CHBr

$CHBr$

1971

Rossi-Sonnichsen, Inga;
et al.

(и.к. спектр)
(ν, band)

„C. R. Acad. Sci, Ser. C."
1971, <u>273</u>, N1, 19-22.

(см $CHCl_3$; $\overline{\underline{III}}$)

40426.6623

Th. Ch. Ph

HCBr стр. ик-сп

DCBr 54969 0.8

1974.

4-4646

Eysel Hans Hermann, Lehmann Walter J., Lucas Kai, Müller Achim, Schmidt Karlheinz. Die Anwendbarkeit verschiedener Näherungsmethoden zur Berechnung von Kraftkonstanten bei Säkulargleichungen der Ordnung $n > 2$. "Z. Naturforsch.", 1974, 29a, N 2, 332-337

(нем., рез. англ.)

075 078 092 0100 экз ВИНИТИ

50731.36[illegible]7 /14
TC,Ph,Ch

CHBr 411 Раман спектр

1975
3247

Tsuboi Masamichi, Hirakawa Akiko Y., Muraishi Shuichi. A possible correlation between a Jahn-Teller coupling and a Raman scattering. "J.Mol.Spectrosc.", 1975, 56, N 1, 146-158

(англ.) 0424 пнх

394 395 [illegible] 1 [illegible] ВИНИТИ

$CHBr$ 1977

Bauschlicher C. W. et al.

геометрия, эл. расчет.

J. Amer. Chem. Soc. 1977, 99, 7106–10

●

(см. CH_2, II)

СНВг

от. 24135

1986

Scuseria G. E., Durán M.,
Maclagan R. G. A. R.,
Schaefer H. F.,

геометр.,
синглет-
триплетн.
разделения,
колебат.
частоты

J. Amer. Chem. Soc.,
1986, <u>108</u>, N 12, 3248-
● -3253.

$HCBr^-$ (OM. 31024) 1988

Murray K.K., Leopold D.G. et al.,

Фото-электр. спектр

J. Chem. Phys. 1988, 89, N 9, 5442-5453.

Photoelectron spectroscopy of the halocarbene anions

HCF^-, $HCCl^-$, $HCBr^-$, HCl^-, CF_2^-, and CCl_2^-.

$HCBr^-$ DM 36443 1992

Gilles M.K., Ervin K.M. et al.,

Фото-
электр.
спектр

J. Phys. Chem. 1992, <u>96</u>, N3, 1130-1141.

Negative Ion photoelectron spectroscopy of HCF^- $HCCl^-$;

$HCBr^-$, and HCI^-: photoelectron Agular Distributions and Neutral Triplet Excitation Energies.

$CHBr$ 1992

Irikura Karl K.,
Goddard W. A., (III). et al.

м. п. J. Amer. Chem. Soc. 1992.
114, N1. с. 48–57.

(см. ● CH_2; III)

$CHBr$

1993

Gobbi A., Frenking G.,

низшие
синглет.
и
триплет.
состоян.,
теорет.
расчет

Bull. Chem. Soc. Jpn.,
1993, <u>66</u> (11), 3153-65

(см. NF_2^+; <u>III</u>)

$CH^{79}Br$ 1993

120: 40753a The perpendicular $\nu_4^{\mp} + \nu_6^{\pm1}$ component of the rovibrational $\nu_4 + \nu_6$ band of bromomethane ($CH_3^{79}Br$), studied in a high resolution FTIR spectrum from 3870 cm^{-1} to 4110 cm^{-1}. Ben Sari-Zizi, Najate; Alamichel, Claude (Fac. Sci., Univ. Mohammed V, Rabat, Morocco). *Mol. Phys.* 1993, 80(3), 515-23 (Eng). 860 Rotational lines of the almost unperturbed $\nu_4^{\mp1} + \nu_6^{\pm1}$ component of the $\nu_4 + \nu_6$ band of $CH_3^{79}Br$ have been assigned in spite of overlaps with several other bands. Only a few sub-bands ($K\Delta K$ = 1, −7, −8, −9) are subject to slight resonances. An RMS deviation of 0.0039 cm^{-1} has been achieved by a least-squares fit of 742 lines. As expected, the A', B', D'_J, D'_{JK} and D'_K mol. consts. have been found quite close to those of the parallel component. The comparison between the centers of both components of the $\nu_4 + \nu_6$ band allowed the authors to measure two anharmonicity consts.: x_{46} = −5.25 cm^{-1} and g_{46} = 0.89 cm^{-1}.

