$CH_3J$ 1992

Waits L.D., Daniel R.G.
et al.

м.п.

47th Ohio State Univ. Int. Symp. Mol. Spectrosc., Columbus, Ohio, June 15-19, 1992. С. 114.

Изучение резонансной многофотонной ионизации $CF_3J$

Р. Ж. Х. N9, 1993, 9Б1086.

$CH_3J$

1993

Lee Meng-Rong, Ben-Amotz D.;

сдвиги частот колебаний

J. Chem. Phys., 1993, <u>99</u>, N 12, c. 10074-10077.

(см. $C_2H_6$; $\overline{\underline{III}}$)

$CH_3I$

1993

**118: 48258x** **The effect of nuclear quadrupole hyperfine interaction on the infrared absorption band $\nu_6$ of iodomethane.** Paso, Risto; Alanko, Seppo (Dep. Phys., Univ. Oulu, [illegible] Finland). *J. Mol. Spectrosc.* **1993**, 157(1), 122-31 [illegible]. A high-resoln. absorption spectrum of the perpendicular fundamental [illegible] $\nu_6$ of $^{12}CH_3I$ was recorded. The band was analyzed essentially as [illegible] unperturbed perpendicular band, although a small Coriolis interaction with $2\nu_3$ was taken into account. A least-squares fit with [illegible] parameters was performed. The splittings and shifts in line positions caused by the nuclear quadrupole hyperfine effect were investigated, and the influence of this effect on the results of the least-squares fit was studied. The correction of the hyperfine effect increases the amt. of acceptable lines by more than 10% in the least-squares fit. The influence of these addnl. observations on the mol. consts. [illegible] generally within the statistical error limits, but for some higher [illegible] parameters the changes are more considerable.

($\nu_6$)

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

$CH_3I$ 1994

Chen Cheng, Lu Li-Hwa, et al.

I, теорет. расчёт

THEOCHEM 1994, 116 (1-3), 219-27.

(см. $I_2$; III)

$CH_3I$ 1994

Geng Zhi-Yuan,
Wang Yong-Cheng,
et al.

м.п. Acta chim. sin. 1994.
52, N 5. c. 417-420.

(см. $CH_3F$; III)

1995

F: CH3I
P: 3

4Б1286. Низшая фундаментальная полоса 'ню'[3] {13}CH[3]I. Одновременный анализ уровней v[3]=1, v[6]=1 и v[3]=2. The lowest fundamental band 'ню'[3] of {13}CH[3]I: Simultaneous analysis of the levels v[3]=1, v[6]=1, and v[3]=2 / Alanko Seppo, Karhu Juha // J. Mol. Spectrosc. - 1995. - 174, N 1. - C. 215-222. - Англ.

В области 470-550 см{-1} исследован ИК-спектр метилиодида, отнесенный к полосе 'ню'[3]. Частоты более 1500 переходов отнесены к субполосам K=0-12 со значениями J до 79. На основании одновременного анализа полос 'ню'[3], 'ню'[6] и 2'ню'[3] определены вращат. постоянные, силовые постоянные и постоянные Кориолиса.

РЖХ 1997

$^{13}CH_3I$ 1995

**123: 324741g The lowest fundamental band $\nu_3$ of $^{13}CH_3I$: simultaneous analysis of the levels $v_3 = 1$, $v_6 = 1$, and $v_3 = 2$.** Alanko, Seppo; Karhu, Juha (Dep. Physical Sciences, Univ. Oulu, 90570 Oulu, Finland). *J. Mol. Spectrosc.* 1995, 174(1), 215–22 (Eng). The IR spectrum of the lowest fundamental band $\nu_3$ of $^{13}CH_3I$ has been studied in the region 470–550 cm$^{-1}$ at a resoln. of 0.0027 cm$^{-1}$. In this parallel band more than 1500 transitions have been assigned for subbands K = 0–12, including J values up to 79. The band has been analyzed using the upper state energies as observations. In addn. to the vibrational level $v_3 = 1$ the model included the level $v_6 = 1$ in order to study the influence of the Coriolis interaction $v_3/v_6$ on the band parameters. There is also a Coriolis resonance in effect between the upper states of the bands $v_6$ and $2\nu_3$ and accordingly the level $v_3 = 2$ has been added to the model.

