CH_3OH (От 31418) 1989

7 Л131. **Спектр высокого разрешения метанола в области 8—100 см$^{-1}$.** High resolution spectrum of CH_3OH between 8 and 100 cm^{-1} / Moruzzi G., Strumia F., Carnesecchi P., Carli B., Carlotti M. // Infrared Phys.— 1989.— 29, № 1.— С. 47—86.— Англ.

Составлен атлас линий спектра поглощения метанола в области ниже 100 см$^{-1}$, причем интервал 40—100 см$^{-1}$ представлен в атласе впервые. Спектр CH_3OH измерен при давлении 0,75 Тор на фурье-спектрометре с разрешением 0,0019 см$^{-1}$ и точностью калибровки по волн. числу $5 \cdot 10^{-5}$ см$^{-1}$. Дано теоретич. описание спектра, рассмотрена процедура отнесения линий. В таблице приведены коэф. разложения в ряд Тейлора энергетич. уровней для симметрии типа A,

М·Л·

ф. 1989, N 7

E_1 и E_2 и коэф. K-удвоения для симметрии типа A. Приведена схема систематизации измеренных переходов. Для 6720 линий даны квантовые числа нижнего и верхнего состояний, тип симметрии, эксперим. и расчетное значения частоты. Библ. 22. И. Г.

CH_3OH От 31418 1989

ИК спектр высокого разрешения

110: 201833n **High resolution spectrum of methanol between 8 and 100 cm^{-1}.** Moruzzi, G.; Strumia, F.; Carnesecchi, P.; Carli, B.; Carlotti, M. (Dip. Fis., Univ. Pisa, I-56100 Pisa, Italy). *Infrared Phys.* 1989, 29(1), 47–86 (Eng). The FIR spectrum of CH_3OH between 8–100 cm^{-1} was measured by a high resoln. Fourier transform spectrometer. A computer best fit program, based on the Taylor series expansion of the energy levels, was used for the line assignments. The region between 40–100 cm^{-1} is presented for the first time. The region between 8–40 cm^{-1}, covered in a previous work, is revisited in the light of the new measurements at higher frequencies, and new assignments are given. The available microwave and radio-frequency assignments were inserted into the fit program. A catalog of 6725 assigned MW and FIR lines below 101.8 cm^{-1} is presented.

C.A. 1989, 110, N22

CH_3OH (От. 31418) 1989

+ **11 Б1252. Спектр высокого разрешения CH_3OH между 8 и 100 см$^{-1}$.** High resolution spectrum of CH_3OH between 8 and 100 cm^{-1} / Moruzzi G., Strumia F., Carnesecchi P., Carli B., Carlotti M. // Infrared Phys.— 1989.— **29**, № 1.— С. 47—86.— Англ.

С высоким разрешением (0,00125 см$^{-1}$, фурье-спектрометр) измерен ИК спектр поглощения паров CH_3OH в обл. 8—100 см$^{-1}$. Приведено положение и отнесение $(n'K';\ J')v' \leftarrow (n'',\ K'';\ J'')v''$ 6720 переходов в этом диапазоне.

В. М. Ковба

М.Л.

Х. 1989, N 11

CH_3OH ОМ 31913 1989

19 Б1231. Далекая инфракрасная спектроскопия высокого разрешения метанола. Ultrahigh resolution far-infrared spectroscopy of methanol / Moruzzi G., Prevedelli M., Evenson K. M., Jennings D. A., Vanek M. D., Inguscio M. // Infrared Phys.— 1989.— 29, № 2—4.— С. 541—549.— Англ.

На перестраиваемом ИК-спектрометре на базе CO_2-лазера с использованием смешения частот на точечном диоде выполнены измерения в обл. частот 116,2—116,8 см$^{-1}$ и 162,1—163,1 см^{1} с разрешением около 25—35 кГц спектра поглощения метанола, CH_3OH. С учетом данных ИК-фурье-спектроскопии и теорет. расчетов идентифицировано 78 линий спектра поглощения. Из результатов ИК-спектроскопии установлено, что лазерная линия 170 мкм CH_3OH расположена в непосредственной близости от неотнесенной линии поглощения. Использованный лазерный ИК-спектрометр благодаря высокому спектральному разрешению особенно полезен при исследованиях спектров высокой спектральной плотности, таких как спектр метанола. С. Н. Мурзин

М.П. -

Х. 1989, N 19

CH_3OH

от. 31913 1989

11 Л145. Спектроскопическое исследование метанола со сверхвысоким разрешением в дальней ИК-области. Ultrahigh resolution far-infrared spectroscopy of methanol / Moruzzi G., Prevedelli M., Evenson K. M., Jennings D. A., Vanek M. D., Inguscio M. // Infrared Phys. — 1989.— 29, № 2—4.— С. 541—549.— Англ.

С использованием перестраиваемого когер. спектрометра, основанного на смешивании частот, в дальней ИК-области получены 78 линий поглощения метанола с разрешением 20 кГц. Проведено сравнение с полученным ранее фурье-спектром, где эти линии сильно перекрываются. Обнаружено, что лазерная линия метанола 170 мкм расположена очень близко к неинтерпретированной интенсивной линии поглощения, что объясняет особенности штарк-эффекта и зависимости от давления, проявляющиеся на этой лазерной линии. Н. Т.

М.Л.

Ф. 1989, N11

CH_3OH

(Om 31911)

1989

111: 86426p Fourier spectrum of methanol between 950 and 1100 cm⁻¹. Moruzzi, G.; Strumia, F.; Carnesecchi, P.; Lees, R. M.; Mukhopadhyay, I.; Johns, J. W. C. (Dip. Fis., Univ. Pisa, I-56100 Pisa, Italy). *Infrared Phys.* 1989, 29(2-4), 583-606 (Eng). The IR spectrum of MeOH between 950 and 1100 cm⁻¹ was measured by a high resoln. Fourier transform spectrometer. This spectral region is of particular interest because of its overlapping with the CO_2 laser emissions used for exciting the MeOH laser. A catalog of 3410 assigned lines is presented, as well as the Taylor development tables for evaluating the energies of the upper levels of the corresponding transitions.

(UK)

C.A. 1989, <u>111</u>, N10

CH_3OH 1989

Nhu M.D., Allegrini M.,
et al.,

The Partition Function of
Methanol.
Eleventh Colloquium On
High Resolution Mo- 864

lecular Spectroscopy, Giessen,
September 18-22, 1989, A1, J21.

CH_3OH

1989

12 Л188. Спектры ИК—ИК-двойного резонанса $^{13}CH_3OH$ и $^{12}CH_3OH$. Infrared—infrared double-resonance spectra of $^{13}CH_3OH$ and $^{12}CH_3OH$ / Petersen J. C. // J. Opt. Soc. Amer. B.— 1989.— **6**, № 3.— С. 350—355.— Англ.

Исследованы спектры ИК—ИК-двойного резонанса молекул $^{13}CH_3OH$ и $^{12}CH_3OH$ в газовой фазе при возбуждении непрерывным излучением $^{12}C^{16}O_2$-лазера с акустооптич. модуляцией и подстройкой частот излучения и исследуемых вращательных подуровней молекул посредством эффекта Штарка в рабочей кювете с газом. Идентифицированы полосы колебательно-вращательно-крутильных переходов. Рассчитаны значения усредненного постоянного электрического дипольного момента μ для $n=0$ основного состояния, а также величины μ колебательно-возбужденного состояния групп CO и возбужденного состояния групп CH_3, причем величины μ для деф. кол. групп CH_3, меньше значений μ для вал. кол. групп CO на ~0,065 ед. Дебая. Библ. 21.

И. В. А.

м.п.

ф.1989, N 12

$COH_4^{+\cdot}$ 1989

Pius K., Chandrasekhar J.,

ab initio
расчет
стабильн.
и структ.

Int. J. Mass Spectrom.
and Ion Process 1989,
87, N 1, 15-18.

CH_3OH 1989

111: 142981e The oxygen-hydrogen stretching force constant in associated methanol species and the cooperativity effect. Shivaglal, M. C.; Singh, Surjit (Dep. Chem., Indian Inst. Technol., Madras, 600 036 India). *Int. J. Quantum Chem.* 1989, 36(2), 105-18 (Eng). The effect of mol. interaction on the O-H stretching force const. of MeOH is reported for its assocd. species. The various electron donors (D) and acceptors (A) considered include org. mols. such as methanol, di-Me ether, acetone, acetonitrile, DMF, pyridine, and ions such as F^-, Cl^-, Li^+, and H^+. The variation in the O-H stretching force const. of MeO-H...D species on interaction with the electron acceptor such as in the species A-MeOHH...D is explained on the basis of the cooperativity effect. (CE). The effect is discussed in terms of the relationship $CE = (\Delta F/F) \times 100$, where ΔF is the redn. in force const. of the H-bonded O-H stretching mode of the assocd. MeOH..D when the lone pair electrons on O of the MeOH mol. are involved in H bonding with A, and F is the H-bonded O-H stretching force const. of the species when the lone pair electrons are free. The cooperativity effect (CE) increases with electron acceptor and electron donor capacities of A and D. The calcd. force consts. are compared with the exptl. results.

Сил. пост.

C.A. 1989, <u>111</u>, N16

CH_3OH 1989

Тупицын И. Ф.,
Пузанов Ю. В. и др.

м. п. Теор. и эксперим. химия. 1989. 25, N 4. С. 406 – 412.

(см. CH_3NH_2; III)

CH_3OH^+

1990

11 Д130. Оценка частот нормальных колебаний ионов $N_2H_4^+$(г) и CH_3OH^+(г) / Александровская А. М., Журавлева Л. Н., Дмитриева Т. В. // Структура и энерг. молекул: Тр. 5 Всес. совещ. по изуч. структуры молекул в газ. фазе, Иваново, 11—14 июня, 1990: Межвуз. сб. науч. тр.— Иваново, 1990.— С. 46—49

Частоты норм. колебаний ионов $N_2H_4^+$ (симметрии D_{2h}) и CH_3OH^+ (симметрии C_s) оценены путем сравнения данных по частотам нейтральных молекул со значениями частот в характеристич. группах др. молекул и соответствующих им ионов.

М·Л·

☒ (11) $N_2H_4^+$

ф. 1991, N 11

$CH_3OH^+(г)$ 1990

Александровская А.М.,
Муравлёва Л.Н. и др.,

Структура и энергетика моле-м.л. кул. Труды V Всесоюзного Совещания по изучению структур молекул в газовой фазе, Иваново, 1990.

$^{13}CH_3OH$ ОМ. 34758 1990

113: 200763q The millimeter- and submillimeter-wave spectrum of methyl-carbon-13 alcohol revisited. Anderson, Todd; Herbst, Eric; De Lucia, Frank C. (Dep. Phys., Duke Univ., Durham, NC 22706 USA). *Astrophys. J., Suppl. Ser.* 1990, 74(2), 647-64 (Eng). The lab. millimeter- and submillimeter-wave spectrum of the sym. (*A*) and degenerate (*E*) substates of $^{13}CH_3OH$ has been extended to include 430 transitions in the *A* species and 411 transitions in the *E* species. For the *A* species, the obsd. transitions now include quantum nos. through $J \leq 10$ and $K \leq 8$ in the ground torsional state ($v_t = 0$) and through $J \leq 10$ and $K \leq 7$ in the $v_t = 1, 2$ excited torsional states. For the *E* species, the obsd. transitions now include quantum nos. through $J \leq 10$ and $|K| \leq 8$ in the ground torsional state and through $J \leq 10$ and $|K| \leq 6$ in the $v_t = 1, 2$ excited torsional states. Modification of the extended internal axis method (IAM) Hamiltonian as in earlier work has reduced the overall root-mean-square deviation to the level of exptl. accuracy. The new spectral consts. derived from the nonlinear least-squares fit to the data were used to predict the frequencies of an addnl. 562 transitions of $^{13}CH_3OH$ for $v_t = 0, 1, 2$ and rotational quantum no. $J \leq 12$.