Вращат. пост. в колеб сост.

С.А. 1994, 120, N 4

1994

HCBr
DCBr

3 Б1161. Получение галогенметиленов при расширении в свободной струе из горячего сопла: отождествление и характеристика HCBr и DCBr **с помощью спектроскопии возбуждения флуоресценции, индуцированной лазером.** Production of halomethylenes in free-jet expansions from a hot nozzle: Identification and characterization of HCBr and DCBr by laser-induced fluorescence excitation spectroscopy /Xu Songlin, Beran Kyle A., Harmony Marlin D. //J. Phys. Chem. .— 1994 .— 98 ,№ 11 .— С. 2742—2743 .— Англ.

Продемонстрирован эффективный синтез хлорметилена и бромметилена путем пиролиза в горячем сопле и последующего расширения в сверхзвуковой свободной струе. Впервые измерены спектральные св-ва возбуждения ФЛ, индуцированной лазерным излучением, для бромкарбена. Получены спектры HCBr и DCBr, к-рые согласуются с теор. прогнозами геометрии этих соединений: нелинейной в основном и квазилинейной в возбужденном состояниях. В протонированных соединениях частота изгиба в возбужденном состоянии близка к 840 см$^{-1}$ при $\nu_2=5$, а частота вал. кол. C — Br $\nu_3 \approx 783$ см$^{-1}$.

Н. Н. Морозов

М-Л-

Х.1995, №3

HCBr

1996

125: 259976n High resolution near–infrared electronic spectroscopy of HCBr. Chang, Bor–Chen; Sears, Trevor J. (Dep. Chem., Brookhaven Natl. Lab., Upton, NY 11973–5000 USA). *J. Chem. Phys.* **1996**, 105(6), 2135–2140 (Eng). The rotationally resolved spectrum of the HCBr $\tilde{A}^1A''(0,2,0)$ $K_a = 0 - 1$ transition between 12760 and 12850 cm^{-1} was obtained for the 1st time at Doppler–limited resoln. using a transient frequency–modulation absorption technique. Rotational structure of HC^{79}Br and HC^{81}Br was identified and analyzed. The anal. shows R'' (C–Br) = 1.85$_2$ Å and R' (C–Br) = 1.74$_9$ Å. The obsd. band indicates a linear–bent transition. This yields an upper limit of ~1600 cm^{-1} for the barrier to linearity above the zero–point energy for the $\tilde{A}^1A''$ state. Perturbations caused by singlet–triplet interactions were also found in the obsd. spectrum. The anal. of these perturbations indicates a very low–lying $\tilde{a}^3A''$ state.

ИК спектр,
М.П.

C.A. 1996, 125, N 20

2000

F: CHBr
P: 3
133:111619 Near-infrared spectroscopy of bromomethylene in a slit-jet expansion. Chang, Bor-Chen; Costen, Matthew L.; Marr, Andrew J.; Ritchie, Grant; Hall, Gregory E.; Sears, Trevor J. Dep. Chem., Brookhaven National Lab. Upton, NY 11973-5000, USA J. Mol. Spectrosc., 202(1), 131-143 (English) 2000. Several rotational subbands of the bromomethylene (HCBr) and deuterated bromomethylene (DCBr) A1A.ltwarw.X1A' origin band at 830-840 nm were recorded under slit-jet cooled conditions that result in rotational and translational

temps. of ~20 K. The radical was formed by 193-nm laser photolysis of bromoform in the early stages of the expansion and detected by absorption of a single-frequency Ti:sapphire ring laser. The spectral simplification achieved compared to earlier measurements at ambient temp. allowed a nearly complete rotational anal. The data were combined with addnl. measurements at room temp. to det. rotational consts. and est. a structure for the radical in its ground state. With the exception of K' = 0, the excited state levels suffer multiple perturbations due to interactions with the manifold of excited X state levels caused by Renner-Teller and anharmonic coupling. At. Br transitions from the 4P5/2 level at 63,400 cm-1 were also obsd. in the source following absorption of at least two 193-nm photons by the precursor.