ИК спектр, $\nu_i$

C. A. 1995, 123, N24

1995

F: CH3I
P: 3

1Б1160. Образование отрицательных ионов из CH[3]I электронным ударом. Negative ion formation from CH[3]I by electron impact / Nagesha K., Marathe V. R., Krishnakumar E. // Int. J. Mass Spectrom. and Ion Process. - 1995. - 145, N 1 - 2. - C. 89-96. - Англ.

Методом пересекающихся пучков изучали образование отрицательных ионов при столкновениях e+CH[3]I в интервале энергий электронов 0-50 эВ. В дополнение к I{-}, наблюдали H{-} и CH{-} при специфических резонансных энергиях. Измерены сечения. Проведены неэмпирич. расчеты поверхностей потенциальной энергии CH[3]I и CH[3]I{-}.

РЖХ 1997

1995

F: CH3I-
P: 3

1Б1160. Образование отрицательных ионов из CH[3]I электронным ударом. Negative ion formation from CH[3]I by electron impact / Nagesha K., Marathe V. R., Krishnakumar E. // Int. J. Mass Spectrom. and Ion Process. - 1995. - 145, N 1 - 2. - С. 89-96. - Англ.

Методом пересекающихся пучков изучали образование отрицательных ионов при столкновениях e+CH[3]I в интервале энергий электронов 0-50 эВ. В дополнение к I{-}, наблюдали H{-} и CH{-} при специфических резонансных энергиях. Измерены сечения. Проведены неэмпирич. расчеты поверхностей потенциальной энергии CH[3]I и CH[3]I{-}.

РЖХ 1997

1995

F: H3CI
P: 3

7Б1258. Чисто колебательное силовое поле для молекул типа XY[3]Z(C[3v]). Pure vibrational force field for XY[3]Z (C[3v]) molecules / Rajamanickam N., Fernandez-Liencres M. P., Lopez J. J., Fernandez M., Escribano R. // 10th Int. Conf. Fourier Transform Spectrosc., Budapest, Aug. 27 - Sept. 1, 1995: Book Abstr. and Program. - Budapest, 1995. - C. B2.7. - Англ.

В рамках модели т. н. чисто колебат. силового поля проведен анализ силовых полей моногалогенметанов H[3]CX (симметрии C[3v]), рассмотрено выполнение правила сумм и корреляции между величинами силовых постоянных и геометрическими параметрами.

Р.Ж.Х. N7, 1996.

$CH_3J$

1996

**125: 180056d A detailed analysis of the $\nu_2/\nu_5/\nu_3 + \nu_6$ band system of $^{13}CH_3I$ and $^{12}CH_3I$.** Alanko, Seppo (Dep. Phys. Sci., Univ. Oulu, SF-90570 Oulu, Finland). *J. Mol. Spectrosc.* 1996, 177(2), 263–279 (Eng). The IR spectra of $^{13}CH_3I$ and $^{12}CH_3I$ in the region of the bands $\nu_2$, $\nu_3$, and $\nu_3 + \nu_6$, 1200–1600 $cm^{-1}$, were studied at an effective resoln. better than 0.0025 $cm^{-1}$. The excited states of these bands form a complicated level system with a no. of resonances coupling the levels. Accordingly, the bands were analyzed by diagonalizing the complete energy matrixes with all the interactions simultaneously taken into account. The computational procedure is discussed. In the case of $^{13}CH_3I$, 6302 observations including 145 perturbation-allowed transitions were least-squares fitted by using a model with 44 free parameters. The std. deviation of the fit was 0.00014 $cm^{-1}$. For $^{12}CH_3I$, 7161 transitions including 351 forbidden lines were fitted using practically the same model is above. The std. deviation in this case was 0.00015 $cm^{-1}$.

ИК спектр

C.A.1996, 125, N14

1996

F: CH3I
P: 3

6Б1299. Вращательная спектроскопия высокого разрешения CH[3]I с использованием нового метода, свободного от допплеровского уширения. High-resolution rotational spectroscopy of CH[3]I using a novel doppler-free technique / Carocci S., Di Lieto A., Menciassi A., Minguzzi P., Tonelli M. // J. Mol. Spectrosc. - 1996. - 175, N 1. - C. 62-67. - Англ.