Кеттле М.Л.

C.A. 1990, 113, N 22

CH_3OH (оп 33752) 1990

112: 242594v **Additional measurements and a refined analysis of the millimeter- and submillimeter-wave spectrum of methanol.** Anderson, Todd; De Lucia, Frank C.; Herbst, Eric (Dep. Phys., Duke Univ., Durham, NC 27706 USA). *Astrophys. J., Suppl. Ser.* 1990, 72(4), 797-814 (Eng). The lab. millimeter- and submillimeter-wave spectrum of the sym. (*A*) and degenerate (*E*) substates of $^{12}CH_3OH$ was extended to include 437 transitions through $J \leq 10$ and $K \leq 8$ in the 1st 3 torsional states ($v_t = 0, 1, 2$) of the *A* species and 419 transitions through rotational quantum nos. $J \leq 10$, $|K| \leq 8$ in the $v_t = 0$ torsional state, and $|K| \leq 6$ in the $v_t = 1, 2$ torsional states of the *E* species. Modification of the extended internal axis method (IAM) Hamiltonian to include more cross terms which describe the interaction of rotation and torsion as well as the sepn. of the fits of the A and the E species have reduced the overall root-mean-square deviation to the level of the exptl. uncertainty. This makes possible a very significant improvement in the calcn. of the rotational-torsional spectrum of MeOH in this spectral region. The spectral consts. generated by the fit were used to predict an addnl. 569 lines of $^{12}CH_3OH$ for $v_t = 0, 1, 2$ and rotational quantum no. $J \leq 12$.

вр. спектр,
М.П.

С.А. 1990, 112, N 26

CH_3OH Оп. 34255 1990

Carrick P., Curl R.F. et al.,

Vo J. Mol. Struct. 1990, 223,
171-184.

The OH stretching funda-
mental of methanol.

CH_3OH 1990

Dang-Nhu M., Allegrini M., et al.,

J. Mol. Spectrosc. 1990, <u>141</u>, N2, 348-350.

Intensities of the CO stretch

Band of CH_3OH at 9.7 μm

CH_3OH от 34297 1990

Коцаренко А.А., Эфенди-Агаев Н.Л.,

$(\rho, \Delta H_v)$ Изв. вузов. Нефть и газ. 1990, №1, 59–61.

CH_3OH От·34037 1990

ab initio расчет

Larkins F.P., Seen A.J., Phys. Scr. 1990, <u>41</u>, N6, 827-832

Ab initio studies of molecular X-Ray Emission

Processes: Methanol.

$CH_3{}^{18}OH$

1990

114: 155559m FIR lasing and spectroscopy in the methyl group-rocking band of methanol-^{18}O. Lees, R. M.; Zhao, Saibei; Rommens, M. A.; Johns, J. W. C., Lewis Bevan, W.; Young, C.; Lees, T. J. (Dep. Phys., Univ. New Brunswick, Fredericton, NB Can. E3B 5A3). *Proc. SPIE-Int. Soc. Opt. Eng.* 1990, 1514(Conf. Dig. - Int. Conf. Infrared Millimeter Waves, 15th, 1990), 729-31 (Eng). A weak IR band above the strong C-O stretching band in $CH_3{}^{18}OH$ is identified as the in-plane CH_3-rocking mode. Numerous P, Q and R branches have been assigned in the high-resoln. FTIR spectrum. The energy level pattern in the excited state shows that the torsional barrier height increases markedly by in going from the ground to the excited state. The band overlaps well with the 9.6 µm CO_2 laser band, and six CH_3-rock FIR laser transition systems are identified.

спектр,
Di

C.A. 1991, 114, N16

CH_3OH 1990

Margreiter D.,
Deutsch H., et al

сечение
ионизации,
теор.
расчет

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

(см. H_2; III)

CH_3OH

Om 35157

1990

11 Б1285. Спектр CH_3OH между 100 и 200 $см^{-1}$. Торсионные и «запрещенные» переходы. The spectrum of CH_3OH between 100 and 200 cm^{-1}: Torsional and «forbidden» transitions / Moruzzi G., Riminucci P., Strumia F., Carli B., Carlotti M., Lees R. M., Mukhopadhyay I., Johns J. W. C., Winnewisser B. P., Winnewisser M. // J. Mol. Spectrosc.— 1990.— **144**, № 1.— С. 139—200.— Англ.

На трех ИК-фурье-спектрометрах в областях частот 8—200 $см^{-1}$ с разрешением 0,0025 $см^{-1}$, 80—350 $см^{-1}$ с разрешением 0,004 $см^{-1}$ и 30—1250 $см^{-1}$ с разрешением 0,0025 $см^{-1}$ измерен колебательно-вращат. спектр CH_3OH. Выполнено сопоставление трех наборов спектроскопич. данных в области частот 100—200 $см^{-1}$ для 6000 линий поглощения, а также для 955 линий в области ниже 100 $см^{-1}$. Большинство линий принадлежит возбужденному торсионному уровню основного колебат. состояния. Часть линий отнесена к «запрещен-

М. Л.

Х. 1991, № 11

ным» переходам $\Delta K=0$, $\Delta n=1$ Q-ветви вблизи 184,2 $см^{-1}$. Наряду с данными об абс. частотах переходов получены точные значения вращательно-торсионных уровней энергии, для расчета к-рых использовано разл. по вращат. и общему квантовым числам. Полученные результаты м. б. использованы в кач-ве втор. стандарта волновых чисел в ИК-области спектра.

С. Н. Мурзин

CH_3O^0

1990

19 Б1335. Спектр высокого разрешения обертонной полосы валентного колебания CO метилового спирта. High-resolution spectrum of the C—O stretch overtone band in methyl alcohol / Mukhopadhyay I., Ozier I., Lees R. M. // J. Chem. Phys.— 1990.— 93, № 10.— С. 7049—7053.— Англ.

В области первого обертона вал. кол. CO газ. MeOH получен ИК-фурье спектр с разрешением 0,004 см$^{-1}$. Спектр разрешен на *J* мультиплетов, каждый из к-рых имеет сложную подструктуру, обусловленную торсионно-колебательно-вращат. вз-виями. Внутри этой структуры выделены *R* и *P* ветви, соотв-щие переходам $K=0$ и $K=1$ торсионных колебаний типов *A* и *E* для $J\leqslant 24$. С помощью использования комбинац. разностей, известных для основного состояния, выполнено отнесение линий. Найдены вращат. постоянные и главные члены торсионно-вращат. гамильтониана второго возбужденного состояния вал. кол. CO. Величина торсионного барьера в этом состоянии равна 395,5 см$^{-1}$.

Б. С. Авербух

М. П.

Х. 1991, N 19

CH_3OH Om·33955 1990

Petersen J.C.,

J. Opt. Soc. Am. B 1990,

7, N2, 159–163

Infrared radio-frequency double-resonance spectra of

CH_3OH in the CH_3 deformation state and torsionally excited states.

CH_3OH Оп. 33938 1990

Rauk A., Dutler R.,
et al.,
Can. J. Chem. 1990,
<u>68</u>, N 2, 258-266.
Infrared and [illegible] vibrational

circular dichroism intensities of model systems CH_3OH, CH_3NH_2, NH_2NH_2, NH_2OH, and $HOOH$ and the deuterated species, ND_2ND_2, $DOOH$, and $DOOD$: A theoretical study using the vibronic coupling formalism.

CH_3OH

1990

5 Д72. Газофазные кислотности и молекулярные геометрии H_3SiOH, H_3COH и H_2O. Gas phase acidities and molecular geometries of H_3SiOH, H_3COH, and H_2O / Sauer Joachim, Ahlrichs Reinhart // J. Chem. Phys.— 1990.— 93, № 4.— С. 2579—2583.— Англ.

Расчеты проводились квантовомеханич. методом с использованием больших базисов. Геометрии, полученные для H_2O и CH_3OH, согласуются с экспериментальными в пределах точности эксперимента. Предсказанная равновесная геометрия силанола (пикометры, градусы): $r(SiO) = 165{,}0$; $r(OH) = 95{,}76$; $r(SiH) = 146{,}8$ (в плоскости), $r(SiH) = 147{,}6$ (вне плоскости); угол $(SiOH) = 117{,}7$. Газофазные кислотности ($\Delta H_{298}{}^0$) (в ккал/моль) 392,3 (H_2O), 384,5 (CH_3OH) и 359,3 (SiH_3OH). Наилучшие теоретич. оценки $\Delta H_{298}{}^0$ для H_2O $391{,}0 \pm 2{,}5$ ккал/моль. Это указывает на высокую точность проведенных исследований. Эксперим. исследования молекулы силанола затруднены в связи с высокой реакционной способностью. Г. К.

М.П.

ф. 1991, N5

CH_3OH

1990

11 Б1294. Анализ вращательного спектра метанола при помощи улучшенного гамильтониана Накагава—Тсунекава—Коджима. Analysis of the rotational spectrum of methanol by an improved Nakagawa—Tsunekawa—Kojima Hamiltonian / Sżtraka L. // 4th Austr.-Hung. Conf. Recent Develop. Infrared and Raman Spectrosc. [and] Austr. Hung. Int. Conf. Vibrat. Spectrosc., Veszprém, Apr. 18—20, 1990. 3rd Circ.— [Veszprém], 1990.— С. P32.— Англ. Место хранения ГПНТБ СССР

В результате обобщения теор. модели Уотсона с использованием улучшенного гамильтониана Накагава—Тсунекава—Коджима получены выражения для постоянных центробежного искажения 1-го и 2-го порядков в случае молекул, подобных молекуле метанола. На основе полученного гамильтониана выполнена обработка микроволнового, миллиметрового и субмиллиметрового спектров метанола (Herbst E. et al. // J. Mol. Spectr.— 1986.— **116**.— С. 120; DeLucia F. C. al. // J. Mol. Spectr.— 1989.— **134**.— С. 394). С. Н. Мурзин

М·Л·

Х. 1991, N 11

H_3COH 1990

Sauer Joachim,
Ahlrichs R.

м.п.

J. Chem. Phys. 1990. 93,
N 4. С. 2575–2583.

(см. H_3SiOH; III)

CH_3OH (Оп 84957) 1990

Von Nagy-Felsobuki E.I.,
Kimura K.,

Ар,
ab initio
расчет

J. Phys. Chem. 1990,
<u>94</u>, N21, 8041–8044.

CH_3OH 0m 36368 1991

15 Б1177. Чисто вращательные спектры газофазных метанолов. Pure rotational Raman spectra of vapor phase methanols / Forneris R., da Silva S. C., Hase Y. // Spectrosc. Lett.— 1991.— **24**, № 9.— С. 1237—1246.— Англ.

Исследован чисто вращат. спектр КР (в области 120—5 см$^{-1}$) газ. метанолов CH_3OH (**I**), CH_3OD (**II**), CD_3OH (**III**) и CD_3OD (**IV**). Идентифицированы эквидистантные линии с интервалами 3,2; 3,0; 2,6; 2,5 для **I—IV**, соотв. Спектральный анализ проведен для модели нежесткого симм. волчка, идентифицированы линии чисто вращат. переходов *S*-ветвей **I—IV**. Обработкой МНК из эксперим. данных получены величины вращат. постоянных *B*, равные (0,80±0,1); (0,76±0,01); (0,64±±0,2); (0,61±0,02) см$^{-1}$ для **I—IV**, соответственно.

Г. М. Курамшина

М.Л.

