

1996

метастаб.
состоян.

125: 98493k **Characterization of a metastable state of ozone by high−resolution Fourier transform spectrometry.** Bouvier, A. J.; Bacis, R.; Bussery, B.; Churassy, S.; Inard, D.; Nota, M.; Brion, J.; Malicet, J.; Anderson, S. M. (Universite Claude Bernard, Lyon I, Laboratoire de Spectrometrie Ionique et Moleculaire, UMR 5579 du CNRS, 43 Bd du 11 Novembre 1918, 69622, Villeurbanne, Fr.). *Chem. Phys. Lett.* 1996, 255(4,5,6), 263−266 (Eng). A high−resoln. study of the Wulf bands of O_3 is reported. A preliminary anal. of the rotational structure in 2 vibronic bands yields the band origin $T_0 = 9555.49 \pm 0.25$ cm^{-1}, the bending frequency $\omega_2 = 530.9 \pm 0.4$ cm^{-1} and geometries (R, θ) for the corresponding bound vibrational levels of the upper state, which is most likely to be $^3A_2$. Rotational levels extend to ≥1090 cm^{-1} above T_0. The radiative lifetime is −0.1−0.01 s, indicating the state's metastable character.

C. A. 1996, 125, N8

O_3

1996

(ик спектр)

124: 245187y Infrared spectra of ${}^{18}O$-enriched ozones in liquid oxygen solution. Bulanin, K. M.; Bulanin, M. O.; Tsyganenko, A. A. (Peterhof, Russia 198904). *Chem. Phys.* 1996, 203(1), 127–36 (Eng). FTIR spectra of 6 ozone isotopomers are studied in liq. O_2 soln. at 77 K in the spectral range 650–3200 cm^{-1}. Full vibrational assignment is given and relative transition strengths are measured for many previously unobserved absorption bands of ${}^{18}O$-enriched species. Whenever such comparison is possible, most but not all of the relative strengths in soln. are in agreement with the rotationless transition moments in the gas phase. An order of magnitude enhancement obsd. for the hybrid-type ν_1 transitions in asym. ${}^{16}O^{16}O^{18}O$ and ${}^{16}O^{18}O^{18}O$ mols. is consistent with the calcd. off-diagonal vibrational dipole matrix elements for the fundamental transitions in C_{2v} and C_s isotopomers. Probably enhancement of transitions into the states with the even vibrational quantum no. v_3 may serve as a sensitive criterion for an interaction-induced asym. distortion of the O_3 potential energy surface by intermol. interactions via terminal O atoms.

C.A. 1996, 124, N 18

1996

F: O3
P: 3
14Б1280. Инфракрасное поглощение O[3] при лазерном возбуждении CO[2]. Infrared absorption of O[3] under CO[2] laser excitation / Codnia Jorge, Azcarate M. Laura [Optical Engineering] // Opt. Eng. - 1996. - 35, N 1. - C. 86-93. - Англ.

РЖХ 1997

1996

F: O3
P: 3
6Б1276. Анализ с высоким разрешением 5'ню'[3], 3'ню'[1]+'ню'[2]+'ню'[3] и 'ню'[1]+4'ню'[3] полос {16}O[3]. Положения линий и интенсивности. High resolution analysis of the 5'ню'[3], 3'ню'[1] + 'ню'[2] + 'ню'[3], and 'ню'[1] + 4'ню'[3] bands of {16}O[3]: Line positions and intensities / Flaud J. M., Barbe A., Camy-Peyret C., Plateaux J. J. // J. Mol. Spectrosc. - 1996. - 177, N 1. - C. 34-39. - Англ.
На ИК-фурье-спектрометре с разрешением 0,008 см{-1} измерены колебательно-вращат. спектры полос 3'ню'[1]+'ню'[2]+'ню'[3] и 5'ню'[3] вблизи 2,1 мкм и горячей полосы 'ню'[1]+4'ню'[3]-'ню'[3] вблизи 2,5 мкм молекулы озона {16}O[3]. Анализ спектров выполнен с учетом квартичного и секстичного центробежного искажения, резонансов ангармонизма между вращат. уровнями (005)- и (311)-состояний, кориолисовых резонансов между (005)- и (104)-состояниями и (104)- и (311)-состояниями. Для более чем 126 линий измерены интенсивности, согласующиеся с результатами модельного расчета.

РЖХ 1997

$^{16}O_3$

1996

125: 70467f High resolution analysis of the $5\nu_3$, $3\nu_1 + \nu_2 + \nu_3$, and $\nu_1 + 4\nu_3$ bands of $^{16}O_3$: line positions and intensities. Flaud, J. M.; Barbe, A.; Camy–Peyret, C.; Plateaux, J. J. (Laboratoire Phys. Moleculaire Applications, Univ. Pierre Marie Curie, 75252 Paris, Fr.). *J. Mol. Spectrosc.* **1996**, 177(1), 34–39 (Eng). Using a Fourier transform spectrum of ozone recorded in the 2.1 μm region at a resoln. of 0.008 cm^{-1}, it was possible to perform the 1st high resoln. anal. of the $3\nu_1 + \nu_2 + \nu_3$ and $5\nu_3$ bands of $^{16}O_3$. These results, together with those derived from the anal. of the $\nu_1 + 4\nu_3 = \nu_3$ hot band in the 2.5 μm region, were used to derive a large set of exptl. rotational energy levels (up to J = 47 and K_a = 14) for he three vibrational states (005), (311), and (104). These levels were satisfactorily fitted using a Hamiltonian model which takes into account both the anharmonic interactions between the levels of (005) and (311) and the Coriolis–type interactions between the levels of (005) and (104) and of (311) and (104), and a precise set of vibrational energies and rotational and coupling consts. was derived. In particular, the following band centers were obtained: ν_o (005) = 4919.2034 cm^{-1}, ν_0 (311) = 4897.2766 cm^{-1}, ν_0(104) = 4922.5717 cm^{-1}. Also, 126 line intensities were measured and fitted leading to the detn. of transition moment consts. for the 3 bands $5\nu_3$, $3\nu_1 + \nu_2 + \nu_3$, and $\nu_1 + 4\nu_3$. These consts., together with the Hamiltonian consts. derived were finally used to generate a comprehensive list of line positions and intensities.

(ν_i)

C. A. 1996,
125, N 6

O_3

ОТ 38505 1996

126: 162516v Low-lying ionization potentials of O_3 and NO_2 using the multiconfigurational spin tensor electron propagator method. McKellar, Alexander J.; Yeager, Danny L.; Nicholas, Jeffrey A.; Golab, Joseph T. (Chemistry Department, Texas A&M University, College Station, TX 77843-3255 USA). *J. Chem. Phys.* 1996, 105(22), 9927-9932 (Eng), American Institute of Physics. The multiconfigurational spin tensor electron propagator method (MCSTEP) is a single particle Green's function (or electron propagator) method for detg. the low-lying principal vertical ionization potentials (IPs) and electron affinities (EAs) of atoms and mols. It was specifically designed to handle cases where the initial state has nondynamical correlation and/or is open shell. We have applied MCSTEP for the first time to triat. mols. composed entirely of second row atoms. The two cases we present are O_3 and NO_2 – for the former nondynamical correlation is present in the ground (initial) state and for the latter the ground (initial) state is open shell. MCSTEP results are accurate compared to expt. and other forefront theor. techniques.

(Э)

теор. расчет

(А)

NO_2

C.A. - 1997, 126, N 12

O_3

1996

22Б1345. Ультрафиолетовый спектр поглощения озона. Структурный анализ и изучение изотопического эффекта в системе Хэртли. UV absorption spectrum of ozone: structure analysis and study of the isotope effect in the Hartley system / Parisse C., Brion J., Malicet J. // Chem. Phys. Lett.— 1996.— **248**, № 1-2.— С. 31–36.— Англ.

Спектр поглощения озона в области длин волн 195–350 нм с шагом 0,01 нм записан с точностью 1–3% при пяти т-рах 218–295 К для $^{16}O_3$ и $^{18}O_3$. Исследована колебат. структура системы Хэртли с точностью около 10 см$^{-1}$ для обоих изотопомеров. Полученные результаты представляют интерес для атмосферной оптики.

С. Н. Мурзин

М.Л.

Х. 1997, N22

O_3

1996

128: 225076r New structure of ozone. Rao, B.; Prakash, Om (Division of Standards, National Physical Laboratory, New Delhi, 110 012 India). *Asian J. Phys.* **1996**, 5(4), 487–491 (Eng), Anita Publications. A new structure of ozone was proposed and discussed from studies reported in the literature. Some of the obsd. properties of ozone such as diamagnetic nature etc. can be explained satisfactorily by this structure.

новая структура

C.A. 1998, 128, N18

O_3

1996

124: 245294f **Vibrational spectra of the $^{16}O/^{17}O/^{18}O$ substituted ozone molecule isolated in matrixes.** Schriver-Mazzuoli, L.; Schriver, A.; Lugez, C.; Perrin, A.; Camy-Peyret, C.; Flaud, J.-M. (Laboratoire Physique Moleculaire Applications, Universite Pierre Marie Curie, 75252 Paris, Fr.). *J. Mol. Spectrosc.* 1996, 176(1), 85-94 (Eng). IR spectra of $^{16}O/^{17}O/^{18}O$ enriched O_3 were recorded both in Ar and N matrixes using Fourier transform spectroscopy. The fundamental bands ν_1, ν_2 and the combination band $\nu_1 + \nu_3$ were analyzed from 2 mixts. with different isotopic abundances. Most of the obsd. absorption peaks were assigned, and a change in the relative intensities of the 3 fundamental modes was evidenced for unsym. isotopic species. The present study was undertaken to better understand possible mechanisms of isotopic enhancements obsd. in the stratosphere.