Предложен новый спектроскопич. метод двойного резонанса с субдопплеровским разрешением и высокой чувствительностью, в к-ром селекция по скоростям осуществляется за счет коллинеарного распространения излучения двух частот. При использовании излучения CO[2]-лазера и миллиметрового излучения измерены вращат. и колебат. переходы CH[3]I, а также впервые измерен электрич. дипольный момент в возбужденном v[6]=1 колебат. состоянии, равный 'мю'[6]=1,6295(6) Д.

PMX 1997

$CH_3J$

1996

**124: 159079h High-resolution rotational spectroscopy of $CH_3I$ using a novel Doppler-free technique.** Carocci, S.; Di Lieto, A.; Menciassi, A.; Minguzzi, P.; Tonelli, M. (Dip. Fis., Univ. Studi, I-56126 Pisa, Italy). *J. Mol. Spectrosc.* **1996**, 175(1), 62-7 (Eng). A new exptl. approach to double resonance spectroscopy is discussed in detail. The method uses collinear propagation of radiation of two frequencies to achieve velocity selection; it does not rely on nonlinear effects and it has a great sensitivity. Some examples of its application to the IR-microwave region are described. By using a $CO_2$ laser and a mm-wave klystron we measured the frequency of rotational and vibrational transitions of $CH_3I$ with sub-Doppler resoln. We also obtained the first measurement of the elec. dipole moment in the $\nu_6 = 1$ excited vibrational state and result is $\mu_6 = 1.6295(6)$ D.

(Сек. вращат. спектр)

C. A. 1996, 124, N 12.

$CH_3J$

1996

9 **6Б1299. Вращательная спектроскопия высокого разрешения $CH_3I$ с использованием нового метода, свободного от допплеровского уширения.** High-resolution rotational spectroscopy of $CH_3I$ using a novel doppler-free technique / Carocci S., Di Lieto A., Menciassi A., Minguzzi P., Tonelli M. // J. Mol. Spectrosc.— 1996 .— **175**, № 1 .— С. 62—67 .— Англ.

Предложен новый спектроскопич. метод двойного резонанса с субдопплеровским разрешением и высокой чувствительностью, в к-ром селекция по скоростям осуществляется за счет коллинеарного распространения излучения двух частот. При использовании излучения $CO_2$-лазера и миллиметрового излучения измерены вращат. и колебат. переходы $CH_3I$, а также впервые измерен электрич. дипольный момент в возбужденном $v_6=1$ колебат. состоянии, равный $\mu_6=1,6295(6)$ Д. С. Н. Мурзин

М.Л.

Х. 1997, N6

$CH_3J$

1396

125: 70500m **A new approach to double−resonance spectroscopy: The method of Doppler splitting.** Minguzzi, P.; Carocci, S.; Di Lieto, A.; Menciassi, A.; Quochi, F.; Tonelli, M. (Dipartimento di Fisica dell'Universita, I−56126 Pisa, Italy). *Laser Spectrosc., Int. Conf., 12th* 1995 (Pub. 1996), 216−219 (Eng). Edited by Inguscio, Massimo; Allegrini, Maria; Sasso, Antonio. World Scientific: Singapore, Singapore. The authors describe some examples of the application of a new Doppler−free spectroscopic method to the study of vibrational and rotational transitions of $CH_3I$. The authors discuss the speed dependence of collision broadening, the measurement of mm−wave and IR frequencies and the est. of the elec. dipole moment in the $v_6$ excited vibrational state.

C. A. 1996, 125, N6

$CH_3J$

1996

**6Б1298. Детальный анализ системы полос $\nu_2/\nu_5/\nu_3+\nu_6$ $^{13}CH_3I$ и $^{12}CH_3I$.** A detailed analysis of the $\nu_2/\nu_5/\nu_3+\nu_6$ band system of $^{13}CH_3I$ and $^{12}CH_3I$ / Seppo A. // J. Mol. Spectrosc.— 1996 .— 177, № 2 .— С. 263—279 .— Англ.

На ИК-фурье-спектрометре в области частот 1200—1600 см$^{-1}$ с разрешением 0,0025 см$^{-1}$ измерены колебательно-вращат. спектры полос $\nu_2$, $\nu_5$ и $\nu_3+\nu_6$ двух изотопомеров $^{12}CH_31$ и $^{13}CH_31$. Анализ спектров выполнен в приближении модели $C_{3v}$ с учетом колебательно-вращат. взаимодействий, включая кориолисов резонанс, резонанс Ферми и резонанс l-типа. С использованием 44 свободных спектроскопич. параметров измеренные переходы описаны в данной модели с точностью 0,00015 см$^{-1}$.