(+3) ☒

X. 1992, N 15

CH_3OH Dm 36368 1991

115: 265735t **Pure rotational Raman spectra of vapor phase methanols.** Forneris, R.; Da Silva, S. C.; Hase, Y. (Inst. Fis., Univ. Sao Paulo, 01418 Sao Paulo, Brazil). *Spectrosc. Lett.* 1991, 24(9), 1237–46 (Eng). The rotational Raman spectra of four vapor phase isotopic methanols, CH_3OH, CH_3OD, CD_3OH, and CD_3OD, are reported in the wavenumber regions from 5 to 100–120 cm^{-1}. The major parts of the spectra consist of equidistant bands at 3.19, 3.04, 2.56, and 2.46 cm^{-1} intervals, resp., and are interpreted as the pure rotational S-branch transitions.

Вр. спектр,
м.п.

$$\underbrace{CH_3OD,\ CD_3OH,}\ CD_3OD$$

(+1) (+2) ☒

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

$^{13}CH_3{}^{17}OH$ 1991

115: 101780c Microwave spectrum of methanol ($^{12}CH_3{}^{17}OH$). Hoshino, Yoshiaki; Ohishi, Masatoshi; Takagi, Kojiro (Dep. Phys., Toyama Univ., Gofuku, Japan 930). *J. Mol. Spectrosc.* 1991, 148(2), 506-8 (Eng). The microwave spectra, rotational consts., mol centrifugal distribution, potential barrier height and inertial consts. are presented for methanol-^{17}O.

Мв. спектр,

м.п.

C.A. 1991, 115, N10

CH_3OH

1991

115: 122736h Torsion-rotation absorption line assignments in the symmetric CH-stretch fundamental of methanol. Hunt, R. H.; Shelton, W. N.; Cook, W. B.; Bignall, O. N.; Mirick, J. W.; Flaherty, F. A. (Dep. Phys., Florida State Univ., Tallahassee, FL 32306 USA). *J. Mol. Spectrosc.* 1991, 149(1), 252–6 (Eng). The sym. CH-stretch fundamental band of methanol vapor was examd. between 2800 and 2880 cm^{-1} by means of a 1.25-m path difference Fourier transform spectrometer. Ten parallel-type subbands were identified–8 of these arise from torsional states with principal quantum no. $n = 0$ and 2 with $n = 1$. Most of these subbands exhibit strong rotational perturbations. An approx. anal. of the subband origins yields a band center at 2843.39 cm-11 and a hindering potential barrier height in the excited state of 379 cm-11 as compared with the ground state value of 373 cm^{-1}.

ИК-спектр,
м.п.

C.A. 1991, 115, N 12

CH_3OH 1991

115: 290055d The infrared spectrum of methanol: evidence for state mixings. Moruzzi, Giovanni; Moraes, Joao Carlos Silos; Strumia, Franco; Lees, Ronald M.; Mukhopadhyay, Indranath; Winnewisser, Brenda P.; Winnewisser, Manfred (Dip. Fis., Univ. Pisa, I-56126 Pisa, Italy). *Proc. SPIE-Int. Soc. Opt. Eng.* 1991, 1576(Conf. Dig. - Int. Conf. Infrared Millimeter Waves, 1991), 246-7 (Eng). A study of state mixings is made in a continuing high resoln. IR spectral study of methanol.

ИК-спектр,

М.Л.

C.A. 1991, 115, N26.

CH_3OH ОП 35805 1991

12 Д196. Критическое исследование сродства к протону, предсказанного из рентгеновских фотоэлектронных спектров (РФС). A critical investigation of XPS predicted proton affinities / Nordfors D., Mårtensson N., Ågren H. // J. Electron Spectrosc. and Relat. Phenom.— 1991.— **56**, № 3.— С. 167—187.— Англ.

Для ряда тестовых случаев, в частности, для молекул CH_3OH, CH_3FH^+, CH_3F, CH_4, NH_4^+, NH_3 исследована применимость термохимич. модели (ТХМ) для определения протонного сродства ПС в газовой фазе из энергий остовной ионизации. Отклонение величин ПС от экспериментальных, полученных из данных РФС, приписано наличию различных узлов протонирования, эффектам геометрич. релаксации и химич. эффектам. Проведено сопоставление результатов ТХМ с данными расчетов методом МК ССП, включающих оптимизацию геометрии и использующих аналитические молекулярные градиенты и гессианы. Для протонирования молекулы NH_3 ТХМ и

М.П.

⊞ ⑮

ф. 1991, №12

данные расчетов в приближении МК ССП согласуются. Подчеркнута важность включения энергий колебаний в нулевой точке в расчеты как остовной ионизации, так и ПС. Показано, что ошибка, связанная с геометрией молекул, мала для протонирования азота, но составляет ~1 эВ для фтора.

$CH_3{}^{18}OH$

Дм 36475

1991

115: 290023s Double-resonance spectra of oxygen-18-labeled methanol. Petersen, J. C.; Choi, S. E. (Dan. Inst. Fundam. Metrol., Lyngby, 2800 Den.). *J. Opt. Soc. Am. B: Opt. Phys.* 1991, 8(11), 2256–9 (Eng). Two double-resonance techniques were used to confirm previously proposed assignments of IR transitions in the $Me^{18}OH$ mol. The techniques involve a cw CO_2 laser, and they complement each other. The IR–IR double-resonance technique is used for probing accidental coincidences between the CO_2 laser lines and Stark-tuned levels of *E* symmetry. Two such coincidences were assigned, and the permanent elec. dipole moment components μ_a'' and μ_a' were detd., for the 1st time in this mol. for the ground state and the CO stretch state, resp. The IR radio-frequency double-resonance technique was used to probe a level of *A* symmetry. This observation has permitted a more accurate detn. of mol. asymmetry parameters with $(n,K) = (0,3)$ in both vibrational levels.

М.п.

C.A. 1991, 115, N26.

CH_3OH 1992

116: 70994q Microwave and submillimeter-wave rotational spectrum of methyl alcohol in the ground torsional state. Baskakov, O. I.; Pashaev, M. A. (Dep. Radiophys., Kharkov State Univ., 310077 Kharkov, USSR). *J. Mol. Spectrosc.* 1992, 151(2), 282-91 (Eng). The frequencies of 440 transitions of the spectrum of the ground torsional-vibrational state of Me alc. were measured in the microwave and submillimeter regions, 130 of these belonging to the main isotopomer CH_3OH ($J \leq 42$, $K \leq 8$), 190 to the isotopomer CD_3OH ($J \leq 37$, $K \leq 10$), and 120 to CD_3OD ($J \leq 27$, $K \leq 5$). For the first time, all the transitions were identified on the basis of directly calcd. frequencies. These results were obtained through the use of a new effective torsional-rotational Hamiltonian. Its parameters were calcd. based on the frequencies of all earlier known and new transitions of microwave and submillimeter-wave spectra of the ground torsional-vibrational state of methanol. The root-mean-square deviation is 710 kHz (800 lines) for the main isotopomer, 144 kHz (370 lines) for CD_3OH, and 316 kHz (150 lines) for CD_3OD.

(Мв спектр)

C. A. 1992, 116, N 8

CH_3OH

1992

7 Б1049. Теоретическое исследование энергий диссоциации метанола. Theoretical study of the bond dissociation energies of methanol /Bauschlicher Charles W., Langhoff Stephen R., Walch Stephen P. //J. Chem. Phys. .—1992 .—**96** ,№ 1 .—С. 450—454 .—Англ.

Неэмпирическими методами рассчитаны энергии диссоциации D_c и D_0 молекулы CH_3OH. На предварит. стадии вычислены также энергии диссоциации HO—H и O—H. Энергии определены в приближениях связанных пар (модифицированный и усредненный варианты) с орбиталями, оптимизированными одно- или многоконфигурац. методами ССП. Рассмотрено несколько вариантов базисов, включая наборы натуральных АО. Сделан вывод, что модифицированный метод функционала связанных пар для подобных систем приводит к погрешности в энергии диссоциации в пределах 4 ккал/моль. Значения D_0 (без поправок) составили 101 ккал/моль для $CH_3OH \rightarrow CH_3O + H$, 94,2 для $CH_3OH \rightarrow CH_2OH + H$ и 83,7 для $CH_3OH \rightarrow CH_3 + OH$. Наибольшую трудность при учете корреляц. эффектов представляет расчет диссоциации по связи C—O.

А. В. Немухин

(D_0)

Х. 1993, N 7

$CH_3OH^{·+}$

1992

2 Б1108. Улучшенная термохимия для катион-радикала метанола ($CH_3OH^{·+}$) и его дистонического изомера ($CH_2OH_2^{·+}$). Refined thermochemistry for the methanol radical cation ($CH_3OH^{·+}$) and its distonic isomer ($CH_2OH_2^{·+}$) //J. Phys. Chem .—1992 .—96 ,№ 14 .—С. 5804—5807 .—Англ.

Неэмпирическим методом ССП, а также с учетом электронной корреляции в рамках теории возмущений Меллера—Плессета вплоть до четвертого порядка и квадратичным методом конфигурац. вз-вия с учетом одно-, двух- и трехкратных возбуждений, с использованием расширенных базисных наборов вплоть до 6—311 ГФ, дополненных тремя наборами ф-ций *f*- и *d*-типа, а также двумя наборами ф-ций *p*-типа и диффузными ф-циями, в рамках теории «Gaussian-2» проведены расчеты электронного и геометрич. строения молекулы метанола (I), катион-радикала метанола ($CH_3OH^{·+}$) (II) и его дистонич. изомера ($CH_2OH_2^{·+}$) (III) и оценена энер-

И.П., энергии ионизации, термохим

☒ ③

Х. 1993, №2

гия ионизации (ЭИ) I и разность в энергии (Δ) между II и III. На наивысшем уровне расчета найдено, что ЭИ молекулы I равны 1051 кДж/моль (эксперим.: 1047 кДж//моль), а Δ равна 27 кДж/моль (эксперим.: 30 кДж/моль). Обсуждено влияние кач-ва базисного набора и учета электронной корреляции на результаты расчетов и проанализированы источники ошибок на низших уровнях расчета.

И. Н. Сенченя

CH_3OH 1992

Bauschlicher C.W., (Z),
Langhoff S.R., et al.,

J. Chem. Phys., 1992, 96,
N 1, C. 450-454.

М.Л.

(см. H_2O; III)

CH_3OH

1992

[illegible] **200796k The infrared absorption spectra and normal coordinate analysis of methanol $^{13}CH_3OH$, $^{13}CD_3OH$, and $^{13}CD_3OD$.** Cruz, F. C.; Scalabrin, A.; Pereira, D.; Vazquez, P. A. M.; Hase, Y.; Strumia, F. (Inst. Fis. "Gleb Wataghin", UNICAMP, [illegible] Campinas, Brazil). *J. Mol. Spectrosc.* 1992, 156(1), 22-38 (Eng). The IR absorption spectra of the gas-phase ^{13}C-methanol isotopomers, $^{13}CH_3OH$, $^{13}CD_3OH$, and $^{13}CD_3OD$, were measured in the wavenumber region between 400 and 4000 cm^{-1}, at instrumental resolns. of 4 and 0.12 cm^{-1}. The fundamental vibrational wavenumbers were assigned from the spectra with the aid of a normal coordinate anal. using the valence force consts. recently detd. for the gas-phase ^{12}C isotopomers. Using the fundamental wavenumbers of both ^{12}C and ^{13}C-methanol isotopomers, the authors obtained a new set of force consts. for the methanol mol. by a simultaneous least-squares adjustment to a total of 67 obsd. wavenumbers.