(ИК в матриц.)

C.A. 1996, 124, N 18

O_3 OM 38461 1996

(Ap)

125: 177883r Calculation of proton affinities and absolute gas basicities of X_3 Group VI triatomics: a density functional study. Toscano, Marirosa; Russo, Nino; Rubio, Jaime (Dipartimento Chimica, Universita Calabria, I-87030 Arcavacata di Rende, Italy). *J. Chem. Soc., Faraday Trans.* **1996**, 92(15), 2681–2684 (Eng). Proton affinities (PA) and abs. gas basicities (GB) of O_3, S_3, Se_3 and Te_3 have been computed using the linear combination of Gaussian-type orbitals-d. functional method (LCGTO-DF) employing local and non-local exchange-correlation functionals. Comparison with previous exptl. and theor. results shows that the gradient cor. results are able to reproduce the exptl. proton affinities of ozone. PA and GB predictions for the other X_3 Group VI triatomics are consistent with the expected periodic trends. The computed geometrical and spectroscopic consts. for the X_3 systems, in both C_{2v} and D_{3h} symmetry, agree well with the available exptl. data.

(+3) ☒ S_3, Se_3, Te_3

C.A. 1996, 125, N14

O_3

1997

127: 181340v Global potential energy surfaces for the lowest two $^1A'$ states of ozone. Atchity, G. J.; Ruedenberg, K. (Department Chemistry, Iowa State Universty, Ames, IA 50011 USA). *Theor. Chem. Acc.* **1997**, 96(3), 176−194 (Eng), Springer. The global features of the potential energy surfaces of the lowest 2 $^1A'$ states of O_3 are established and detailed information is detd. for the crit. regions. Contour maps are generated on a variety of planes and curved surfaces cutting through the 2 energy surfaces in various directions to obtain a full understanding of the 3D characteristics of both surfaces. Perimetric internal coordinates are used so that the 3 atoms are treated on an equal footing. The $1^1A'$ state, the ground state, has a ring min. and 3 equiv. open min., all lying in C_{2v}−restricted coordinate spaces. Direct dissocn. to O_2 + O is only

потенц.
поверхност
2х $^1A'$ сост.

C. A. 1997, 127, N 13

possible from the open min. The lowest energy path from the ring min. 1st leads to an open min. before going to dissocn. The transition states between the ring min. and the open min. also have C_{2v} symmetry. Close to these transition states lie the 3 open min. of the $2^1A'$ state, which has no ring min. Isomerization between the open min. is highly unlikely in the ground state, but not excluded in the excited state. Both states dissoc. into the same state of $O_2 + O$, namely the ground state $O(^3P) + O_2(^3\Sigma_g^-)$ whose energy lies between that of the $1^1A'$ and $2^1A'$open min. There exists an extended, interestingly shaped region in coordinate space in which the 2 states come very close to each other. It contains an intersection seam between the 2 states consisting of 4 branches connected by 3 knots. Radiationless transitions between the 2 states can be expected.

O_3

1997

128: 81544s Infrared spectrum of ozone in the 4600 and 5300 cm^{-1} regions: high order accidental resonances through the analysis of $\nu_1 + 2\nu_2 + 3\nu_3 - \nu_2$, $\nu_1 + 2\nu_2 + 3\nu_3$, and $4\nu_1 + \nu_3$ bands. Barbe, A.; Plateaux, J. J.; Mikhailenko, S.; Tyuterev, Vl. G. (Groupe de Spectrometrie Moleculaire et Atmospherique, Equipe associee au CNRS D 1434, UFR Sciences, 51687 Reims, Fr.). *J. Mol. Spectrosc.* **1997**, 185(2), 408–416 (Eng), Academic Press. The very weak bands $\nu_1 + 2\nu_2 + 3\nu_3$ and $4\nu_1 + \nu_3$ of $^{16}O_3$ have been obsd. for the first time, using the Fourier transform spectrometer (FTS) of Reims and the usual exptl. setup providing a large product p × 1 of approx. 38 Torr × 36 m. The upper levels of these A–type bands which are rather close in energy (they appear resp. at 5291.722 and 5307.790 cm^{-1}) belong to two different sets of interacting polyads. To correctly reproduce the rotation–vibration energy levels and account for the obsd. perturbations, both bands are treated in a dyad approxn.: the (123) state in the Coriolis resonance with the (330) state, and the (401) state in the Coriolis resonance with the (024) state. The assignments of the rotation–vibration levels of the (123) state are confirmed by measurements of line positions of the hot band $\nu_1 + 2\nu_2 + 3\nu_3 - \nu_2$ which has also been obsd. for the first time. The fits are very satisfactory: the r.m.s. deviation for 249 energy levels of the (123) state is 2.4×10^{-3} cm^{-1} and is 2.0×10^{-3} cm^{-1} for 266 levels of the (401) state. These r.m.s. are near exptl. accuracy. Transition moments for the three obsd. bands are detd. from measured line intensities.

ИК в

обл.

4600-5300 см-1

Vi

C.A.1998,

128, N7

O_3

1997

127: 312563v **First observation of the $v_2 = 3$ state of ozone: the (131) state through analysis of cold and hot bands. Study of v_2 behavior.** Barbe, A.; Mikhailenko, S.; Plateaux, J. J. (Groupe de spectrometrie Moleculaire et Atmospherique, Equipe Associee au CNRS D 1434, 51687 Reims, Fr.). *J. Mol. Spectrosc.* 1997, 184(2), 448–453 (Eng), Academic. The vibration–rotation energy levels of the (131) state of ozone were obtained, covering the whole range of J up to 33 and K_a up to 9, from the anal. of the hot band, obsd. for the 1st time $\nu_1 + {}_{\nu 3} + \nu_3 - \nu_2$ in the 3400 cm⁻¹ region. The assignments were confirmed by the anal. of the cold band $\nu_1 + 3\nu_2 + \nu_3$ recorded in the 4100 cm⁻¹ region. This enabled the authors also to derive the transition moment $\varphi_z^{000-131} = 1.8 \times 10^{-4}$ D. The anal. was performed using single state Watson's Hamiltonian where the 164 levels are fitted with 10 parameters with a root–mean–square deviation of 1.9×10^{-3} cm⁻¹, near the exptl. accuracy. Note that the anal. involving simultaneously three interacting states of the Triad {(230), (131), (032)} also was performed which however did not result in an improvement of the root–mean–square deviation of the fit. This work allows the authors to observe a quasi–linear variation of $A(1v_21)$, $B(1v_21) + C(1v_21)$ and $\Delta_k(1v_21)$ with respect to v_2. This result is of 1st importance to derive band centers of perturbing.

(ν_i)

C.A.1997, 127, N 22

O_3

1997

127: 10485s **Analysis of the $2\nu_1 + \nu_2 + 2\nu_3$ band of ozone.** Barbe, A.; Mikhailenko, S.; Plateaux, J. J.; Tyuterev, Vl. G. (Groupe Spectrometrie Moleculaire Atmospherique, Equipe Associee CNRS–URA D 1434, 51687 Reims, Fr.). *J. Mol. Spectrosc.* **1997,** 182(2), 333–341 (Eng), Academic. The $2\nu_1 + \nu_2 + 2\nu_3$ band of ozone, occurring in the 4780 cm^{-1} region, was obsd. for the 1st time, using a Fourier transform spectrometer, at 0.008 cm^{-1} resoln. and using a large path length pressure product. Assignments of vibration–rotational transitions were made up to $J = 48$ and $K_a = 9$. As a few levels with $K_a = 1$ or 2 are perturbed, it was necessary to take into account the Coriolis resonance between the (212) and (141) vibrational states. With the effective Hamiltonian explicitly accounting for the interaction between these 2 states, the fit on 165 energy levels leads to the root–mean–square deviation of 1.9×10^{-3} cm^{-1}, which is near the exptl. accuracy. Line intensities of the $2\nu_1 + \nu_2 + 2\nu_3$ band were measured and calcd. The set of spectroscopic parameters for interacting bands, as well as transition moment consts., is given. A complete list of line positions and intensities, with a cutoff of 1×10^{-26} $cm^{-1}/mol.{\cdot}cm^{-2}$ at 296 K up to $J = 65$ and $K_a = 15$, was generated, which leads to the integrated band intensity $S_\nu(2\nu_1 + \nu_2 + 2\nu_3) = (5.1 \pm 2.0) \times 10^{-23}$ $cm^{-1}/mol.{\cdot}cm^{-2}$.

(ν_i)

C. A. 1997, 127, N 1

O_3

1997

127: 225454s The calculation of the bound and quasibound vibrational states for ozone in its $^1B_2$ electronic state. Bludsky, Ota; Jensen, Per (FB 9–Theoretische Chemie, Bergische Universitat–Gesamthochschule Wuppertal, D–42097 Wuppertal, Germany). *Mol. Phys.* 1997, 91(4), 653–661 (Eng), Taylor & Francis. The bound and quasibound vibrational states of ozone in the $^1B_2$ electronic state were calcd. using the stabilization method. The calcn. was based on an ab initio potential energy function from the literature. From the topol. of this surface, the authors det. the mol. symmetry group of $^1B_2$ O_3 to be $C_{2v}(M)$. The parameters of resonances in the 750–2750 cm^{-1} energy range relative to the $O_2(^1\Delta_g) + O(^1D)$ dissocn. limit are given. The effective vibrational consts. obtained by fitting the calcd. vibrational energy levels are compared with the corresponding exptl. values. The agreement is satisfactory and supports the assignment of the Huggins band to the $^1B_2 - X^1A_1$ electronic transition.