С. Н. Мурзин

М.Л.

Х. 1997, N 6

$H_3CI$ 1997

Fernandez-Liencres M.P.,
Fernandez G.M. et al.

сил.
пост.

J. Mol. Struct. 1997,
407 (2-3), 101-116.

(см. $H_3CF$; III)

$^{13}CH_3J$

1998

128: 236528r **Infrared spectrum of $^{13}CH_3I$ in the 2770–3200 cm$^{-1}$ region: rotational analysis of the fundamentals $\nu_1$ and $\nu_4$ together with $2\nu_5$ and $\nu_3 + \nu_5 + \nu_6$.** Alanko, Seppo (Dep. Physical Sciences, Univ. Oulu, FIN–90571 Oulu, Finland). *J. Mol. Spectrosc.* **1998,** 188(1), 43–62 (Eng), Academic Press. The high resoln. IR spectrum of $^{13}CH_3I$ in the region of the fundamental bands $\nu_1(A_1)$ and $\nu_4^{\pm1}(E)$ near 3000 cm$^{-1}$ were studied in detail with an effective resoln. better than 0.0040 cm$^{-1}$. In addn. to these fundamentals, an overtone band $2\nu_5^0$ and a PAPE band $\nu_3 + \nu_5^{\mp1} + \nu_6^{\pm1}$ were identified in the region. The excited states of these four bands, together with $2\nu_2 + \nu_3$, $\nu_2 + 2\nu_6^{\mp2}$, $\nu_2 + \nu_5^{\pm1}$, $\nu_2 + \nu_3 + \nu_6^{\pm1}$, $2\nu_5^{\mp2}$, $\nu_3 + \nu_5^{\mp1} + \nu_6^{\mp1}$, $2\nu_3 + 2\nu_6^{0,\mp2}$, and $3\nu_3 + \nu_5^{\pm1}$, form a complicated level system with a no. of resonances coupling the levels. Accordingly the bands were analyzed by diagonalizing the complete energy matrixes with all the interactions simultaneously taken into account. Special care was paid to eliminate the effects of the near–lying vibrational levels on the consts. of the fundamentals. Esp. the influence of the strong Fermi resonance $\nu_1/2\nu_5^0$ was studied. The model with 60 free parameters could reproduce the 4610 exptl. transitions with only fairly modest std. deviation of $4.3 \times 10^{-3}$ cm$^{-1}$. The phys. reasonable values for the parameters were considered more important than just the final std. deviation of the least squares fit.

(ИК, Di)

CA. 1998, 128, N19

$CH_3J$

1998

**129: 337074r The molecular constants of $^{12}CH_3I$ in the ground and $v_6 = 1$ excited vibrational state.** Carocci, S.; Di Lieto, A.; De Fanis, A.; Minguzzi, P.; Alanko, S.; Pietila, J. (Dipartimento di Fisica dell'Universita, Instituto Nazionale di Fisica della Matezia, I−56126 Pisa, Italy). *J. Mol. Spectrosc.* 1998, 191(2), 368−373 (Eng), Academic Press. A set of 26 new measurements were recorded by a Doppler−free double−resonance technique, with a relative accuracy of ~1−$^{-8}$. These data are combined to previous FTIR measurements to refine the mol. consts. of $^{12}$MeI. All the available literature data were revisited, a few assignments updated, and some frequencies changed according to new laser stds. A simultaneous fit to all the measurements of IR, microwave, and radiofrequency transitions produced an improved set of parameters, independent of previously detd. consts. (c) 1998 Academic Press.

(М.П.)

C.A. 1998, 129, N 25

**F: $CH_3I$**
**P: 3**

2001

135:24954 **Theoretical Calculation of Bond Dissociation Energies and Enthalpies of Formation for Halogenated Molecules.** Lazarou, Yannis G.; Prosmitis, Alexandros V.; Papadimitriou, Vassileios C.; Papagiannakopoulos, Panos. Institute of Physical Chemistry, National Center for Scientific Research Demokritos, Aghia Paraskevi, Greece. J. Phys. Chem. A (2001), 105(27), 6729-6742. in English.