(спектр)

C.A. 1992, 117, N 20

CH_3OH 1992

Lee Timothy J., Rice Julia E,

М·Л·

J. Amer. Chem. Soc., 1992,
114, N 21, с. 8247–8256.

(См. CH_3NO_3; III)

CH_3OH

1992

118: 135006g **High-resolution infrared, far-infrared and microwave spectroscopy and far-infrared laser analysis of CD_3OH and CH_3OH.** Mollabashi, Mahmoud (Univ. New Brunswick, Fredericton, NB Can.). 1990. 393 pp. (Eng). Avail. NLC Order No. DANN59449. From *Diss. Abstr. Int. B* 1992, 52(11), 5849.

(ИК спектр)

Ⓗ ☒

CD_3OH

C.A.1993, 118, N14

CH_3OH

1992

116: 244127b **The spectrum of methanol between 200 and 350 cm^{-1}: torsional transitions and evidence for state mixings.** Moruzzi, Giovanni; Strumia, Franco; Moraes, Joao Carlos Silva; Lees, Ronald M.; Mukhopadhyay, Indranath; Johns, John W. C.; Winnewisser, Brenda P.; Winnewisser, Manfred (Dip. Fis., Univ. Pisa, I-56126 Pisa, Italy). *J. Mol. Spectrosc.* 1992, 153(1-2), 511-77 (Eng). In the framework of a systematic investigation of the IR and far IR spectrum of CH_3OH by high-resoln. Fourier transform spectroscopy, a catalog is presented of 8800 absorption lines between 200 and 352 cm^{-1}. The Taylor expansion coeffs. for evaluating the energies of the levels involved in the transitions are also given. All of the lines occurring in the 200-352 cm^{-1} region correspond to transitions between torsionally excited states. Some forbidden lines ($\Delta n \neq 0$; $\Delta K = 0$), indicating state mixings, were found.

Фурье ИК
спектр

C.A. 1992, 116, N 24

CH_3OH

1992

116: 264604h **New infrared–infrared double resonance spectra of methanol.** Petersen, J. C. (Dan. Inst. Fundam. Metrol., Lyngby, 2800 Den.). *Opt. Commun.* 1992, 88(4-5-6), 357-63 (Eng). Several new Stark tuned IR–IR double resonance spectra were obsd. when the CH_3OH mol. was investigated using an acousto-optic modulated single-mode continuous-wave CO_2 laser. The observations confirmed the assignments of 3 previously reported IR absorption transitions. New assignments are proposed for 3 transitions while partial assignments have been obtained for 3 transitions and a previously obsd. double resonance was reassigned. The results allowed the detn. of the permanent elec. dipole moment components μ_a'' and μ_a' for several ground state and CO stretch state levels including excited torsional state levels. Assignments of optically pumped far-IR laser lines assocd. with 2 of the IR transitions are proposed.

(M) ИК спектр

C.A. 1992, 116, N 26

CH_4O^+

1992

117: 258378s **The chemistry of gas-phase ions: a theoretical approach.** Radom, Leo (Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601 Australia). *Int. J. Mass Spectrom. Ion Processes* 1992, 118-119, 339-68 (Eng). A review with 59 refs. The various means by which ab-initio-MO theory can be used to study the chem. of gas-phase ions are discussed. Topics discussed include: the prediction of mol. structures, vibrational spectra, stable isomeric structures, reaction pathways, heats of formation, gas-phase acidities, ionization energies, appearance energies, reverse activation energies, isotope effects, and ion/neutral complexes. Systems examd. in detail include: ionized methanol and its rearrangement and fragmentation products [CH_4O^+], protonated ethanol [$C_2H_7O^+$], and the ion dimer of ammonia with mol. hydrogen [NH_5^+].

структур. парамет., ν_i, стабилн. изомеров; J, обзор. ② ☒

$C_2H_7O^+$, NH_5^+

C.A. 1992, 117, N26.

CH_3OH

1992

116: 264593d **Infrared–radiofrequency double–resonance Stark spectroscopy of methyl alcohol using a carbon dioxide laser.** Takagi, Kojiro; Kuse, Masaya; Kido, Tsuyoshi; Furuta, Mitsuhiro (Dep. Phys., Toyama Univ., Toyama, Japan 930). *J. Mol. Spectrosc.* 1992, 153(1–2), 291–302 (Eng). An IR–radiofrequency double–resonance technique using a CO_2 laser was applied to observe direct radiofrequency transitions between Stark components in torsion–rotational states of CH_3OH. A double–resonance cell consisting of a pair of parallel glass plates coated with a conductive thin film and a radiofrequency transmission line outside the parallel plates was developed and used over a wide range of values of frequency and elec. field. The a–component of the elec. dipole moment, μ_a, was detd. for various torsion–rotational levels in the ground state and in the excited CO stretching and CH_3 rocking (A') vibrational states.

(Ч)

C. A. 1992, 116, N26

$CH_3{}^{18}OH$

1992

118: 134966h FTIR spectroscopy of the lower vibrational modes of O-18 methanol. Zhao, Saibei; Lees, R. M.; Johns, J. W. C.; Chan, C. P. (Dep. Phys., Univ. New Brunswick, Fredericton, NB Can. E3B 5A3). *Proc. SPIE-Int. Soc. Opt. Eng.* 1992, 1929(Conf. Dig. – Int. Conf. Infrared Millimeter Waves, 7th, 1992), 240–1 (Eng). The high-resoln. Fourier transform-IR spectrum of $CH_3{}^{18}OH$ was investigated from 1100–1600 cm^{-1}. Broad absorptions occur in this region with poorly-defined structure yet to be conclusively identified. Various sub-branches have been assigned and linked together by combination differences. From 1100–1400 cm^{-1}, they involve excited torsional levels of the CH_3-rock interacting with the OH-bend, and above 1400 cm^{-1} the out-of-plane CH_3-deformation mode in Coriolis resonance with the sym. CH_3-bend. The vibrational energy pattern is discussed, along with improvements to far-IR laser wavenumbers.

(ИК спектр)

C.A. 1993, 118, N 14

CH_3OH

1993

120: 147468p Methanol in isolated matrix, vapor and liquid phase: Raman spectroscopic study. Furic, Kresimir; Mohacek, Vlasta; Mamic, Miro (Ruder Boskovic Inst., Zagreb, Croatia 41001). *Spectrochim. Acta, Part A* 1993, 49A(13-14), 2081-7 (Eng). Raman spectra of MeOH suspended in Ar matrixes are reported. A comparison of calcd. values and results for the vapor and liq. phases obtained with the same instrument is included. Observations in the low and high frequency regions are not entirely in agreement with complementary IR studies, but this can be explained by the prevalence of dimeric forms.

спектр
в
матрице

C.A. 1994, 120, N12

CH_3OH 1993

9 Б1190. Молекулярное силовое поле метанола. Molecular force field of methanol /Hase Y., Forneris R., da Silva S. C. //Spectrosc. Lett. .— 1993 .— **26** ,№ 3 .— С. 1497— 1510 .— Англ.

На основе ИК- и КР-спектров газ. фазы, с привлечением данных по дейтерированным молекулам, проведен анализ нормальных колебаний молекулы метанола. Определено 25 параметров силового поля, проводится сравнение с ранее полученными результатами, обсуждается отнесение ИК-полос к смешанным колебаниям. Особое внимание уделено низкочастотной области. Л. В. Серебренников

М.Л.

Х. 1994, №9

$H-CH_2OH$ От. 37380 1993

Ruscic B., Berkowitz J.,

До J. Phys. Chem., 1993,
97, 11451–11455

CH_3OH

1993

121: 21226k Fourier transform a-type spectra of $^{13}CD_3OH$ methanol in the 14–50 cm^{-1} range. Xu, Li Hong (Phys. Dep., Univ. New Brunswick, Fredericton, NB Can. E3B 5A3). *Proc. SPIE-Int. Soc. Opt. Eng.* **1993**, 2250, 48–9 (Eng). The FTIR spectra of $^{13}CD_3OH$ MeOH was recorded at 14–50 cm^{-1} on the modified DA3.002 Bomem spectrometer at a resoln. of 0.002 cm^{-1} at the Herzberg Inst. of Astrophys., Natl. Res. Council, Ottawa. Clear ground state a-type J-multiplets are seen in this region. Assignments of these J-multiplets were combined with ground state information obtained from assocd. IR fundamental band studies to form a solid base of ground state data over an extensive range of torsion-rotation quantum nos. The data were useful for further IR studies and FIR (far-IR) laser assignments for this isotopic species of MeOH. Global fitting of the new FIR observations together with previous microwave measurements has yielded an improved set of a-type mol. parameters.

ММ, МБ
спектр

C.A. 1994, 121, N2

CH_3OH

1993

121: 21227m Microwave and millimeter spectra of O-17 and O-18 methanol. Xu, Li Hong; Bance, P. M.; Lees, R. M.; Styger, C.; Gerry, M. C. L. (Phys. Dep., Univ. New Brunswick, Fredericton, NB Can. E3B 5A3). *Proc. SPIE-Int. Soc. Opt. Eng.* **1993**, 2250, 94-5 (Eng). Microwave and mm-wave spectra of Me^{17}OH and Me^{18}OH were studied at 30-40 GHz. Me^{17}OH was studied with a pulsed-mol.-beam Fourier transform spectrometer operating in the X and K$_u$ bands to examine the quadrupole hyperfine structure of certain transitions.

Мм, Мв
спектр

C.A. 1994, 121, N2

CH_3OH

1994

122: 276865f The equilibrium absorption spectrum of an excess electron in methanol. The effect of deuteration on the band shape. Abramczyk, Halina; Barut, Marek; Kroh, Jerzy (Inst. Applied Radiation Chem., Technical Univ. Lodz, 93-590 Lodz, Pol.). *Bull. Pol. Acad. Sci., Chem.* 1994, 42(1), 131–40 (Eng). The visible absorption spectra of excess electrons in CH_3OH, CD_3OH, CH_3OD and CD_3OD were measured at 77 K. The Raman spectra of deuterated methanols were measured at 77 K and 293 K. The theor. spectra were calcd. in terms of the electron–vibron coupling and compared with the exptl. ones. The deuteration effect of intramol. vibrational modes on the absorption band shape has been discussed.

(CKP)

C.A. 1995, 122, N 22

CH_3OH 1994

Illenberger E.
NATO ASI Ser., Ser.
(Ae) B 1994, 326, 355-76.
обзор

(см. CF_3I; III)

CH_3OH

1994

Вращат. спектр

120: 230218a **Absolute frequency measurements of methanol from 1.5 to 6.5 THz.** Matsushima, Fusakazu; Evenson, Kenneth M.; Zink, Lyndon R. (Dep. Phys., Toyama Univ., Gofuku, Japan 930). *J. Mol. Spectrosc.* 1994, 164(2), 517-30 (Eng). Frequencies of 446 MeOH rotational transitions at 1.5-6.5 THz were measured with an accuracy of 1 ppb. The far-IR radiation used for the measurements was generated from the radiation of 2 CO_2 lasers using a MIM diode as a nonlinear mixer. The high resoln. and sensitivity of the spectrometer enabled forbidden Q branch transitions ($\Delta n = 1$ and $\Delta K = 0$) for $J = 12$-26 to be obsd.

C.A. 1994, 120, N 18

1995

F: CH3OH
P: 3
2Б1253. Вращательно-торсионный спектр высокого разрешения метанола от 0,55 до 1,2 ТГц. The high-resolution rotational-torsional spectrum of methanol from 0.55 to 1.2 THz / Belov S. P., Winnewisser G., Herbst Eric // J. Mol. Spectrosc. - 1995. - 174, N 1. - C. 253-269. - Англ.

На субмиллиметровом спектрометре в области частот 0,55-1,2 ТГц с точностью около 10 кГц измерен вращательно-торсионный спектр метанола CH[3]OH в трех наинизших торсионных состояниях. Выполнен глобальный анализ данных и определены молекулярные постоянные.