сост. $^1B_2$, стр-ра

C.A. 1997, 127, N 16

F: O3
P: 3

1997

22Б1175. Нарушение правила неполного непересечения между полностью симметричными состояниями с замкнутыми оболочками в валентно-изоэлектронном ряду O[3], S[3], SO[2] и S[2]O. Violation of the weak noncrossing rule between totally symmetric closed-shell states in the valence-isoelectronic series O[3], S[3], SO[2] and S[2]O / Ivanic Joseph, Atchity Gregory J., Ruedenberg Klaus // J. Chem. Phys. - 1997. - 107, 11. - C. 4307-4317. - Англ.

С использованием многоконфигурационного метода ССП в полном валентном пространстве и базисов cc-pVTZ исследованы поверхности потенциальной энергии (ПЭ) указанных в заглавии систем в основных и низших возбужденных ({1}A[1]) состояниях. Показано, что во всех случаях взаимопревращение изомеров с открытой и циклической структурой происходит с помощью переходных состояний C[2v], вблизи которых наблюдается коническое пересечение 1{1}A[1]- и 2{1}A[1]-поверхностей ПЭ.

РЖХ, 1998, №22

O_3

OM 39130

1997

128: 94729f Molecular geometry and vibrational frequencies of ozone from compact variational wave functions explicitly including triple and quadruple substitutions. Leininger, Matthew L.; Schaefer, Henry F., III (Center for Computational Quantum Chemistry, University of Georgia, Athens, GA 30602 USA). *J. Chem. Phys.* **1997**, 107(21), 9059–9062 (Eng), American Institute of Physics. The performance of a multireference CISD method, CISD[TQ], is compared to that of other approaches which include a large degree of electron correlation, including Brueckner methods. The CISD[TQ] method selects as refs. all single and double substitutions within an active orbital space. Certain triple and quadruple substitutions from the Hartree–Fock ref. are included in the CISD[TQ] wave function as singles and doubles from the selected ref. set. This wave function has previously been shown in simpler cases to provide results near to those predicted by the CI wave function, including all single, double, triple, and quadruple substitutions (CISDTQ). For the challenging multireference case of ozone, the CISD[TQ] wave function yields geometries and harmonic vibrational frequencies with an accuracy similar to the full CCSDT method. These promising results suggest that for difficult multireference problems the CISD[TQ] wave function provides an efficient and accurate approach for approximating the complete CISDTQ.

структ,
Vi, теор
расчет

CA 1998, 128, N8

1997

O_2–O

127: 25186u **Photofragment excitation spectrum for O(^{1}D) from the photodissociation of jet-cooled ozone in the wavelength range 305–329 nm.** Takahashi, Kenshi; Kishigami, Masahiro; Taniguchi, Nori; Matsumi, Yutaka; Kawasaki, Masahiro (Institute for Electronic Science, and Graduate School of Environmental Science, Hokkaido University, Sapporo, Japan 060). *J. Chem. Phys.* 1997, 106(15), 6390–6397 (Eng), American Institute of Physics. The photofragment excitation (PHOFEX) spectrum for O(^{1}D) prodn. from the photolysis of O_3 under supersonic free-jet conditions was measured, scanning the photodissocn. wavelength at 305–329 nm and probing the O(^{1}D) atoms by vacuum UV laser induced fluorescence at 115.2 nm. The bond dissocn. energy $D_0^0(O_2-O)$ is 101.53 ± 0.25 kJ mol^{-1} from the cut-off wavelength in the PHOFEX spectrum for the photodissocn. of jet-cooled O_3 (T_{rot} = 5 K) to O(^{1}D) + O_2(a $^1\Delta_g$). The cut-off wavelength for vibrationally hot band excitation to the dissociative continuum of O(^{1}D) + O_2(a $^1\Delta_g$) was also obsd. in the PHOFEX spectrum. The active mode for the hot band excitation was the antisym. stretching mode ν_3 in the ground electronic state of O_3. Sharp peaks corresponding to vibrational bands in the Huggins system were also obsd. in the PHOFEX spectrum of the O(^{1}D) atoms produced via the spin-forbidden dissocn. process, O(^{1}D) + O_2(X $^3\Sigma^-_g$). The spectral widths of the vibronic bands in the Huggins system are discussed in terms of the dissocn. dynamics.

D_0

C.A. 1997, 127, N2

O_3

1997

128: 27060t theoretical studies of the potential energy surface and the vibrational excited state of ozone. Xian Hui; Xie, Daiqian; Yan, Guosen (Dep. Chem., Sichuan Univ., Chengdu, Peop. Rep. China 610064). *Wuli Huaxue Xuebao* **1997**, 13(10), 865–867 (Ch), Beijing Daxue Chubanshe. The excited vibrational states of the ozone mol. are studied using the vibrationally SCF–CI (SCF–CI) procedure. In order to reproduce the obsd. vibrational band origins well, the potential energy surface for the electronic ground state of O_3 is optimized using the recently obsd. vibrational band origins up to 4400 cm^{-1}. The root-mean-square error of this fitting for the 30 obsd. vibrational energy levels is 0.47 cm^{-1}. All the calcd. band origins are within 1.0 cm^{-1} of the obsd. values.

Колб. эл. сост.,
потенц.
пов-сть,
теор. расч.

CA 1998, 128, N3

O_3

Отт. 40081

1998

128: **222886u The ozone molecule: electronic spectroscopy.** Bacis, R.; Bouvier, A. J.; Flaud, J. M. (Laboratoire de Spectrometrie ionique et moleculaire, UMR CNRS no. 5579, Universite Claude Bernard, 69622 Villeurbanne, Fr.). *Spectrochim. Acta, Part A* **1998**, 54A(1), 17–34 (Eng), Elsevier Science B.V.. A review with 112 refs., dealing with five lowest–lying excited electronic states of ozone, UV excited states, vacuum–UV absorption, photoionization, photoelectron spectra, and photodissocn. products.

обзор,
электрон.
спектр,
нижние
эл. сост.

C.A. 1998, 128, N18

O_3

1998

130: **30639k The $2\nu_2$ and $3\nu_2 - \nu_2$ bands of ozone.** Barbe, A.; Chichery, A.; Tyuterev, Vl. G.; Taskhun, S.; Mikhailenko, S. (Groupe de Spectrometrie Moleculaire et Atmospherique, UPRESA CNRS Q 6089, UFR Sciences, 51687 Reims, Fr.). *Spectrochim. Acta, Part A* **1998**, 54A(12), 1935–1945 (Eng), Elsevier Science B.V.. The IR spectra of $^{16}O_3$ in the range 1300–1500 cm^{-1} were recorded at high resoln. (0.007 cm^{-1}), with a large product $p \times l = 32.4$ torr × 3212 cm, and a good S/N ratio ≃ 500. This enables the authors to observe the $2\nu_2$ band with high values of rotational quantum nos., resp. $J \leq 57$ and $K_a \leq 16$, and also to observe for the 1st time the hot band $3\nu_2 - \nu_2$. The IR data, combined with the 24 known microwave transitions in the (020) state, lead to a new set of Hamiltonian parameters. Statistical aspects of the simultaneous fit of microwave and IR data are discussed and predictions of microwave transitions in the (020) state are given. The Hamiltonian

(спектр)

C. A. 1999, 130, N3

parameters for (030) are reported, leading to an observation of a quasi linear dependence of rotational consts. and the centrifugal distortion const. Δ_K with respect to the v_2 quantum no. Transition moment parameters are given for the $2\nu_2$ and $3\nu_2 - \nu_2$ bands. A complete final calcn. of line positions and intensities up to $J \leq 65$ and $K_a \leq 20$ leads to the integrated band intensity S_v $(2\nu_2) = (5.328 \times 10^{-22}$ $cm^{-1})/(cm^{-2}$ $mol.^{-1})$ at 296 K, with a cut−off of 2×10^{-26}.

O_3

1998

128: 236424d First study of the $\nu_2 = 3$ dyad {(130), (031)} of ozone through the analysis of hot bands in the 2300−2600 cm^{-1} region.

Barbe, A.; Mikhailenko, S.; Plateaux, J. J.; Tyuterev, Vl. G. (Groupe de spectrometrie Moleculaire et Atmospherique, UPRESA CNRS Q 6089, UFR Sciences, 51687 Reims, Fr.). *J. Mol. Spectrosc.* 1998, 187(1), 70−74 (Eng), Academic Press. Hot bands $\nu_1 + 3\nu_2 - \nu_2$ and $3\nu_2 + \nu_3 - \nu_2$ of $^{16}O_3$ in the region 2300−2600 cm^{-1} and the cold band $3\nu_2 + \nu_3$ in the region 3050−3110 cm^{-1}, corresponding to the $\nu_2 = 3$ dyad {(130), (031)}, were obsd. for the 1st time, using the Fourier Transform Spectrometer (FTS) at Reims and the usual exptl. setup providing a large product pressure × path length, p × l. Three hundred sixty-five rovibration energy levels of the upper states were obtained with J and K_a up to 46 and 9, resp. The fit of these data gives a root-mean-square deviation of 1.93×10^{-3} cm^{-1}. The ν_2 dependence of the rotational parameters A, B, and C for the $(1\nu_2 0)$ and $(0\nu_2 1)$ states is discussed.