1999

F: HCBr
P: 3 131:65156 Vibronic Reassignment of the A1A'' .ltwarw. X1A' Band System of Bromomethylene. Marr, Andrew J.; Sears, Trevor J. (Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973-5000, USA). J. Mol. Spectrosc., 195(2), 367-370 (English) 1999 In recent months the authors have obsd. the 1st hot band spectra of bromomethylene (M. and S., in press) and searched for and obsd. other vibronic bands of DCBr in previously unaccessed NIR regions (M. and S., submitted for publication). From their examn. it was realized that all previous vibronic assignments for both HCBr and DCBr were incorrect. New

assignments which place the zero point level of the A1A'' state at ~11,97 cm' (compared to 11,130 cm-1 previously) and which agree with all previously obsd. band positions were detd. Described herein are the details of that vibronic reassignment and the spectroscopic and dynamical evidence that confirm it.

CHBr

Оп · 40107

1999

ab initio
расчет
геометр.
колебан-
частот,
$\Delta_f H$(расч)

Martin Schwartz
and Paul Marshall*,

J. Phys. Chem. A 1999,
<u>103</u>, 7900 – 7806

$HCBr$
$DCBr$

OM-40985

2000

Bor-Chen Chang,
Matthew L. Costen et al.,

J. Mol. Spectrosc., 2000,
202, 131-143.

Near-Infrared Spectroscopy

Bromomethylene
in a Slit-Jet Expansion

HCBr

(Ã–X̃)

2001

135: 248867h Laser excitation and dispersed fluorescence spectra of the HCBr Ã–X̃ vibronic transition. Tsai, Tsung–Chuan; Chen, Chun–Wei; Chang, Bor–Chen (Department of Chemistry, National Central University, Chung–Li, Taiwan 32054). *J. Chem. Phys.* **2001**, 115(2), 766–770 (Eng), American Institute of Physics. We recorded the laser–induced fluorescence (LIF) excitation spectra of several HCBr Ã–X̃ vibronic transitions between 580 nm and 630 nm in a d.c. (DC) discharge supersonic free jet expansion. Dispersed fluorescence spectra, following excitation of these HCBr Ã–X̃ vibronic transitions were successfully obtained for the first time. The anal. of the dispersed fluorescence spectra reveals the details of the vibrational structure of the X̃ $^1A'$ state as well as that of the ã $^3A''$ state. The vibrational frequencies were detd. as 1119 cm−1 (bend), 676 cm−1 (C–Br stretch) for the X̃ $^1A'$ state and 994 cm−1 (bend), 733 cm−1 (C–Br stretch) for the ã $^3A''$ state. In addn., based upon the observation of the triplet state levels, the value of the triplet–singlet energy gap (the zero–point level energy gap) could be extd. from the dispersed fluorescence spectra and is to be approx. 2006 ± 8 cm^{-1}(5.73 ± 0.02 kcal/mol).

лазервозб.
флуоресц.

C.A. 2001, 135, N17

HCBr

2001

$(\tilde{A}A'' - \tilde{X}\,^1A')$

135: 363881v Experimental and theoretical studies of the near-infrared spectrum of bromomethylene. Yu, Hua-Gen; Gonzalez-Lezana, Tomas; Marr, Andrew J.; Muckerman, James T.; Sears, Trevor J. (Department of Chemistry, Brookhaven National Laboratory, Upton, NY 11973-5000 USA). *J. Chem. Phys.* 2001, 115(12), 5433-5444 (Eng), American Institute of Physics. New measurements in the $\tilde{A}\ ^1A''-\tilde{X}\ ^1A'$ band system of HCBr at near-IR wavelengths are reported. Rotationally resolved spectra of HCBr and DCBr for both naturally occurring Br isotopes are analyzed and provide accurate energies for the low-lying bending vibrational levels in both the $\tilde{A}$ and $\tilde{X}$ states. The exptl. results are compared to extensive ab initio calcns. of these 2 states and the low-lying $\tilde{a}\ ^3A''$ state. The ab initio T_{00} value for the $\tilde{A}-\tilde{X}$ system is

C.A. 2001, 135, N25

calcd. within 500 cm^{-1} of the exptl. results. For the triplet state, T_{00} ($\tilde{a}-\tilde{X}$) is 1833 cm^{-1}. The measurements of the bending intervals in the $\tilde{X}$ $^{1}A'$ state suggest that this is ~250 cm^{-1} too low. With this shift and inclusion of spin–orbit coupling between the $\tilde{a}$ and $\tilde{X}$ states, the calcd. bending vibrational levels in the $\tilde{X}$ state reproduce the observations, and the calcns. make testable predictions of the position of the triplet and other singlet state vibronic levels. Combining the exptl. and computational results, the triplet, $T_{00}(\tilde{a}-\tilde{X})$, excitation energy is estd. as 2028 cm^{-1}.