Pжх 1997

CH_3OH 1995

123: 324744k **The high-resolution rotational-torsional spectrum of methanol from 0.55 to 1.2 THz.** Belov, S. P.; Winnewisser, G.; Herbst, Eric (I. Physikalisches Inst., Univ. Koeln, D-50937 Cologne, Germany). *J. Mol. Spectrosc.* 1995, 174(1), 253–69 (Eng). The rotational-torsional spectrum of gas-phase methanol (CH_3OH) has been studied at high resoln. in the frequency range 0.55–1.2 THz. Over 450 new spectral lines belonging to 14 Q branches and 3 R branches in the lowest three torsional states (v_1 = 0–2) have been measured and analyzed. The lines have been added to previously measured transitions at lower frequency to comprise a global data set, which has been fit via an extended internal axis method in which transitions belonging to the A and E symmetry species are analyzed sep.

кол. вр. спектр
высокого
разрешен.

С.-А. 1995, 123, N 24-

CH_3OH

1995

122: 145666u **Precise laboratory measurements of methanol rotational transition frequencies in the 5 to 13 GHz region.** Breckenridge, S. M.; Kukolich, S. G. (Department of Chemistry, University of Arizona, Tucson, AZ 85721 USA). *Astrophys. J.* **1995**, 438(1, Pt. 1), 504–5 (Eng). Rotational transitions for MeOH were measured at 5–13 GHz with a precision and accuracy of a few kHz or less using a Flygare–Balle type pulsed-beam Fourier transform microwave spectrometer. The accurate center frequencies for transitions measured should be useful in detg. accurate Doppler shifts and making pos. mol. identification in radio astronomy.

Вращат-
переходы

C. A. 1995, 122, N 12

1995

F: CH3OH
P: 3
2Б1231. Анализ с программой "Ритц" фурье-спектра C[3]O между 350 и 950 см{-1}. "Ritz" analysis of the fourier spectrum of CH[3]OH between 350 and 950 cm{-1} / Ioli N., Moruzzi G., Riminucci P., Strumia F., Silos Moraes J. C., Winnewisser B. P., Winnewisser M. // J. Mol. Spectrosc. - 1995. - 171, N 1. - С. 130-144. - Англ.

Новая программа "Ritz" расчета и идентификации вращательно-колебат. спектров использована для анализа почти 9600 линий фурье-спектра C[3]O в области 350-950 см{-1}, полученного с разрешением 0,0012 см{-1}. Программа расчета основана на комбинационном принципе Ридберга-Ритца, учитывает резонансы Ферми и кориолисовы взаимодействия с учетом торсионных переходов 'ДЕЛЬТА'n=1, 2, 3 в основном колебат. состоянии.

Р.Ж.Х. N2, 1996.

1995

F: CH3OH
P: 3
1Б1258. "Ритц" анализ фурье-спектра {13}CH[3]OH от 25 до 350 см{-1}. "Ritz" analysis of the Fourier spectrum of {13}CH[3]OH from 25 to 350 cm{-1} / Moraes Joao Carlos S., Pereira Daniel, Scalabrin Artemio, Moruzzi Giovanni, Strumia Franco, Winnewisser Brenda P., Winnewisser Manfred, Mukhopadhyay Indranath, Kumar Gupta Pradeep // J. Mol. Spectrosc. - 1995. - 174, N 1. - C. 177-195. - Англ.
На ИК-фурье-спектрометре в области частот 25-350 см{-1} с разрешением 0,004-0,007 см{-1} измерен спектр поглощения изотопомера метанола {13}CH[3]OH. Анализ данных выполнен с использованием расчетной программы "Ритц", включая торсионно-возбужденные уровни основного колебательного состояния. Библ. 44.

PЖX 1997

CH_3OH

1995

123: **324739n "Ritz" analysis of the Fourier spectrum of $^{13}CH_3OH$ from 25 to 350 cm^{-1}.** Moraes, Joao Carlos S.; Pereira, Danial; Scalabrin, Artemio; Moruzzi, Giovanni; Strumia, Franco; Winnewisser, Brenda P.; Winnewisser, Manfred; Mukhopadhyay, Indranath; Gupta, Pradeep Kumar (Dep. Fisica Quimica, UNESP, Ilha Solteira, Brazil). *J. Mol. Spectrosc.* **1995,** 174(1), 177–95 (Eng). The "Ritz" program has been used for the investigation of the absorption spectrum of the $^{13}CH_3{}^{16}OH$ isotopomer of methanol from 25 to 350 cm^{-1}. This allowed us to assign some perturbed level sequences which could not be followed by the Taylor expansions used in a previous program. Altogether, more than 13,800 lines have been assigned in the investigated region, and the energies of 1363 levels of A symmetry and 2006 levels of E symmetry have been evaluated. A comparison with the energy level values of the parent species $^{12}CH_3OH$ is presented. Some forbidden transitions, due to state mixings, have been obsd. Taylor expansion coeffs. for evaluating the energies of the levels involved in the transitions are also given. All of the lines presented in this paper correspond to transitions involving torsionally excited levels within the ground vibrational state.

ИК Фурье спектр

C. A. 1995, 123, N24

F: CH3OH

P: 3

1995

9Б1303. Микроволновый и миллиметровый спектры {13}CD[3]OH. Microwave and millimeter-wave spectra of {13}CD[3]OH / Mukhopadhyay I., Sastry K. V. L. N., Lees R. M., Winnewisser M. // J. Mol. Spectrosc. - 1995. 172, N 1. - C. 108-115. - Англ.

Измерены спектры поглощения {13}CD[3]OH в микроволновой и миллиметровой области (18-116 ГГц). Отнесены все линии мультиплетов R-ветвей переходов А-типа J=1'<-'0, 2'<-'1 и 3'<-'2 для трех нижних торсионных состояний. Большое расщепление в мультиплетах объясняется сильным торсионно-вращательным взаимодействием. Отнесены также переходы b-типа, включая серии K=1'<-'0 E[1], K=1'<-'2 E[1] и асимметрично расщепленные K=3'<-'2 A (Q-ветви). При анализе использован полуэмпирический торсионно-вращательный гамильтониан и определены точные спектроскопические параметры а-типа: (B+C)/2, F[V], G[V], L[V], D[J] D[JK], I[b], I[c], I[ab], 'альфа', 'ро' (система обозначений дана в работе//J. Chem. Phys.-1968.-48.-C. 5299).

Р.ЖХ.N9, 1996

1995

F: CH3OH
P: 3

1Б1253. Спектроскопия обертонов метилового, этилового спиртов и цианидов. Overtone spectroscopy of methyl, ethyl alcohols and cyanides / Prasad V. J., Rai S. B. // Indian J. Phys. B. - 1995. - 69, N 5. - С. 471-476. - Англ.

В области 5500-16 000 см{-1} получены ИК-спектры метанола, этанола, метил- и этилцианида. Их спектры в области 15 900-17 550 см{-1} получены с помощью метода тепловой линзы. Измеренные частоты отнесены к обертонам с v=2-6 колебаний C-H и O-H и использованы для вычисления нулевых частот колебаний, постоянных ангармоничности и энергий диссоциации этих связей. Обсуждено влияние H-связей.

РЖХ 1997

$CH_3{}^{18}OH$

1995

123: 68909s Fourier transform spectroscopy of $CH_3{}^{18}OH$: the in-plane CH_3-rocking band. Zhao, Saibei; Lees, R. M.; Johns, J. W. C.; Chan, C. P.; Gerry, M. C. L. (Phys. Dep., Univ. New Brunswick, Fredericton, NB Can. E3B 5A3). *J. Mol. Spectrosc.* **1995**, 172(1), 153–75 (Eng). The IR Fourier transform spectrum of $CH_3{}^{18}OH$ has been recorded in the region from 1020 to 1620 cm^{-1} at high resoln. in order to study the low-lying bending modes, including the CH_3-rocking, OH-bending, and CH_3-deformation fundamental bands. More than 10,000 lines have now been assigned in this region. The present paper focuses on the n = 0 ground torsional subbands of the in-plane CH_3-rocking fundamental. This band is principally of parallel a-type character, due to mixing of the predominantly parallel CO-stretching and OH-bending coordinates with the perpendicular rocking coordinate. Some b-type character was also obsd., with partial assignments of a no. of weak perpendicular subbands. The parallel subbands have been fitted to J(J+1) power-series expansions to obtain the subband origins, as well as compact representations of the data in terms of phenomenol. state-specific expansion coeffs. The n = 0 excited state energies calcd. from the subband origins follow a similar oscillatory pattern with K to that of the ground vibrational state but with significantly reduced amplitude. Anal. with our basic torsion-rotation Hamiltonian yields an effective torsional barrier height for the rocking state of 474.5 ± 2.8 cm^{-1}, a 27% increase over the ground state value. The vibrational energy is found to be 1058.46 ± 0.62 cm^{-1}. An interesting

ИК Фурье спектр, м.п.,

V_0

С.А. 1995; 123, N6

J-localized level-crossing resonance between the CH_3-rocking and CO-stretching modes has also been obsd. through perturbations in the spectrum.

1995

F: CH3OH
P: 3

5Б1359. Фурье-спектроскопия CH[3]{18}OH. Полоса плоскостного маятникового колебания группы CH[3]. Fourier transform spectroscopy of CH[3]{18}OH: The in-plane CH[3]-rocking band / Zhao Saibei, Lees R. M., Johns J. W. C., Chan C. P., Gerry M. C. L. // J. Mol. Spectrosc. 1995. - 172, N 1. - С. 153-175. - Англ.

Исследованы ИК-фурье-спектры поглощения (в области 1020-1620 см{-1}, с разрешением 0,002-0,004 см{-1}, при комн. т-ре) CH[3]{18}OH (I). Интерпретированы более 10 000 линий, идентифицированы крутильные подсистемы и положения их начал (для основного состояния n=0) для плоскостного маятникового колебания группы CH[3] I. Результаты эксперим. отнесения подсистем включены в схему для теор. анализа ПФВВ I с использованием колебательно-вращат. гамильтониана, рассчитаны параметры ПФВВ, асимметричного расщепления уровней A, возмущения анализируемого колебат. состояния.

Р. Ж. Х. N5, 1996.

CH_3OH^+ 1996

24Б1143. Структура метанольного катион-радикала. Неестественно короткая длина связи С—О в расчетах на уровне МП2. The structure of the methanol radical cation: An artificially short C—O bond with MP2 theory / Gauld James W., Glukhovtsev Mikhail N., Radom Leo // Chem. Phys. Lett.— 1996.— **262**, № 3-4.— С. 187–193.— Англ.

В рамках теор. коррелированных методов квантовой химии различного уровня проведено повторное исследование структуры $CH_3OH^{\cdot+}$ (I) и на наиболее высоком уровне расчета (CCSD(T)/6–311G(*df, p*)) показано, что катион-радикал I имеет заслоненную конформацию с диной связи С—О, равной 1,370 Å. Показано также, что приближение МП2 с использованием расширенных базисов переоценивает эффект сопряжения в I и приводит к значению длины С—О, равному менее 1,3 Å. Н. С.

М.Л.

Х.1997, №24

1996

F: CH3OH
P: 3

97 13Б1276. Изучение инфракрасных спектров - ацетона и метанола, изолированных в матрицах из аргона. Infrared matrix izolation study of acetone and methanol in solid argon / Han Sang Woo, Kim Kwan // J. Phys. Chem. - 1996. - 100, N 43. - C. 17124-17132. - Англ.

Место хранения ГПНТБ Изучены ИК-спектры смесей ацетона и метанола в матрицах из аргона при 9К. В области полос обеих молекул найдены полосы комплексов состава 1:1, что подтверждено изучением концентрационных зависимостей. Обсуждается строение комплексов, проведены неэмпирические расчеты различного уровня. Найдено, что наиболее стабильна плоская структура с шестичленным циклом. Библ. 59.