ν_2, A, B, C

CA 1998, <u>128</u>, N 19

O_3

1998

128: 198019r **Analysis of high resolution measurements of the $2\nu_1+3\nu_3$ band of ozone: Coriolis interaction with the $\nu_1+3\nu_2+2\nu_3$ band.** Barbe, A.; Plateaux, J. J.; Tyuterev, Vl. G.; Mikhailenko, S. (Groupe Spectrometrie Moleculaire Atmospherique, Equipe Associee CNRS UPRESA D 1434, UFR Sciences, 51687 Reims, Fr.). *J. Quant. Spectrosc. Radiat. Transfer* 1998, 59(3–5), 185–194 (Eng), Elsevier Science Ltd.. The $2\nu_1+3\nu_3$ band of ozone, which occurs in the 5080 cm^{-1} region, was obsd. for the 1st time using a Fourier transform spectrometer, operating at 0.008 cm^{-1} resoln. and with a large path–length x pressure product (3616 cm x 42.8 torr). Assignment of rotation–vibration transitions was done for $J = 40$ and $K_a = 14$. It was necessary to account for the Coriolis coupling between the levels of the (203) and (132) states to correctly reproduce the energy levels, particularly for states with $K_a = 4$. In this way, the authors have obtained a very satisfactory root–mean–square error of 1.8×10^{-3} cm^{-1}, close to the exptl. accuracy. Line intensities of the $2\nu_1+3\nu_3$ band were measured and calcd., and transition moment consts. derived. Finally a complete list of line positions,a dn intensities was calcd., leading to a total band intensity of $S\nu=0.133 \times 10^{-21}$ cm^{-1}/mol cm^{-2} at 296 K.

(UK)

C.A. 1998, 128, N16

O_3

1998

129: 195049k **Infrared high−resolution spectra of ozone in the range 5500−5570 cm^{-1}: analysis of $\nu_2 + 5\nu_3$ and $\nu_1 + \nu_2 + 4\nu_3$ bands.** Barbe, A.; Chichery, A.; Tyuterev, Vi G.; Taskhun, S. A.; Mikhailenko, S. N. (Groupe de Spectrometrie Moleculaire et Atmospherique, Equipe Associee au CNRS UPRESA Q 6089, Universite de Reims, UFR Sciences, 51687 Reims, Fr.). *J. Phys. B: At., Mol. Opt. Phys.* 1998, 31(11), 2559−2569 (Eng), Institute of Physics Publishing. The $\nu_2 + 5\nu_3$ and $\nu_1 + \nu_2 + 4\nu_3$ bands of ozone, which occur in the 5500 cm^{-1} region, were obsd. for the 1st time using a Fourier transform spectrometer, operating at 0.008 cm^{-1} resoln. and with a large path length × pressure product (3216 cm × 28.3 torr). The assignment of rotation−vibration transitions was done for J up to 35 and Ka up to 12, for the $\nu_2 + 5\nu_3$ band and up to J = 40 and Ka = 2 for the $\nu_1 + \nu_2 + 4\nu_3$ band resp. The effective Hamiltonian used in calcns. accounts for the 1st−order Coriolis coupling between these two bands. As the levels corresponding to Ka = 5 are perturbed, it was necessary to account for anharmonic resonance with the (321) state. Also, to correctly reproduce the levels of (015) with Ka = 8, 9, 10 it was necessary to include a Coriolis coupling with (080) state in the model. In this way, the authors have obtained a very satisfactory root−mean−square deviation of 2.4×10^{-3} cm^{-1}, near the exptl. accuracy. Rovibrational line intensities of $\nu_2 + 5\nu_3$ and $\nu_1 + \nu_2 + 4\nu_3$ bands were measured and the value of the principal transition moment consts. were recovered. Finally a complete list of line positions and intensities was calcd. leading to the integrated band intensity of $S_\nu = 9.33 \times 10^{-23}$ cm^{-1}/mol. cm^{-2} for the $\nu_2 + 5\nu_3$ band and $S_\nu = 1.44 \times 10^{-23}$ cm^{-1}/mol. cm^{-2} for the $\nu_1 + \nu_2 + 4\nu_3$ band at 296 K with a cut−off of 3×10^{-26}.

(спектр)

C.A. 1998,
128, N15

O_3

1998

(ν_i)

130: 73147r **The $2\nu_1 + \nu_2 + 3\nu_3$ band of $^{16}O_3$: line positions and intensities.** Barbe, A.; Chichery, A. (Groupe Spectrometric Mol. Atmospherique, Equipe Associee, CNRS, 51687 Reims, Fr.). *J. Mol. Spectrosc.* 1998, 192(1), 102−110 (Eng), Academic Press. The $2\nu_1 + \nu_2 + 3\nu_3$ band of ozone, which occurs in the 5700−cm^{-1} region, was obsd. for the 1st time using a Fourier Transform Spectrometer, operating at 0.008 cm^{-1} resoln. and with a large pathlength × pressure product (3216 cm × 28.3 torr). The assignment of rotation−vibration transitions was done for J up to 38 and Ka up to 11, resp., after many difficulties due to a Coriolis coupling between (213) and (420) states. This 1, which occurs between closed band centers (4 cm^{-1}) but corresponds to $\Sigma_i\Delta\nu_i = 6$, strongly perturbs energy levels and leads to a difficulty in assignments. In particular the authors show the deviations for various types of J and

C. A. 1999, 130, N6

Ka as large as 1 cm^{-1}, with respect to the calcns. performed without account of this resonance. The final calcn. for the 212 rovibrational states is very satisfactory, as the root−mean−square is 2.5×10^{-3} cm^{-1}, near the exptl. accuracy, with meaningful spectroscopic Hamiltonian parameters. Rovibrational lines intensities of the $2\nu_1 + \nu_2 + 3\nu_3$ band were measured, and the value of the transition moment was recovered. Finally a complete list of line positions and intensities was calcd. (with a cut−off of 3×10^{-26} cm^{-1}/mol. cm^{-1}) leading to a total band intensity of $S_\nu = 3.118$ 10^{-23} cm^{-1}/mol. cm^{-2} at 296 K. (c) 1998 Academic Press.

O_3 Om. 39477 1998

Bouvier A.J., et al.,

J. Mol. Spectrosc.,

M.n. 1998, <u>190</u>, 189-197

O_3 Bouvier A. J.; 1998

Analusis 1998, 26(4), M69-M72

Near infrared absorption spectra of ozone by high-resolution Fourier transform spectroscopy.

$(^3A_2 \leftarrow \tilde{X}\,^1A_1)$
FTIR

Получены структур
паром., и спектр.
постоянн

C.A. 1998, 129, N18, 237045p

O_3

1998

(Vi)

129: 33874y **Vibrational relaxation study of O_3 in rare gas and nitrogen matrixes by time resolved infrared–infrared double resonance spectroscopy.** Dahoo, P. R.; Jasmin, D.; Brosset, P.; Gauthier–Roy, B.; Abouaf–Marguin, L. (Laboratoire de Physique Moleculaire et Applications, Universite Pierre et Marie Curie, 4 place Jussieu, 75252 Paris, Fr.). *J. Chem. Phys.* 1998, 108(20), 8541–8549 (Eng), American Institute of Physics. A time resolved IR–IR double resonance technique is used to study the vibrational relaxation of O_3 in rare gas and N matrixes. A tunable IR pulsed source excites the $\nu_1+\nu_3$ level of O_3 in the ground electronic state. A continuous wave (cw) CO_2 laser probes the populations of the fundamental and $v_2 = 1$ levels as a function of time. After minimization of thermal effects, the relaxation signal can be analyzed. At fixed probe frequency, the behavior of the rise time of the signals with the pump frequency shows spectral diffusion to occur inside the inhomogeneous profiles. At high concn. in Ar (O_3/Ar = 1/250), intermol. energy transfer is obsd. between the 2 sites. In Xe matrixes, it has time to take place at concns. 1/2000. The relaxation rates of the $v_2 = 1$ level to the ground state are measured at different concns. in rare gas and N matrixes. At high diln., a max. relaxation time, called intrinsic relaxation time τ_i, is detd. in the different matrixes: it covers 3 orders of magnitude, from a few hundred nanoseconds in Ne to 320 μs in Xe. The results are discussed and compared with literature data within the frame of the isolated binary collision model.

C. A. 1998, <u>129</u>, N 3

O_3

1998

эм:40080

Обзор. ИК
и м/в
спектр

128: 222885t **The ozone molecule: infrared and microwave spectroscopy.** Flaud, J. M.; Bacis, R. (Laboratoire de Photophysique Moleculaire, CNRS, Universite Paris–Sud, 91405 Orsay, Fr.). *Spectrochim. Acta, Part A* 1998, 54A(1), 3–16 (Eng), Elsevier Science B.V.. A review with 84 refs. is given on vibrational state, mol. rotation and transition moment transitions for ozone mols. An effect of the isotopic substitution is discussed.

CA· 1998, 128, N18

$^{18}O_3$

$^{16}O_3$

1998

are discussed.

128: 276409j **Rotational structure in the absorption spectra of $^{18}O_3$ and $^{16}O_3$ near 1 μm: A comparative study of the $3A_2$ and $3B_2$ states.** Gunther, Jurgen; Anderson, Stuart M.; Hilpert, Georg; Mauersberger, Konrad (Bereich Atmospharenphysik, Max–Planck–Institut fur Kernphysik, Heidelberg, Germany). *J. Chem. Phys.* 1998, 108(13), 5449–5457 (Eng), American Institute of Physics. Absorption spectra for $^{16}O_3$ and $^{18}O_3$ near 1 μ were recorded to explore the rotational structure assocd. with the $^3A_2$ and $^3B_2$ electronic states of ozone. Rotational features within the $^3A_2$ $^1A_1$ 1–0 band respond predictably to isotopic substitution, enabling detn. of the upper state adiabatic electronic energy and asym. stretching frequency via isotope shift techniques. The authors find an adiabatic energy of 9963 ± 4 cm^{-1}, in excellent agreement with that detd. earlier from vibronic isotope shifts obsd. at lower resoln., 9990 ± 70 cm^{-1}. The authors also find an asym. stretching frequency of 367 ± 17 cm^{-1}, indicating that the $^3A_2$ state potential energy surface is bound against dissocn. to $O+O_2$ despite the fact that it lies above the corresponding dissocn. limit. Rotational structure assocd. with transitions to the $^3B_2$ state is detected for the 1st time. It responds anomalously to ^{18}O substitution. The geometry of the upper state for $^{18}O_3$ appears to differ markedly from that for $^{16}O_3$ ($\Delta\theta \approx -4$ deg, or $\Delta r_e \approx +0.07$ A), suggesting that the $^3B_2$ surface is strongly anharmonic and precluding a straightforward anal. of the isotope shifts.