The bond dissocn. energies and the enthalpies of formation of halogenated mols. were theor. calcd., and the results were compared with the corresponding exptl. values in order to examine the reliability of a large no. of levels of theory in thermochem. calcns. D. functional theory using a multitude of exchange and correlation functionals, Moller-Plesset perturbation theory, and QCISD(T) and CCSD(T) methods were employed, with all-electron and effective-core potential basis sets of varying complexity. A small set of 19 mols. was selected, consisting of $X_2$, HX, and $CH_3X$ (X = F, Cl, Br, and I), the mixed-halogen mols. ClF, BrF, BrCl, IF, and ICl, and $H_2$ and $CH_4$. The calcd.

bond dissocn. energies were cor. for basis set superposition errors and the first-order spin-orbit coupling in the 2P state of halogen atoms. In addn., the enthalpies of formation of all mols. in the set as well as those of Me (CH3) and halomethyl radicals (CH2X) were also calcd. by using the corresponding atomization reactions, cor. for the spin-orbit coupling in the 3P state of carbon atom and the 2P state of halogen atoms. Levels of theory employing the B3P86 functional with moderately large basis sets, augmented with diffusion and polarization functions, were found to be sufficiently reliable in the calcn. of bond dissocn. energies of closed-shell halogenated mols. In particular, the B3P86/6-311++G(2df,p) level of theory was found to be the most accurate, with an RMS deviation of 6 kJ·mol-1 for 23 bond dissocn. energies, with a negligible dependence of the accuracy on the level of theory chosen for the geometry optimization. In addn., the B3P86 functional in combination with small basis sets was found to be superior to B3LYP and MP2 in the calcn. of mol. structures. Regarding the calcd. enthalpies of formation, G2 theory was the most accurate, with an RMS deviation of 9 kJ·mol-1, followed by several combinations of the B3PW91 and B3LYP functionals with mostly large basis sets. However, the B3P86 functional tends to overbind open-shell species, resulting in an underestimation of the enthalpies of formation for polyat. mols. Extension of the bond dissocn. energy calcns. at levels of theory employing the B3P86 functional to a larger set of 60 bonds in 41 halogen-contg. mols. revealed systematic errors dependent on the mol. size. Therefore, the calcd. bond dissocn. energies at the B3P86/6-311++G(2df,p) level of theory were empirically improved by increasing the abs. energies of the radicals by the quantity 9 × 10-5·Ne Hartrees (Ne = total no. of electrons of the radical), with a subsequent lowering of the RMS deviation in the larger set to 8.0 kJ·mol-1.

2001

**F: CH3I**
**P: 3**

135:38602 **Separation of neutral versus cationic dissociation processes in an ultracompact double time-of-flight spectrometer: first results on CH3I.** Lehr, L.; Weinkauf, R.; Schlag, E. W. Institut fur Physikalische und Theoretische Chemie, TU-Munchen, Garching, Germany. Int. J. Mass Spectrom. (2001), 206(3), 191-199. English.

The authors present a simple exptl. setup, which allows simultaneous detection and anal. of photoions and photoelectrons. In short, the app. is a hybrid of a time-of-flight mass spectrometer and a time-of-flight magnetic bottle photoelectron spectrometer. For ions and electrons the same field-free drift region as well as the same multichannel plate detector is used. Mass resoln. m/Δm is .apprx.1000. Electron energy resoln. ΔE decreases with abs. energy and is 50 meV at

0.5 eV. For lower electron energies the resoln. is limited by the bandwidth of the 200 fs laser pulse. The app. is tested at the known A~ state dynamics of Me iodide by femtosecond pump-probe excitation and ionization. The obsd. fragment ions can have 2 different origins. They can be formed (1) either by parent cation photodissocn. or (2) by ultrafast neutral fragmentation with subsequent fragment ionization by the intense probe laser. Because of the different ionization energies of MeI and I, neutral, and cationic dissocn. pathways can be distinguished by electron energy anal. This tool is very important for interpretation of mass and femtosecond laser pump-probe spectra of short-lived mol. systems. Because of the comparable detection probability for ions and electrons the app. would allow electron-ion coincidence measurements at kilohertz laser repetition rates.

$(CH_3I)_2$ От. 41742 2003

Bogdanchikov G.A., Baklanov A.V. et al.,

ab initio расчет

Chem. Phys. Lett., 2003, <u>376</u>, 395-402