PHYX 1997

CH_3-OH
CH_3-OH^+
CH_3-OH^-

ОП 38522

1996

Harold Basch, Pinchas Aped et al.,

Mol. Phys., 1996, 89, N 2, 331-354

De,

Re,

ab initio расчет

$CH_3{}^{18}OH$

1996

125: 233604q Laboratory microwave spectrum of $CH_3{}^{18}OH$. Hoshino, Y.; Ohishi, M.; Akabane, K.; Ukai, T.; Tsunekawa, S.; Takagi, K. (Department Physics, Toyama University, Toyama, Japan 930). *Astrophys. J., Suppl. Ser.* 1996, 104(2), 317–328 (Eng). The microwave spectrum of $CH_3{}^{18}OH$ at 9–95 GHz was studied in the lab. One hundred ninety-seven lines were obsd., including all the transitions of $J \leq 30$, $|K| \leq 6$ in the torsional ground state ($v_1 = 0$) and some lines from torsionally excited states up to $v_1 = 3$. The spectrum was analyzed by using the Hamiltonian proposed by De Lucia et al. and was fitted to 33 mol consts. with an root-mean-square deviation of the fit, 0.22 MHz, by treating the A and E substates simultaneously.

МВ спектр

CH_3OH

1996

125: 287610g Fourier transform spectroscopy of torsionally excited C-13 methanol in the CO-stretching band. Lees, R. M.; Mukhopadhyay, I.; Predoi, Andriana; Lewis-Bevan, W.; Johns, J. W. C. (Dep. Phys., Univ. New Brunswick, New Brunswick, Can. E3B 5A3). *J. Chem. Phys.* **1996**, 105(9), 3406-3418 (Eng). Torsionally excited $n = 1$ and $n = 2$ subbands of the CO-stretching fundamental were assigned in the FTIR spectrum of $^{13}CH_3OH$ recorded at a resoln. of 0.002 cm^{-1}. For the $n = 1$ torsional state, subbands with $K \leq 7$ were identified for A torsional symmetry and ≤ 5 for E symmetry. For $n = 2$, 4 subbands were so far assigned. Subband origins were obtained by fitting the obsd. wavenos. to $J(J + 1)$ power-series expansions. The expansion parameters represent the data compactly to close to the exptl. uncertainty in the absence of line blending or perturbations. Significant downshifting of the $n = 1$ origins is obsd., correlated closely with proximity to the $n = 0$ OH-bending state. J-localized perturbations were obsd. and characterized for several subbands. Two of the far-IR laser lines optically pumped by the 10R(14) CO_2 laser line were assigned.

(спектр)

C.A. 1996, 125, N22

1996

F: CH3OH
P: 3
1Б1259. Отнесение длинноволновых ИК-лазерных линий от оптически накачиваемого {13}CH[3]OH. Assignments of FIR laser lines from optically pumped {13}CH[3]OH / Moraes J. C. S., Carelli G., Moretti A., Moruzzi G., Strumia F. // J. Mol. Spectrosc. - 1996. - 177, N 2. - C. 302-306. - Англ.
Заново выполнено отнесение длинноволновых ИК-лазерных линий, излучаемых оптически накачиваемым {13}CH[3]OH. С использованием улучшенной версии программы расчета "Ритц" для фурье-спектра поглощения {13}CH[3]OH дано новое отнесение для 11 ИК-лазерных линий и подтверждено 11 ранее сообщенных отнесений. ИК- и длинноволновые ИК-частоты переходов оценены с точностью 10{-4} см{-1}.

РЖХ 1997

Метанол ОП 38972 1996

CH_3OH

ИК спектр
в
матрице

Sang Woo Han and
Kwan Kim+,

J. Phys. Chem. 1996,
100, N 43, 17124-132.

Infrared Matrix Isolation study of Acetone and Methanol in Solid Argon

1996

F: CH3OH
P: 3

17Б1289. Определение дипольного момента {18}O метанола при помощи микроволновой штарковской спектроскопии. Determination of the dipole moment of O-18 methanol by microwave stark spectroscopy / Sastry K. V. L. N., Mukhopadhyay I., Gupta P. K., VanderLinde J. // J. Mol. Spectrosc. - 1996. - 176, 1. - C. 38-44. - Англ.

На штарковском микроволновом спектрометре в области частот 36-48 ГГц со штарковскими полями от 0 до 1500 В с точностью 10 кГц измерены частоты девяти вращат. переходов первых четырех торсионных состояний в основном колебат. состоянии для {18}O-изотопомера метанола. Определены компоненты дипольного момента для основного торсионного состояния 'мю'[a]=0,8992(8) и 'мю'[b]=1,4226(3) Д. Установлено, что величина дипольного момента возрастает при торсионном возбуждении.

PWAX 1997

CH_3OH

1997

127: 226670w **Fourier transform spectrum of the in-plane CH_3-rocking fundamental and vibrational coupling in C-13 methanol.** Predoi, Adriana; Lees, R. M.; Johns, J. W. C. (Centre Laser Applications Molecular Science, Dep. Physics, Univ. New Brunswick, Fredericton, NB Can. E3B 5A3). *J. Chem. Phys.* 1997, 107(6), 1765-1778 (Eng), American Institute of Physics. The Fourier transform IR spectrum of the in-plane CH_3-rocking fundamental of $^{13}CH_3OH$ has been investigated at 0.002 cm^{-1} resoln. The rocking band is principally of parallel character and has a double-peaked Q branch and relatively wide spread subbands indicative of a substantial change in torsional barrier height. All A subbands from $K = 0$ to 11 and all but one E subband from $K = 0$ to 9 have been assigned in the $n = 0$ torsional state and fitted to $J(J + 1)$ power-series expansions to obtain the subband origins and excited-state energy structure. The effects of vibrational interactions between the CH_3-rocking and CO-stretching modes are prominent in the spectrum. Coriolis coupling between rocking $(K - 1)$ and CO-stretching K levels is observable for $K \geq 6$, and makes significant contributions to

(UK)

C.A. 1997, 127, N16

the subband origins and effective B values. Several J−localized perturbations due to level−crossing resonances with CO−stretch states have been obsd. and characterized. Two reported strong far IR laser lines optically pumped by the 10R(26) CO_2 laser line have been found to arise through such a $\Delta K = 3$ level crossing resonance. Modeling of the rocking−state torsion−K−rotation energies yields a height of $V_3^r = 469.2(38)\ cm^{-1}$ for the torsional potential barrier, a 26% increase over the ground state. The asymmetry K−doubling pattern in the excited state is qual. consistent with this barrier for $K = 2$ to 4, but the $K = 5$ rocking substate displays strongly enhanced splitting.

CH_3OH

1997

126: 284105f **Microwave spectra of molecules of astrophysical interest. XXIV. Methanol (CH_3OH and $^{13}CH_3OH$).** Xu, Li-Hong; Lovas, F. J. (Dep. of Physical Sciences, University of New Brunswick, Saint John, NB Can. E2L 4L5). *J. Phys. Chem. Ref. Data* 1997, 26(1), 17–156 (Eng), American Chemical Society. The available microwave and mm-wave spectra of MeOH and its most abundant isotopomer, $^{13}CH_3OH$, are reviewed with 41 refs. and supplemented with spectral frequency calcns. derived from rotation–internal rotation analyses. For both species, global analyses of the torsional ground state, $\nu_t = 0$, and the 1st excited torsional state, $\nu_t = 1$, were carried out in which all obsd. spectral lines are reproduced to within their measurement uncertainties. Refs. are given for all data included. The primary objective of this review is to provide radio astronomers with complete spectral coverage of rotational transitions from 500 MHz to 1 THz, including the lower state energy and line strength for each transition, over the range in rotational quantum no. J = 0–26.

(Мв спектр)

C.A. 1997, <u>126</u>, N 21

CH_3OH 1997

ИК спектр

127: 363656k Sub-Doppler infrared spectra and torsion-rotation energy manifold of methanol in the CH-stretch fundamental region. Xu, Li-Hong; Wang, Xiaoliang; Cronin, Thomas J.; Perry, David S.; Fraser, Gerald T.; Pine, Alan S. (Dep. Phys. Sci., Univ. New Brunswick, Saint John, NB Can. E2L 4L5). *J. Mol. Spectrosc.* **1997,** 185(1), 158–172 (Eng), Academic. The IR spectrum of jet-cooled MeOH in the CH-stretched fundamental region was studied by 2 sub-Doppler laser techniques: optothermally-detected mol.-beam elec. resonance and direct-absorption slit-jet spectroscopy. With the aid of microwave-IR double resonance and ground state combination differences. 27 Subbands at 2967–3027 cm^{-1} were analyzed to yield matrix elements of 0.013, 0.041, and 0.75 cm^{-1}, resp. The A–E torsional tunneling splitting for $J = 0$ of the ν_2 vibration of -3.26 cm^{-1} is of opposite sign and a factor of 3 smaller in magnitude than the ground state value of +9.12 cm^{-1}.

C. A. 1997, 127, N 26

CH_3OH

1998

спектр погл;
М.П.

130: 100959r **Torsion–rotation energy levels and the hindering potential barrier for the excited vibrational state of the OH–stretch fundamental band v_1 of methanol.** Hunt, R. H.; Shelton, W. N.; Flaherty, Francis A.; Cook, W. B. (Department of Physics, The Florida State University, Tallahassee, FL 32306 USA). *J. Mol. Spectrosc.* 1998, 192(2), 277–293 (Eng), Academic Press. The absorption spectrum of MeOH vapor was recorded at room temp. from 3200 to 4200 cm^{-1} with a 1.24–M path–difference Fourier transform spectrometer. Over 10,000 transitions to the torsion–rotation states $n, \tau J, K$ of the OH stretching fundamental band v_1 were assigned, thereby greatly expanding the results of previous studies. Approx. 4000 of the cleaner lines were used to det. 665 excited state torsion–rotation levels with

С.А. 1999, 130, N8

principal torsional quantum no. $n = 0$ as well as 494 levels with $n =$ 1,286 levels with $n = 2$, and 14 levels with $n = 3$. These levels correspond to 86 values of the quantum nos. n, τ, K. Most of the levels of a given n, τ, K are perturbed resulting in irregular P−, Q−, and R−branch series. The $J = 0$ origins for 64 values of n, τ, K have fitted and a value of 410 cm^{-1} obtained for the hindering potential barrier. This in agreement with a previous study of grating spectra but is lower than that obtained in more recent anal. of $n = 0 - 0$ transitions obsd. for $K \leq 3$ in very low temp. spectra. The criteria used there to select states to be fitted and the difficulties in estg. the $J = 0$ origins because of the many perturbing level crossings are discussed. (c) 1998 Academic Press.

CH_3OH 1998

$^{13}CH_3OH$

Jackson, Michael,
(New Mexico univ, Las Cruces, NM USA) 1998, 145pp
From Diss. Abstr. Int.,
B1999, 59(7), 3524

(ик спектр)

(см. CD_3F; III)

CH_3OH

1998

(спектр)

129: 222572j **Assignment and power series analysis of tne FIR Fourier transform spectrum of cyanamide using a multimolecule Ritz program.** Moruzzi, Giovanni; Jabs, Wolfgang; Winnewisser, B. P.; Winnewisser, Manfred (Dipartimento di Fisica, Universita di Pisa and INFM, I-56126 Pisa, Italy). *J. Mol. Spectrosc.* 1998, 190(2), 353–364 (Eng), Academic Press. The Ritz program, originally written for the anal. of the Fourier transform spectra of the MeOH isotopomers and presented in previous papers, was extended to analyze the spectra of other mols. This program evaluates the term values involved in the assigned transitions by the Rydberg–Ritz combination principle, and can tackle such perturbations as Fermi–type resonances or Coriolis interactions. As a 1st application of the extended version, the authors present a study of the Fourier transform spectrum of cyanamide between 25 and 980 cm^{-1}. More than 16,000 lines were assigned. Ritz database now comprises a list of >19,000 assigned lines (including of the microwave and FIR lines available in the JPL database) and >3900 term values. All of the lines presented in this paper correspond to transitions within the ground and 1st excited inversion levels of the ground vibrational state of the small–amplitude modes. (c) 1998 Academic Press.