Вращат.
спектр
вблизи
1μ

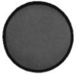
C.A. 1998, 128, N22

O_3 От. 40078 1998

Inard D., et al.,

Chem. Phys. Lett.,
1998, 287, 575-524.
Absorption cros[illegible]s- sections
and lifetime of [illegible] the $^3A_2$ „meta-

stable" state of ozone.



O_3

1998

129: 101293k **Theoretical investigation of Wulf and Chappuis bands in the spectrum of ozone.** Minaev, B. F.; Kozlo, E. M. (Cherkassk Engineering and Technological Institute, Ukraine). *J. Struct. Chem.* 1997 (Pub. 1998), 38(6), 895–900 (Eng), Consultants Bureau. The ground state and some lowest excited states of ozone are calcd. by the semiempirical MNDO method using CI to explain the Wulf near-IR absorption band and photodissocn. of ozone. The results of calcns. show that $^3A_2(1^3A)$ is the lowest excited triplet state of O_3; a transition to this state from the ground X^1A_1 state is responsible for the weak Wulf absorption. The oscillator strength (f = 3.2×10^{-7}) and the radiative lifetime of the $^3A_2$ state ($\tau = 0.01$ s) are in agreement with recent ab initio calcns.

$^3A_2(1^3A)$ – нижнее возб. сост., Σ

CA, 1998, 129, №8

O_3

1398

теор. расчет изомеров

129: 250407c. A systematic ab initio investigation of the open and ring structures of ozone. Muller, Thomas; Xantheas, Sotiris S.; Dachsel, Holger; Harrison, Robert J.; Nieplocha, Jaroslaw; Shepard, Ron; Kedziora, Gary S.; Lischka, Hans (Institut fur Theoretische Chemie und Strahlenchemie, Universitat Wien, A-1090 Vienna, Austria). *Chem. Phys. Lett.* 1998, 293(1,2), 72-80 (Eng), Elsevier Science B.V.. The energy difference between the open and the ring isomer of ozone as well as the dissocn. energy ($O_3(X,{}^1A_1) \rightarrow O_2(X,{}^3\Sigma^-_g) + O({}^3P)$) have been detd. at the CCSD(T), MR-CISD and MR-AQCC levels of theory. Using correlation consistent basis sets up to quintuple-zeta quality, the estd. complete basis set limits for CCSD(T) and MR-AQCC lie within 1 kcal/mol of the exptl. value of 26.1 ± 0.4 kcal/mol and place the ring isomer by 4.8 and 5.3 kcal/mol, resp., above the dissocn. limit. Zero-point vibrational corrections increase the latter two values by 1.4 kcal/mol.

С. А. 1998, 129, N 19

O_3

1998

Энергии ионизации

130: 86380m **Single−reference electron propagator calculations on vertical ionization energies of ozone.** Ortiz, J. V. (Department of Chemistry, Kansas State University, Manhattan, KS 66506−3701 USA). *Chem. Phys. Lett.* 1998, 297(3,4), 193−199 (Eng), Elsevier Science B.V.. Vertical ionization energies of ozone are calcd. with electron propagator methods that employ a single ref. configuration. Ref. determinantal wave functions are defined by Hartree−Fock orbitals or by approx. Brueckner orbitals from a coupled−cluster wave function. An accurate description of the lowest $^2A_1$, $^2B_2$, and $^2A_2$ cationic states requires retention of terms in the superoperator Hamiltonian matrix that have been safely neglected in calcns. on the ionization energies of typical, closed−shell mols.

C.A. 1999, 130, N 7

O_3 1998

129: 32536c A refined potential energy surface and the rovibrational states for the electronic ground state of ozone. Yan, Guosen; Xian, Hui; Xie, Daiqian (Department of Chemistry, Sichuan University, Chengdu, Peop. Rep. China 610064). *Mol. Phys.* **1998**, 93(6), 867–872 (Eng), Taylor & Francis Ltd.. A potential energy surface for the electronic ground state of ozone was optimized by using a variational procedure with the exact vibrational Hamiltonian in bond–length–bond–angle coordinates. In the optimization, the ab initio force field of P. Borowski et al. (1992, J. Chem. Phys., 97, 5568) was taken as the starting point taking into account the recently obsd. vibrational band origins up to 4900 cm^{-1} reported by J. Floud et al. (1996, J. molec. Spectrosc., 177, 34). The root mean square error of this fit for the 39 obsd. vibrational energy levels is 0.83 cm^{-1}. In order to test the refined potential, the rovibrational energy levels up to J = 15 were calcd. and compared with the obsd. values.

потенц пов-ть, Di, теор расч

C. A. 1998, 129, N3

1998

F: O3
P: 3
22Б1388. Фурье-спектры высокого разрешения NO[2] и O[3] в области частот 12500-40000 см{-1} при атмосферных температурах и давлении. High-resolution Fourier transform spectra of NO[2] and O[3] in the 12500-40000 cm{-1} range at atmospheric temperatures and pressures / Voigt Susanne, Orphal Johannes, Burrows John P. // 53rd Ohio State Univ. Int. Symp. Mol. Spectrosc., Columbus, Ohio, June 15-19, 1998. - [Columbus (Ohio)], 1998. - C. TB10. - Англ.

ФЖХ, 1998, №22

F: O3
P: 3

em. 40091

1999

132:56344 A comparative rotational analysis of the 000 bands of the 3A2 X1A1 Wulf transition for the isotopomers 16O3 and 18O3 of ozone by high resolution Fourier transform spectrometry. Bouvier, A. J.; Veyret, V.; Russier, I.; Inard, D.; Churassy, S.; Bacis, R.; Brion, J.; Malicet, J.; Judge, R. H.

Laboratoire de Spectrometrie Ionique et Moleculaire (associe au CNRS U.M.R. 5579) Universite Claude Bernard Lyon I Villeurbanne 69622, Fr.

Spectrochim. Acta, Part A, 55A(14), 2811-2821 (English) 1999 A high resoln. Fourier transform spectrometry comparative anal. of the rotational structure of the 000 absorption band of the 3A2 X1A1 Wulf transition for the isotopomers 16O3 and 18O3 of the ozone mol. is presented. With a near pure case (b) coupling model for the upper triplet state, the

C.A.-2000, 132

for the 3A2 state to <100 unperturbed rotational lines in the range 9100-9550 cm-1 for each band. Using for each of them the well defined ground state parameters, the authors obtained a std. deviation of ~0.050 cm-1 in the fits to the lines. The rotational consts. A, B, C, the 3 rotational distortion terms .DELTA.K, .DELTA.K, .DELTA.J, the spin-rotation consts. a0, a, and b and the spin-spin const. .alpha. are detd. for the (0 0 0) vibrational level of the 3A2 state and of the 2 isotopomers. The parameter .beta. arbitrarily fixed for 16O3 was successfully calcd. for 18O3 and this last result justifies the .beta. value adopted for 16O3. The geometrical parameters of the 3A2 state for the 2 isotopomers are close, r = 1.343 A, .theta. = 98.8.degree. for 18O3 and r = 1.345 A, and .theta. = 98.9.degree. for 16O3 and so are the .DELTA. and .kappa. values. The origin of the 18O3 000 band is blue shifted by 20.6(4) cm-1 with respect to the 16O3 000 band. For the congested parts of the spectra comparisons of both isotopic species has to be done in a special way through sub-band contours. The authors justify the existence of perturbations in the 1st vibrational levels of the 3A2 state by several crossings with high vibrational levels of the ground state.

F: O3
P: 3

1999

132:56347 Spectroscopy of O3 trapped in rare gas matrices. I. Theoretical model for low-lying vibrational levels. Dahoo, P. R.; Lakhlifi, A.; Chabbi, H. Laboratoire de Physique Moleculaire et Applications du CNRS, Universite Pierre et Marie Curie Paris 75252, Fr. J. Chem. Phys., 111(22), 10192-10201 (English) 1999 A theor. model is elaborated which allows methods used in gas phase to be applied to calc. the vibrational energies and transition moments for low-lying levels of O3 trapped in rare gas matrixes. The model used in a previous work allowed only one mode to be handled at a time. With the new approach, an overall treatment of low-

C.A. 2000, 132

lying levels is achieved. The trapping site, a single or double substitutional 1 is distorted to minimize the free energy of the mol.-matrix system. The mol. is considered to be submitted to the net elec. field present in the site as the result of the distortion and polarization of the matrix atoms. New harmonic and anharmonic consts. that lead to matrix dependent calcd. energy levels and transition moments can then be detd. Besides confirmation of 2 trapping sites, a single (S1) and a double (S2) substitutional site in a distorted fcc. lattice structure, 2 other S1 sites in Ar and Kr in a distorted hexagonal-closed-packed (hcp.) lattice structure are possible. A fit within exptl. uncertainty is reached between obsd. and calcd. frequencies for fundamental bands v1, v2, and v3.