C. A. 1998, 129, N 17

$^{13}CH_3OH$

1998.

129: 101335a Fourier Transform infrared spectroscopy of the first CO−stretch overtone band of $^{13}CH_3OH$. Predoi−Cross, Adriana; Mellau, G. C.; Lees, R. M.; Winnewisser, B. P. (Physics Dep., Univ. Toronto, Toronto, ON Can. M5S 1A7). *J. Mol. Spectrosc.* **1998**, 189(2), 144−152 (Eng), Academic Press. This paper presents a high-resoln. FTIR study of the 1st CO−stretch overtone band of $^{13}CH_3OH$. The spectrum was recorded at the Justus−Liebig University, Giessen, Germany on their Bruker IFS 120 HR Fourier transform spectrometer. The authors have assigned parallel subbands in the torsional state n = 0 for K values up to 6. Each individual subband was fitted to a J(J + 1) power series expansion to obtain the subband origin and the state-specific energy expansion coeffs. for the 1st CO−stretch overtone state. The av. rotational const. B in the CO_stretch $\nu_{CO} = 2$ state is 0.768 cm^{-1}, forming a smooth series with that of 0.777 cm^{-1} obtained in the $\nu_{CO} = 1$ state and the ground state value of 0.787 cm^{-1}. Modeling of the excited state torsion−vibration energy level structure derived from the subband origins is then discussed and mol. parameters in the $\nu_{CO} = 2$ state are proposed. The value obtained for the barrier height to internal rotation is 377.06 ± 0.52 cm^{-1}, nearly indistinguishable from the value 378.65 cm^{-1} reported for the CO−stretch $\nu_{CO} = 1$ state. The vibrational energy is 2020.9 ± 1.4 cm^{-1}. The harmonic wavenumber for the CO−stretch vibration in $^{13}CH_3OH$ is $\omega = 1029.9$ cm^{-1}. The anharmonicity const. of this vibration is $\omega x = 6.5$ cm^{-1}, giving $x = 6.3 \times 10^{-3}$. The authors also obsd. asymmetry−induced K doubling for the subbands of A symmetry for K values from 1 to 3 at sufficiently high J values. The size of the splitting coeffs. is similar to those obsd. for the CO−stretch fundamental (14), with the exception of those for the K = 3A doublet, where the obsd. splitting is ~18% larger than that for the ground and CO−stretch $\nu_{CO} = 1$ states.

FTIR-спектр!

V_0, ω_e

CA 1998, 129, 1

CH_3OH

1998

129: 337072p Fourier transform infrared spectroscopy and vibrational coupling in the OH–bending band of $^{13}CH_3OH$. Predoi–Cross, Adriana; Lees, R. M.; Johns, J. W. C. (Centre for Laser Applications and Mol. Science, Physics Department, Univ. of New Brunswick, Fredericton, NB Can.). *J. Mol. Spectrosc.* 1998, 191(2), 348–361 (Eng), Academic Press. The authors present a high–resoln. FTIR study of the OH–bending vibrational band of ^{13}MeOH. The authors have studied the 1070–1400 cm^{-1} spectral region at 0.002 cm^{-1} resoln. using the modified Bomem DA3.002 Fourier transform spectrometer at the Steacie Institute for Mol. Sciences at the National Research Council of Canada in Ottawa. This study led to (i) detn. of excited–state J(J + 1) subband expansion coeffs. and (II) characterization of a variety of interactions coupling the different vibrational modes, notably a strong Fermi resonance between the OH bend and the torsionally excited Me–rocking mode. The OH–bending band is widely spread with Q subbranches grouped in 2 peaks at ~1312 and 1338 cm^{-1}. The lower levels for all assigned subbands were confirmed using closed loops of IR and FIR transitions. The subbands were fitted to J(J + 1) power–series expan-

(FTIR, ν_i)

C. A. 1998, 129, N25

sions to obtain the subband origins and the state−specific energy expansion coeffs. for both the OH−bending and excited torsional Me−rocking states. The strong interaction between the OH−bending state and the 1st excited torsional Me−rocking state gives rise to several extra forbidden subbands due to intensity borrowing. The asymmetry splitting of the $(n\tau K)^{v} = (122)^{OH}$ A OH−bending doublet is anomalously small, and the splitting of the $(122)^{4}$A Me−rocking doublet is enhanced. The authors have identified a network of intermode interactions causing this unusual behavior, but a quant. anal. of the vibrational coupling is restricted by limited knowledge of the unperturbed positions of the interacting levels. All these interactions provide relaxation channels for intramol. vibrational redistribution among the lower vibrational modes in ^{13}MeOH. Another important finding is that the torsion−K−rotation energy curves in the OH−bending state display an inverted pattern compared to the ground state.

Оттиск № 40047 1999

CH_4O
CF_2Cl_2 (R-12)
NH_3
C_6H_6
CO_2
Термодин. св-ва, теор. расч. (ΔH_v, ρ, S, V, H).

Avsec J., Marčič M.
Acta Chim. Slov. 1999, 46(3)
pp. 375-388

The calculation of the thermodynamical properties in the liquid-gas region.

1999

F: CH3OH
P: 3
131:220495 Torsional motion and vibrational overtone spectroscopy of meth Hanninen, V.; Horn, M.; Halonen, L. Laboratory of Physical Chemistry, University of Helsinki FIN-00014, Finland J. Chem. Phys., 111(7), 3018- 3026 (English) 1999 American Institute of Physics. J. Chem. Phys. 111 7 3018-3026 English 1999 An internal coordinate Hamiltonian simulation, physicochem. has been constructed to simulation, physicochem. torsional motion in the OH stretc vibrational overtone region of methanol, CH3OH. The simulation, physicoc includes harmonic couplings between OH and CH stretching

vibrations and F resonance interactions between OH stretches and COH bends and between CH stretches and CH2 bends. A symmetrized basis set has been used to form b diagonal Hamiltonian matrixes with strong resonance couplings off-diagona Obsd. torsional levels of the excited vibrational states have been used a in a least squares optimization of the simulation, physicochem. parameter of which have been estd. by ab initio calcns. The exptl. obsd. increase effective torsional barrier in moving to highly excited OH stretching sta been explained by the simulation, physicochem. torsional motion vibration overtone spectroscopy methanol

1999

F: CH2DOH
P: 3

132:42041 Vibration-Internal Rotation-Overall Rotation Interactions in CH2DOH and CHD2OH I. Development and Application of the Separation Transformations to the Zeroth-Order Kinetic Energy.

Quade, C. Richard Department of Physics, Texas Tech University Lubbock, TX 79409, USA

J. Mol. Spectrosc., 198(2), 329-347 (English) 1999 The zeroth-order kinetic energy is developed for the vibrating- rotating-internally rotating CH2DOH and CHD2OH mols. using the general th of Guan and Quade for the vibration-rotation-large amplitude internal mot interactions in mols. A T transformation is applied to obtain the necess (G-1)0 vibrational matrix elements in the kinetic energy for

C.A. 2000, 132

the R transformation that separates the internal rotation from the 3N-7 other vibrations. Then, a 2nd T transformation is used to sep. rotation from t 3N-7 other vibrations in zeroth order in the kinetic energy. The overall rotation and internal rotation remain coupled in zeroth order. All zerot order kinetic energy coeffs. are calcd. from the mol. structure and masse for the Me alc. mols. The phys. significance of the transformations is discussed. This paper reports the results of the 1st segment of the 3 segments that are necessary in the calcn. of the full soln. to the proble

1999

F: CH3OH
P: 3

131:249581 Infrared-microwave double-resonance spectroscopy of CH3OH by u sidebands of CO2 laser lines. Sun, Zhen-Dong; Matsushima, Fusakazu; Tsune Shozo; Takagi, Kojiro Department of Physics, Toyama University Toyama 930 8555, Japan J. Opt. Soc. Am. B, 16(9), 1447-1454 (English) 1999 An IR-microwave double-resonance technique using microwave sidebands of CO2 laser lines as an IR source was applied for observation of rotational of the MeOH mol. Frequencies of >50 rotational lines in the excited C-O stretching vibrational state (vco = 1) were measured with good precision were compared with those reported in IR studies. Many of them agree with several megahertz, although some lines show differences of >10 MHz. The pressure dependence of the double-resonance signals for 2 low-J microwave transitions belonging to the ground and the vco = 1 states, resp., were o for sample pressures .ltoreq.0.4 torr. For the former transition the sig obsd. to change its sign at higher pressures. Rate equation anal. explai obsd. pressure dependence quant. and allows one to understand the phys. processes involved in the double resonance.

1999

F: CH3OH
P: 3

130:251953 On the physical interpretation of torsion-rotation parameters methanol and acetaldehyde: Comparison of global fit and ab initio results Xu, Li-Hong; Lees, Ronald M.; Hougen, Jon T. (Department of Physical Sciences, University of New Brunswick, Saint John, NB E2L 4L5, Can.). J. Chem. Phys., 110(8), 3835-3841 (English) 1999 Equil. structural consts. and certain torsion-rotation interaction parameters have been detd. for methanol and acetaldehyde from ab initio c using GAUSSIAN 94. The substantial mol. flexing which occurs in going fr bottom to the top of the torsional potential barrier can be quant. relate coeffs. of torsion-rotation terms having a (1-cos 3.gamma.) dependence on torsional angle .gamma.. The barrier height, six equil. structural const characterizing the bottom of the potential well, and six torsion-rotation consts. are all compared to exptl. parameters obtained from global fits t microwave and far-IR data sets for methanol and acetaldehyde. The rather encouraging agreement between the Gaussian and global fit results for met seems both to validate the accuracy of ab initio calcns. of these paramet and to demonstrate that the phys. origin of these torsion-rotation intera terms in methanol lies primarily in structural relaxation with torsion. less satisfactory agreement between theory and expt. for acetaldehyde req further study.