F: O3
P: 3

1999

132:40781 Protonated Ozone: Structure, Energetics, and Nonadiabatic Effec Ceotto, Michele; Gianturco, Franco A.; Hirst, David M. Department of Chemistry, The University of Rome Rome 00185, Italy J. Phys. Chem. A, 103(48), 9984-9994 (English) 1999 Fully correlated calcns. using a multiconfiguration-self-consistent-field (MCSCF) treatment have been carried out to find the most stable structure [O3H]+ and to improve on earlier calcns. on the same system. The results used to evaluate proton affinity (PA) and gas-phase basicity of the ozone quantities which can be compared with exptl. data. The existence of regi nonadiabatic coupling and of charge-exchange effects is evidenced and ana with avoided crossings specifically located for one of the four most stab protonated adducts of ozone. The present study extends the level of accu achieved in earlier calcns. on the possible structures for protonated ozo gives specific suggestions on the microscopic processes for the formation [O3H]+ in the gas phase.

C.A. 20,

1999

F: O3
P: 1

131:122382 New Analysis of 2.nu.1 + .nu.2, .nu.1 + .nu.2 + .nu.3, and .nu 2.nu.3 Bands of Ozone in the 2600-2900 cm-1 Region. Mikhailenko, S.; Barb A.; Plateaux, J. J.; Tyuterev, Vl. G. (Laboratory of Theoretical Spectros Institute of Atmospheric Optics, Tomsk 634055, Russia). J. Mol. Spectros 196(1), 93-101 (English) 1999 The 2600-2900 cm-1 spectral range is revisited for an accurate detn. of l intensities of the 2.nu.1 + .nu.2, .nu.1 + .nu.2 + .nu.3, and .nu.2 + 2.n bands of ozone. The fit on 1702 energy levels of (012), (111), and (210) detd. from obsd. transitions with Jmax .ltoreq. 61 and Ka max .ltoreq. 17 a root-mean-square = 5.6 .times. 10-4 cm-1 and provides a

C.A.1999,131

3^{3} картотека!

satisfactory ag between calcd. and obsd. line positions. Line intensities were measured fitted, leading to the detn. of transition moment parameters for the 3 ba Using these parameters, the authors have obtained the following estns. fo integrated band intensities S(.nu.1 + .nu.2 + .nu.3) = 2.509 .times. 10-2 S(.nu.2 + 2.nu.3) = 0.330 .times. 10-20, and S(2.nu.1 + .nu.2) = 0.0802 . 10-20 cm-1/mol cm-2 at 296 K, with a cutoff of 10-26 cm-1/mol cm-2. The of the .mu.(210)-(000)1 parameter assocd. with the .phi.x operator for 2. .nu.2 band obtained in anal. appears to be 8 times smaller than the previ detd. value of this parameter [M. A. H. Smith, C. P. Rinsland, J. M. Flau Camy-Peyret, and A. Barbe, J. Mol. Spectrosc. 139, 171-181(1990)]. The g line listing of the 2.nu.1 + .nu.2, .nu.1 + .nu.2 + .nu.3, and .nu.2 + 2. bands (up to Jmax = 70 and Ka max = 23) was generated with an intensity c 10-26 cm-1/mol cm-2. The perturbations of (111) and (012) states by the state are discussed

F: O3
P: 3

1999

131:357474 Determination of the Effective Ground State Potential Energy Function of Ozone from High-Resolution Infrared Spectra. Tyuterev, Vl. G. Tashkun, S.; Jensen, P.; Barbe, A.; Cours, T. Groupe de Spectroscopie Moleculaire et Atmospherique, Equipe Associee, UFR Sciences, CNRS UPRESA Reims 51687, Fr. J. Mol. Spectrosc., 198(1), 57-76 (English) 1999

The effective ground state potential energy function of the ozone mol. near the C2v equil. configuration was obtained in a least-squares fit to largest sample of exptl., high-resoln. vibration-rotation data used for t purpose so far. The fitting is based on variational calcns. carried out the extended Morse Oscillator Rigid Bender Internal Dynamics model. The potential function is expanded in Morse-type functions of the stretching variables and in cosine of the bending angle. The present calcn. produce results in significantly better agreement with expt. than previous detns. potential energy surface, and the energies predicted with the new surface sufficiently accurate to be useful for the assignment of new high-resoln. spectra. The root-mean-square deviation of the fit of rovibrational data J = 5 is 0.02 cm-1. For the set of all 60 band centers of the 16O3 mol. included in the Atlas of Ozone Line Parameters, the root-mean-square devi is 0.025 cm-1, and for all band centers detd. so far from high-resoln. sp including those recently obsd. and assigned in Reims corresponding to hig excited stretching and bending vibrations (v1 + v2 + v3 = 6), the root-me square deviation is 0.1 cm-1. The dark states that produce resonance perturbations in the obsd. bands are described with exptl. accuracy up to (v1v2v3) = (080) state. Extrapolation tests demonstrate the predictive p the potential function obtained: rotational extrapolation up to J = 10 fo 11 lowest vibrational states results in an root-mean-square deviation of cm-1. Vibrational energies measured by low-resoln. Raman spectroscopy (w were not included in the input data for the fit) are calcd. within the ex accuracy (root-mean-square = 1.6 cm-1) of the exptl. values up to the dis limit. The statistical anal. suggests that the accuracy of the equil. ge and force consts. of the mol. is considerably improved relative to previo detns. The long-range behavior of the fitted potential at the dissocn. l .fwdarw. O2 + O shows agreement with exptl. data. The new potential ener surface was used to predict the band centers of the isotopomers 17O3 and

1999

F: 03
P: 3

131:248516 Adiabatic states of ozone using Fock space multireference coup cluster method. Vaval, Nayana; Pal, Sourav Physical Chemistry Division, National Chemical Laboratory Poona 411 008, India J. Chem. Phys., 111(9), 4051-4055 (English) 1999 In this paper we present the Fock space multi-ref. coupled cluster theor suitable for calcn. of low-lying adiabatically excited or electron attach states. Low-lying adiabatic as well as vertical excited states of ozone calcd. using this theory in the singles and doubles approxn. The calcd. adiabatic excitation energies are compared with the exptl. values. We al report the adiabatic electron affinity value of ozone.

F: 03
P: 3

2160

133:141877 Infrared Spectroscopy of Neat Solid Ozone and That of Ozone in Interaction with Amorphous and Crystalline Water Ice. Chaabouni, H.; Schriver-Mazzuoli, L.; Schriver, A. Laboratoire de Physique Moleculaire et Applications, Universite Pierre et Marie Curie Paris 75252, Fr. J. Phys. Chem. A, 104(30), 6962-6969 (English) 2000. The interaction of ozone with ice films under high vacuum was studied with single reflection FTIR spectroscopy (incidence angle of 5.degree.). Both amorphous and cryst. ice were studied. On amorphous ice which has a high d. of free surface OH groups two states of ozone were obsd.: one which forms a H bond with the ice surface of the micropores, and a 2nd which is attributed to a physisorbed state. Only the latter state is obsd. on the cryst. ice surface. When chemisorbed ozone is covered by an amorphous film, a temp. increase >60 K leads to diffusion (with a weak yield) of ozone in the H2O lattice. Absorbed ozone remains in the ice bulk until sublimation of the ice film near 155 K.

2000

F: O3
P: 3
132:187010 Intensities of the difference bands .nu.1+.nu.3-.nu.2 and 2.nu .nu.2 of ozone. Comparison with theoretical predictions.

Chichery, A.; Barbe, A.; Tyuterev, V. G.; Sulakshina, O.; Borkov, Y. Faculte des Sciences, Groupe de Spectrometrie Moleculaire et Atmospherique, CNRS Q 60 UPRESA Reims 51687, Fr. J. Mol. Struct., 517-518, 165-170 (English) 2000 The IR spectra of 16O3 in the range 1300-1500 cm-1 were recorded at high resoln. (0.007 cm-1), with a large product p.times.l = 32.4 torr.times.3212 cm, and a good S/N ratio.simeq.500. This enabled one to obsd. the 3.nu.2-.nu.2 band and to extend the measurements of the 2.nu.2 (A. Barbe,

C.A. 2000, 132

A. Chichery, Vl.G. Tyuterev, S. Taskhun, S. Mikhailenko, Spectrochimica Acta 54A (1998) 1935-1945). Two difference bands 2.nu.3-. and .nu.1+.nu.3-.nu.2 were obsd. as well. The positions of the lines are known due to the studies of cold bands 2.nu.1, .nu.1+.nu.3, 2.nu.3 as wel .nu.2. In this region only intensity measurements of the .nu.1+.nu.3-.nu combination band were done so far. Here, due to the large pressure .time pathlength product, the authors are able to observe a large range of transitions for .nu.1+.nu.3-.nu.2 band (up to J = 51 and Ka = 14), and al for the 1st time 2.nu.3-.nu.2 band. The authors have derived the transit moment parameters for 2.nu.3-.nu.2 and estd. an upper limit for 2.nu.1-.n A complete final calcn. is performed for these difference bands. The principal transition moment parameters are compared with theor. predictio

F: O3
P: 3

2000

132:257423 The .nu.1 and .nu.3 bands of the 16O17O17O isotopomer of ozone. Perrin, A.; Flaud, J.-M.; Valentin, A.; Camy-Peyret, C.; Gbaguidi, N.; N'Gom, A. Laboratoire de Photophysique Moleculaire, CNRS, Universite Paris Sud Orsay, Paris 91405, Fr.
J. Mol. Struct., 517-518, 157-163 (English) 2000

C.A. 2000

[illegible] Using 0.002 cm-1 resoln. Fourier transform absorption spectra of an 17O enriched ozone sample, an extensive anal. of the .nu.3 band together with a partial identification of the .nu.1 band of the 16O17O17O isotopomer of ozone was performed for the 1st time. The exptl. rotational levels of the (001) and (100) vibrational states could be satisfactorily reproduced using an Hamiltonian matrix which takes into account the obsd. rovibrational resonances. Actually, as for other Cs-type ozone isotopomers [J.-M. Flaud and R. Bacis, Spectrochimica Acta, A54(1998) 3-16], the (001) rotational levels are involved in both Coriolis and Fermi type resonances with the levels from the (100) vibrational state. Using an Hamiltonian matrix which takes explicitly into account these resonances precise vibrational energies and rotational and coupling consts. were deduced and the following band centers .nu.0(.nu.3)=1017.5336 cm-1 and .nu.0(.nu.1)=1080.153 cm-1 were obtained for the .nu.3 and .nu.1 bands resp.

F: O3
P: 3

2000

133:327523 Photodissociation of O3 around 309 nm.

Taniguchi, Nori; Takahashi, Kenshi; Matsumi, Yutaka Solar-Terrestrial Environment Laboratory and Graduate School of Science, Nagoya University Toyokawa Aichi 442-8507, Japan J. Phys. Chem. A, 104(39), 8936-8944 (English) 2000.

Photodissocn. reaction of O3 following UV photon excitation around the thermodn. threshold of the dissocn. channel of O(1D) + O2(a1.DELTA.g) at 309.44 nm has been studied under room-temp. and jet-cooled conditions. Both O(1D) and O(3P) photoproducts are detected by a technique of vacuum UV laser-induced fluorescence (VUV-LIF) spectroscopy. Photofragment excitation (PHOFEX) spectra for the O(1D) and O(3P) atoms are obtained by scanning the photolysis laser wavelength between 297 and 316 nm while monitoring VUV-

LIF signal intensities at 115 and 130 nm for O(1D) and O(3P), resp. From the behavior of the PHOFEX spectra for the O(3P) and O(1D) atoms around the threshold into O(1D) + O2(a1.DELTA.g), the existence of an exit barrier along the O-O2 dissocn. coordinate in the photoexcited electronic state of O3 is suggested. Anal. of the line widths in the jet-cooled PHOFEX spectra of O(1D) and O(3P) suggests that the quasi-bound states below the barrier and above the threshold have lifetimes of 0.2-0.8 ps. The O(1D) quantum yield values from the O3 photolysis are obtained from the PHOFEX spectrum for O(3P) at 295 K. The O(1D) quantum yields between 297 and 305 nm are almost independent of the photolysis wavelength (.apprxeq.0.89), which is smaller than the current NASA/JPL recommendation for atm. modeling (0.95). The phys. model for O(1D) formation in the photolysis of O3 in the wavelength range 305-329 nm is presented, which can quant. explain the temp. and wavelength dependence of O(1D) quantum yield.

2000

F: O3
P: 3

132:127918 Variational EKE-calculations of rovibrational energies of the ozone molecule from an empirical potential function. Tyuterev, V. G.; Tashkun, S. A.; Schwenke, D. W.; Jensen, P.; Cours, T.; Barbe, A.; Jacon, U.F.R. Sciences, Groupe de Spectroscopie Moleculaire et Atmospherique UPRESA CNRS Q 6089 Reims 51687, Fr. Chem. Phys. Lett., 316(3,4), 271-279 (English) 2000 We report rovibrational calcns. from an empirical potential energy

C. A. 2000, 132

surface (PES) of the electronic ground state of ozone, using an exact kin energy (EKE) operator. The PES was optimized using the EKE Hamiltonian a exptl. spectroscopic high-resoln. data. The RMS deviation of calcns. for exptl. band centers directly obsd. so far in high-resoln. spectra is 0.12 1. The RMS deviation of calcns. of rotational energies up to J.ltoreq.5 0.002 cm-1 for the (000) level and 0.015 cm-1 for five lowest vibrational states. Both rotational and vibrational calcns. are more accurate than presently available EKE-calcns. for O3. The PES shows a phys. meaningful long-range behavior at the dissocn. limit.

2000

F: O3
P: 3

133:258535 Potential function of the ozone molecule: global calculations of the rovibrational states and the dissociation behavior. Tyuterev, Vladimir G.; Cours, T.; Tashkun, Sergey A.; Barbe, Alain; Jensen, P. Groupe de Physique Moleculaire et Atmospherique, UPRESA, CNRS Q 6089, UFR Sci. Reims, Fr. Proc. SPIE-Int. Soc. Opt. Eng., 4063, 142- 151 (English) 2000.

Various empirical and ab initio potential energy surfaces (PES) of ozone are compared with recent accurate PES obtained by a variational fit to spectroscopic data. The value of the dissocn. energy De obtained from this PES agrees well with recent exptl. values. Problems in the normal mode assignment of highly excited vibrational states are discussed.

F: 03
P: 3

2000

132:243300 Measurements of 18O-Enriched Ozone Isotopomer Abundances Using High-Resolution Fourier Transform Far-IR Spectroscopy. Wugt Larsen, R.; Larsen, N. W.; Nicolaisen, F. M.; Sorensen, G. O.; Beukes, J. A. Institut of Chemistry, Department of Molecular Spectroscopy, University of Copenha Copenhagen DK-2100, Den. J. Mol. Spectrosc., 200(2), 235-247 (English) 2000 The distribution of ozone isotopomers in ozone mixts. produced by elec. discharge in mixts. of 16O2 and 18O2 at 77 K was measured by high-resoln. FTIR spectroscopy. It was of key importance to assess not only the total amt. of isotopomers of a certain mass but also the relative amts. of corresponding asym. and sym. ozone species of the same mass given as the

C.A. 2000, 132

ratios [160160180]/[160180160] and [160180180]/[180160180]. For many purposes both ratios were assumed to have the statistical value 2.00. Pu rotational spectra in the far-IR region (30-100 cm-1) were recorded for 3 different 180-enriched ozone mixts., all at 0.00185 cm-1 resoln. All the spectra were cor. for thermal emission. Linestrengths for individual lin in a particular spectrum were measured by a fitting technique taking into account contributions from all other lines in the spectrum. For this pur theor. linestrengths for all 6 ozone species contg. 160 and 180 obtained a quantum-no.-dependent dipole operator were used. The ratios between ob and theor. linestrengths were used to det. the abundances of individual isotopomers in a particular ozone mixt. For one of the ozone samples the abundances of all 6 ozone species were detd. within 1% relative uncertain For the 3 ozone mixts. studied, the ratio between asym. and sym. species mono-180 ozone were 1.99(2), 2.01(2), and 2.10(6). The ratio between asy and sym. species of di-180 ozone were 2.51(4), 2.42(10), and 2.46(3).

$^{16}O_3$

2000

структура, потенц ф-ии, Di, теор.-расч

132: 353043x **Accurate ab initio near−equilibrium potential energy and dipole moment functions of the ground electronic state of ozone.** Xie, Daiqian; Guo, Hua; Peterson, Kirk A. (Department of Chemistry and Albuquerque High Performance Computing Center, University of New Mexico, Albuquerque, NM 87131 USA). *J. Chem. Phys.* 2000, 112(19), 8378−8386 (Eng), American Institute of Physics. We report a highly correlated multireference CI calcn. of the near−equil. potential energy surface of ozone using a large correlation consistent basis set. Three−dimensional anal. expressions are obtained for the potential energy and dipole moment functions using least−squares fits to ab initio points near the C_{2v} equil. geometry. Low−lying

C. A. 2000, 132, №26

vibrational band origins of $^{16}O_3$ and some of its isotopic variants are calcd. using the ab initio potential energy function. The calcd. fundamental frequencies for the sym. stretching and bending vibrations are within about 3 cm^{-1} of the obsd. values, while that for the antisym. stretch deviates from expt. by about 13 cm^{-1}. The agreement with expt. can be significantly improved if the ab initio potential energy function is scaled in the antisym. stretching coordinate. Abs. IR absorption intensities are also calcd. using ab initio elec. dipole moment functions and in good agreement with the available exptl. data.

O_3

2000

поверхность
потенц. функ
ции

132: 353047b Algebraic approach to the potential energy surface for the electronic ground state of ozone. Zheng, Y.; Ding, S. (Institute of Theoretical Chemistry, Shandong University, Jinan, Shandong, Peop. Rep. China). *Chem. Phys.* 2000, 255(2−3), 217−221 (Eng), Elsevier Science B.V. A potential energy surface for the electronic ground state of the O_3 mol. is obtained using U(4) group. This potential energy surface includes the information of bending motion. Addnl., some properties, for example, saddle points, are discussed.

C.A. 2000, 132, N26

O_3

2000

поверхность потенц. ф-ии

132: 353045z **Dynamical symmetric group approach to potential energy surface of molecule O_3.** Zheng, Yujun; Ding, Shiliang (Institute of Theoretical Chemistry, Shandong University, Jinan, Peop. Rep. China 250100). *Chin. Sci. Bull.* 2000, 45(4), 331–334 (Eng), Science in China Press. The Hamiltonian of O_3 mol. is written in terms of Casimir and Majorana operators using coherent states and the corresponding potential energy surface (PES) is obtained. The PES and contours are plotted. The calcd. force consts. and dissocn. energies are in good agreement with exptl. values.

C.A. 2000, 132, №26

^{16}O (тонкая стр-ра)
^{17}O (сверхтонк. стр-ра)
^{18}O

От. 41 152

2001

Blondel C., Delsart C. et al.,

Ae

Phys. Rev. 2001, 64, 052504-1 —— 052504-8

Electron affinities ~~of~~ ^{16}O, ^{17}O,

$^{18}\mathrm{O}$, the fine structure of $^{16}\mathrm{O}^{-}$, and the hyperfine structure of $^{17}\mathrm{O}^{-}$.