1999

F: CH3OH
P: 3

130:251953 On the physical interpretation of torsion-rotation parameters in methanol and acetaldehyde: Comparison of global fit and ab initio results. Xu, Li- Hong; Lees, Ronald M.; Hougen, Jon T. (Department of Physical Sciences, University of New Brunswick, Saint John, NB E2L 4L5, Can.). J. Chem. Phys., 110(8), 3835-3841 (English) 1999 American Institute of Physics. CODEN: JCPSA6. ISSN: 0021-9606. DOCUMENT TYPE: Journal CA Section: 22 (Physical Organic Chemistry) Section cross-reference(s): 73 Equil. structural consts. and certain torsion-rotation interaction parameters have been detd. for methanol and acetaldehyde from ab initio calcns. using GAUSSIAN 94. The substantial mol. flexing which occurs in going from the bottom to the top of the torsional potential barrier can be quant. related to coeffs. of torsion-rotation terms having a (1-cos 3.gamma.) dependence on torsional angle .gamma.. The barrier height, six equil. structural consts. characterizing the bottom of the potential well, and six torsion-rotation consts. are all compared to exptl. parameters obtained from global fits to large microwave and far-IR data sets for

C.A., 199

methanol and acetaldehyde. The rather encouraging agreement between the Gaussian and global fit results for methanol seems both to validate the accuracy of ab initio calcns. of these parameters, and to demonstrate that the phys. origin of these torsion-rotation interaction terms in methanol lies primarily in structural relaxation with torsion. The less satisfactory agreement between theory and expt. for acetaldehyde requires further study.

methanol acetaldehyde torsion rotation parameters ab initio Total energy, Zero-point vibrational energy, ab initio; phys. interpretation of torsion-rotation parameters in methanol and acetaldehyde; Molecular structure, optimized; phys. interpretation of torsion-rotation parameters in methanol and acetaldehyde; MP2 (Moller-Plesset), Torsional barrier, phys. interpretation of torsion-rotation parameters in methanol and acetaldehyde; Hamiltonian, torsion-rotation; phys. interpretation of torsion-rotation parameters in methanol and acetaldehyde; 67-56-1, properties, 75-07-0, properties, phys. interpretation of torsion-rotation parameters in methanol and acetaldehyde

2000

F: CH3OH
P: 3
133:367328 Sub-Doppler Infrared Spectra of the OH-Stretch Fundamental of Methanol. Chirokolava, Andrei; Perry, David S.; Xu, Li-Hong Department of Chemistry, University of Akron Akron, OH 44325-3601, USA J. Mol. Spectrosc., 203(2), 320-329 (English) 2000 High-resoln. IR spectra of the 13C-MeOH OH stretching band, .nu.1, were obtained by slit-jet absorption spectroscopy

at a rotational temp. of 12- Twenty-eight subbands were assigned within the range of upper state quant nos., K' = 0 to 2 and J' = 0 to 10. The upper state energy levels are he perturbed; about half of the assigned subbands are split by perturbations matrix elements in the range 1-3 cm-1. The doubled lines were deperturbe together with the unperturbed lines were fitted to a global torsion-rotat Hamiltonian with root-mean-square deviation of 0.41 cm-1 to yield a torsi barrier height of ~405 cm-1 in the vibrationally excited state

2000

F: CH3OH
P: 3
132:165886 Molecular parameters for 12C and 13C-methanol isotopomers with 16, 17, and 18.

Duan, Yun-Bo; McCoy, Anne B.; Wang, Li; Takagi, Kojiro Department of Chemistry, The Ohio State University Columbus, OH 43210, USA

J. Chem. Phys., 112(1), 212-219 (English) 2000 Torsion-rotational parameters have been detd. for 12C and 13C-methanol isotopomers CH3OH with O-16, 17, and 18 using a recent formulation [Duan Takagi, Phys. Lett. A 207, 203 (1995)] of the centrifugal distortion effe from potential parameters for a mol. contg. a threefold sym.

C.A. 2000, 132

internal rot The calcd. parameters, esp. the consts. representing interactions between torsion and rotation, are used to interpret the relationships among the t in reduced Hamiltonian and in the anal. of the obsd. torsion-rotational spectrum. Mol. parameters are calcd. from potential energy surfaces for methanol to check the quality of these surfaces. The calcd. parameters a compared with parameters obtained from global fits to large exptl. data s The good agreement between the calcd. centrifugal distortion terms and th derived from fits to spectra demonstrates that the derived formulas provi useful tool for understanding the phys. origins and mass dependence of th mol. parameters.

2000

F: CH_3O
P: 3

132:200391 Theoretical study of the Jahn-Teller effect in X 2E CH_3O. Hoper, U.; Botschwina, P.; Koppel, H. Institut fur Physikalische Chemie, Universitat Gottingen Gottingen D-37077, Germany J. Chem. Phys., 112(9), 4132-4142 (English) 2000 The Jahn-Teller effect in X 2E MeO is theor. studied in considerable detail. Making use of ab initio calcns. carried out at the MRC-level the authors present the global shape of the adiabatic potential surfaces. Bo sheets of the

C.A.2000, 132

Jahn-Teller split X 2E electronic state are used to det. th linear, quadratic and bilinear coupling consts. of the e and a1 modes, as well as selected 3rd-order consts. Dynamical calcns. for the vibronic structure were performed with these parameters. The dynamical Jahn-Telle problem is solved by taking into account all the 3 e modes or, alternativ 2 e modes and 2 a1 modes. The resulting vibronic spectra are compared wi those of previous work. Also, ab initio calcd. transition moments for A 2A1.tautm.X 2E are used to give an explanation for the forbidden .DELTA.j (3)/(2) transitions which were found by different exptl. groups.

Om 40 511 2000

F: CH3OH
P: 3
133:301533 The Equilibrium Structure and Torsional Potential Energy Function Of Methanol and Silanol. Koput, Jacek Department of Chemistry, Adam Mickiewicz University Poznan 60-780, Pol. J. Phys. Chem. A, 104(44), 10017-10022 (English) 2000. The mol. parameters of methanol, CH3OH, and its silicon analog silanol, SiH3OH, have been detd. in large-scale ab initio calcns. using the coupled-cluster method, CCSD(T),

and basis sets of double- through (partly) quintuple-zeta quality. The properties studied included the equil. structure, spectroscopic consts., potential energy functions for internal rotation, and harmonic force fields of both mols. The effects of core-electron correlation and of small-amplitude vibrations on the calcd. mol. parameters were investigated. The mol. parameters detd. for methanol are found to be in good agreement with the exptl. data. The accuracy of the theor. predictions for silanol can be assessed.

F: MeO-
P: 3

2000

132:207557 Vibronic structure of alkoxy radicals via photoelectron spectroscopy. Ramond, Tanya M.; Davico, Gustavo E.; Schwartz, Rebecca L.; Lineberger, W. Carl Department of Chemistry and Biochemistry, University of Colorado and National Institute for Standards and Technology, JILA, University of Colorado Boulder, CO 80309-0440, USA J. Chem. Phys., 112(3) 1158-1169 (English) 2000 UV photoelectron spectra of MeO-, EtO-, Me2CHO-, Me3CO-, as well as CD3O- and CD3CD2O- are presented, providing improved electron affinities new information on vibronic coupling in the corresponding neutral radical Jahn-Teller vibronic transitions are assigned to e vibrational modes of X

C.A. 2000, 132

MeO. The excitation energy of the A 2A' state of EtO with respect to the 2A'' state is obsd. directly at 355 .+-. 10 cm-1. Vibronic coupling betw these low-lying electronic states perturbs the obsd. vibronic levels. Features of the Me2CHO- photoelectron spectrum are assigned. The splitti between the X 2A' and A 2A'' states of Me2CHO is 1225 .+-. 65 cm-1. Significant vibronic coupling is not obsd. in Me2CHO. Vibrational assignments are made for the spectral features of Me3CO and no Jahn- Telle effects are obsd. directly. Electron affinities (EAs) for the neutrals (are (in eV); EA(MeO)=1.572 .+-. 0.004; EA(CD3O)=1.559 .+-. 0.004; EA(EtO)=1.712 .+-. 0.004; EA(CD3CD2O)=1.699 .+-. 0.004; EA(Me2CHO)=1.847 0.004; EA(Me3CO)=1.909 .+-. 0.004. Bond dissocn. energies of ROH, D300(R H), along with .DELTA.fH300(RO), .DELTA.fH300(RO-), and .DELTA.fH300(RO+) derived.

2000

F: CD3OD

P: 3

133:43158 Infrared optoacoustic spectroscopy of 13CD3OD around 9p CO2 laser lines. Viscovini, Ronaldo Celso; Scalabrin, Artemio; Pereira, Daniel

Instituto de Fisica, UNICAMP Campinas 13.083-970, Brazil

Int. J. Infrared Millimeter Waves, 21(4), 621-632 (English) 2000

~~73~~— The authors present the results of a study about Doppler limited IR absorbing transitions of the in-plane Me-rocking and the asym. Me deformation modes of 13CD3OD by optoacoustic detection. This is an alternative and attractive technique to be applied to this MeOH isotopomer, in comparison to Fourier transform

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spectroscopy. In fact the contamination problem assocd. with the fast exchange of OD by OH in the mol. limits the use of the Fourier transform technique. Using a waveguide CO2 laser of 290 MHz tunability on each line the authors were able to observe 20 IR absorptions, most of them of large offset. The data will be useful in theor. anal. of this mol., as well as in the generation of FIR laser radiation in optically pumped mol. laser.

2000

F: CD3OH

P: 3

133:43157 Optically pumped far-infrared laser lines of methanol isotopomers: 12CD3OH, 12CH3OD, and 12CH2DOH. Vasconcellos, E. C. C.; Zerbetto, S. C.; Zink, L. R.; Evenson, K. M. Instituto de Fisica, Gleb Wataghin Departamento de Eletronica Quantica, (UNICAMP), Universidade Estadual de Campinas, (UNICAMP) Campinas 13083-970, Brazil Int. J. Infrared Millimeter Waves, 21(4), 477-483 (English) 2000 Twenty-seven new FIR, far-IR, laser lines from the isotopomers of MeOH: 12CD3OH, 12MeOD, and 12CH2DOH, were obtained by optically pumping the mols. with an efficient continuous-wave CO2 laser. The CO2 laser provided

C.A.2000

pumping from regular, sequence, and hot-band CO2 laser transitions. The 2 m long far-IR cavity was a metal-dielec. waveguide closed by 2, flat end mirrors. Several short-wavelength (<100 .mu.m) lines were obsd. The frequencies of 28 laser lines obsd. in this cavity (including new lines and already known lines) were measured with a fractional uncertainty limited by the fractional resetability of the far-IR laser cavity, of 2 parts in 107. optically pumped far IR laser line methanol isotopomer deuteriomethanol Isotope effect, deuterium; optically pumped far-IR laser lines of methanol isotopomers: 12CD3OH, 12CH3OD, and 12CH2DOH;

F: CH3OH
P: 3

2001

134:272897 **Anharmonicity and hydrogen bonding I. A near-infrared study of methanol trapped in nitrogen and argon matrices.** Perchard, J. P.; Mielke, Z. LADIR/Spectrochimie Moleculaire, UMR 7075, Universite Pierre et Marie Curie, Paris, Fr. Chem. Phys. (2001), 264(2), 221-234. CODEN: CMPHC2 ISSN: 0301-0104. in English. AN 2001:109627

The IR spectra of 6 isotopic species of MeOH trapped in solid N and Ar were measured in the domain 7300-300 cm-1. Among the various combinations and overtones obsd., the 2ν1 (OH or OD stretching), 2ν6 (OH or OD bending) and ν1+ν6 transitions were examd. as a function of the concn. and compared to the ν1 and ν6 fundamentals. Most of the bands of monomer and dimer were identified. For aggregates larger than the dimer no absorption assignable to 2ν1 was detected, which, taking into account the accuracy of the intensity measurements, leads to a ν1/2ν1 intensity ratio >1000 for these polymers, to be compared to ≈20 for the monomer and 400 for the proton donor mol. of the dimer. An opposite situation is encountered for the bending mode, the ν6/2ν6 intensity ratio decreasing from monomer to polymers, possibly because of a Fermi resonance between 2ν6 and ν1 whose frequencies get closer in case of aggregation. For the ν1+ν6 combination the effects of H bonding are not as dramatic as in the case of the overtones. From the frequencies and relative intensities some anharmonicity parameters were deduced. Noticeable differences between the spectra of the proton donor and of the proton acceptor mols. of the dimer are explained by changes in the dipole moment function upon H-bond formation.

CH_3OH От 41506 2002

Imre Bako et al.,

ab initio
расчет

J. Mol. Struct. (Theochem)
2002, <u>594</u>, 179–184.

Оп. 41513

2002

$D_{298}(CH_3O-H)$

Kent M. Ervin and
Vincent F. DeTuri,

J. Phys. Chem. 2002, A106,
9947–9956.

2002

CH_3OH
CH_3OD
CD_3OH

Li Wang, Yun-bo Duan et al.,
Chem. Phys. Lett., 2002, 365, 432-439.

комбин-
частоты,
сил. пост.
барьер внутр.
вращ.

Spectroscopic determination

of fundamental molecular parameters for methanol and its isotopomers.