F: O3
P: 3

DM · 41268

2001

134:345856 **Spectroscopy and predissociation of the 3A2 electronic state of ozone 16O3 and 18O3 by high resolution Fourier transform spectrometry.** Bouvier, A. J.; Wannous, G.; Churassy, S.; Bacis, R.; Brion, J.; Malicet, J.; Judge, R. H. Laboratoire de Spectrometrie Ionique et Moleculaire (associe au CNRS U.M.R. 5579), Universite Claude Bernard Lyon I, Villeurbanne, Fr. Spectrochim. Acta, Part A (2001), 57A(3), 561-579. in English.

A high resoln. Fourier transform spectrometry anal. of the rotational structure of the 201 absorption bands of the 3A2←X~1A1 Wulf transition for the isotopomers 16O3 and 18O3 of the ozone mol. is presented. These bands are very intense compared to the 000 bands but the predissocn. is so strong that the main sub-bands appear as continuous contours. Isolated lines and band contour methods were used together to analyze these two rovibrational bands. The lines corresponding to the F2 component are generally the most intense and isolated. The authors' data sets for the (0 1 0) level of the 3A2 state are limited to .apprx.102 weakly or unperturbed rotational lines for the 201 of 16O3 in the range 9620-10140 cm-1 and 123 weakly or unperturbed rotational lines for the same band of 18O3. Using for each of them the well-defined ground state parameters, the authors obtained a std. deviation of .apprx.0.035 cm-1 in the fit to the lines for 16O3 and 0.027 cm-1 in the case of 18O3. The rotational consts. A, B and C, the three rotational distortion terms ΔK, ΔJK and ΔJ, the spin-rotation consts. a0, a and b were successfully calcd. for 16O3 and 18O3 while the spin-spin consts. were fixed to their resp. values obtained for the origin bands. As is the case for the 000 band, the authors have a partial agreement with the isotopic laws for the rotational consts. The geometrical parameters of the (0 1 0) level of 3A2 state for the two isotopomers are close, r = 1.357 .ANG., 0 = 100.7° for 18O3 and r = 1.352 .ANG. and 0 = 100.0° for 16O3. The origin of the 201 band of 18O3 is red shifted by 7.06(4) cm-1 with respect to 16O3 201 band and the two bending mode quanta are, resp., 528.99(9) and 501.34(7) cm-1. A preliminary qual. anal. of the predissocn. is given in the particular case of the F2 spin component of 16O3 for 000 and 201 bands by the measurement of shifts of positions of some rovibrational levels and the evolution of predissocn. broadenings in QQ2 branches. The authors justify the existence of perturbations in the rovibrational levels of 3A2 state through different interaction types: with the dissocn. continuum of the same electronic state or with high vibrational repulsive or weakly bound levels of the ground state.

O_3

2001

135: 142523c Gas−phase proton affinity of ozone: a computational test of the experimental mechanism. Ceotto, M.; Gianturco, F. A. (Dipartimento di Chimica, Citta Universitaria, 00185 Rome, Italy). *THEOCHEM* 2001, 543, 115−122 (Eng), Elsevier Science B.V. Extended ab initio calcns. were carried out for the isolated ozone mol., in its ground

(Ap)

C.A. 2001, 135, N10.

electronic state, and for its protonated adduct. For both systems, the corresponding nuclear geometries of lowest total energies were obtained by multidimensional optimization; different levels of basis set quality and correlation correction were examd. in the two cases. The final results provide very good accord between gas-phase protonation energy data and calcd. quantities. The extensive numerical expts. clearly underline the need for balanced correlation treatments in systems where both static and dynamic correlation effects are important. They further indicate that the existing kinetics expts. on the gas–phase proton affinity of O_3 are not likely to involve the electron transfer channel via a sampling of the conical intersection configuration space that exists in this system.

$^{18}O_3$

2001

135: 99067t Analysis of High−Resolution Spectra of $^{18}O_3$. Chichery, A.; Barbe, A.; Tyuterev, Vl. G.; Bourgeois, M. T. (Groupe de Spectrometrie Moleculaire et Atmospherique, Equipe Associee au CNRS, UPRESA Q 6089, UFR Sciences, 51687 Reims, Fr.). *J. Mol. Spectrosc.* 2001, 206(1), 1−13 (Eng), Academic Press. Using a Fourier transform spectrometer, the authors have recorded the spectra of the $^{18}O_3$ species of ozone in the region 1300−3100 cm^{-1}, with a resoln. of 0.003 cm^{-1}. The large product pathlength × pressure enable one to record 18 bands, 14 for the 1st time. The anal. was performed using effective Hamiltonians for polyads of strongly interacting states for ozone, accounting for Coriolis and anharmonic resonances. The spectral parameters are derived for 16 vibrational states, including the 2 dark states (040) and (130). Various resonances are studied through the mixing coeffs. of rovibrational wavefunctions. Systematic intensity measurements allow detn. of transition moment parameters for 16 bands. Finally, a complete list of all transitions from 1300 to 3100 cm^{-1}, with cutoffs 10^{-26} cm^{-1}/mol cm^{-2} (296 K), is calcd. (c) 2001 Academic Press.

Фурье-спектр
М.П.

C.A. 2001, 135, N7

$^{16}O_3$

2001

абсолютн-
интенсивн-
ν_1 и ν_3

135: 99072r **Absolute Intensities of the ν_1 and ν_3 Bands of $^{16}O_3$:** Claveau, C.; Camy–Peyret, C.; Valentin, A.; Flaud, J.–M. (Laboratoire de Physique Moleculaire et Applications, CNRS, Universite Pierre et Marie Curie, 75252 Paris, Fr.). *J. Mol. Spectrosc.* 2001, 206(2), 115–125 (Eng), Academic Press. New exptl. data on the ν_1 and ν_3 bands of $^{16}O_3$ improving the value of abs. line intensities were obtained. The intensities of 295 lines were measured with an av. accuracy between 2.5% and 3% and the rotational expansion of the transition moment operators for the ν_1 and ν_3 bands was deduced. Finally, a complete listing of line intensities was computed with an intensity cutoff of 1 × 10^{-25} cm^{-1}/mol. cm^{-2}. (c) 2001 Academic Press.

С.А. 2001, 135, N7

O_3

2001

Hathorn B.C., Marcus R.A.

оценка колебат. частот и колебат. плотност.

J. Phys. Chem., A 2001, <u>105</u>, 5586–5589.

Estimation of Vibrational

Frequencies and Vibrational
Densities of States in
Isotopically Substituted
Nonlinear Triatomic Molecules

O_3

2001

135: 159420q The ν_1+ν_3 Bands of the $^{16}O^{17}O^{16}O$ and $^{16}O^{16}O^{17}O$ Isotopomers of Ozone. Perrin, A.; Flaud, J.–M.; Keller, F.; Smith, M. A. H.; Rinsland, C. P.; Devi, V. Malathy; Benner, D. Chris; Stephen, T. M.; Goldman, A. (Laboratoire de Photophysique Moleculaire, Universite Paris Sud, CNRS, 91405 Orsay, Fr.). *J. Mol. Spectrosc.* **2001**, 207(1), 54–59 (Eng), Academic Press. Using 0.002 cm^{-1} resoln. Fourier transform absorption spectra of an ^{17}O enriched ozone sample, an extensive anal. of the $\nu_1 + \nu_3$ bands of the $^{16}O^{17}O^{16}O$ and $^{16}O^{16}O^{17}O$ isotopomers of ozone has been performed for the first time. The exptl. rotational levels of the (101) vibrational states were satisfactorily reproduced using a Hamiltonian matrix that takes into account the obsd. rovibrational resonances. More precisely, for $^{16}O^{17}O^{16}O$, as for the other C_{2v}–type ozone isotopomers, it was necessary to account for the Coriolis type resonances linking the (101) rotational levels with the levels of the (200) and (002) vibrational states and the Darling–Dennison interaction coupling the levels of (200) with those of (002). For the C_s–type isotopomer, namely $^{16}O^{16}O^{17}O$, as for $^{16}O^{16}O^{18}O$ and $^{16}O^{18}O^{18}O$, it proved necessary to also account for an addnl. $\Delta K_a = \pm 2$ resonance involving the rotational levels from (101) and (002) (J.–M. Flaud and R. Bacis, Spectrochimica Acta Part A 54, 3–16 (1998)). Using a Hamiltonian matrix which takes these resonances explicitly into account, precise vibrational energies and rotational and coupling consts. were deduced, leading to the following band centers: $\nu_0(\nu_1 + \nu_3) = 2078.3496$ cm^{-1} for $^{16}O^{17}O^{16}O$ and $\nu_0(\nu_1 + \nu_3) = 2098.8631$ cm^{-1} for $^{16}O^{16}O^{17}O$. (c) 2001 Academic Press.

изото-померы,

$\hat{\nu}_1 + \nu_3$ ([illegible])

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

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

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

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

Оп. 40981

2001

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J. Mol. Spectrosc., 2001, 205, 347-349.

High-Resolution IR Spectra of ^{18}O-Enriched Ozone: Band Centers of $^{16}O^{16}O^{18}O$, $^{16}O^{18}O^{18}O$

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O_3 | Om · 41345 | 2002

Probst M. et al.,

J. Chem. Phys., 2002,
116, N3, 984-992.
Ionization energy stu-
dies for ozo ne and

OClO monomers and dimers.

O_3 (OM. 41450) 2002

Rüdiger Siebert et al.,

J. Chem. Phys., 2002,

116, N 22, 9749......

The vibrational energies ~~of~~
ozone up to the dissociation

threshold: Dynamics calculations on an accurate potential energy surface.