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800 - IV

1957

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Используя видеоспектрометр, измерили вращательный спектр молекулы DCOOD, аппроксимируемой асимметричным волчком, в области частот 7,5—145 *Гц*. Сравнение значений наблюденных и вычисленных частот дало возможность идентифицировать около 80 перехо-

9. 1969. 9Д

дов. Расчеты проведены с помощью теории Кивельсона (Kivelson K., Witson E. B. «J. Chem. Phys.», 1952, 20, 1575), упрощенной введением соотношений Даулинга, где в ф-лах для уровней энергии величины постоянных центробежного искажения τ связаны пятью линейными соотношениями, в результате чего только четыре значения τ являются независимыми, и с помощью теории Ватсона (РЖФиз, 1969, 5Д170). Получено хорошее согласие между теоретич. и эксперим. результатами. Библ. 12.

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8119g Identification of the rotational spectrum of dideuterated formic acid by means of the Kivelson and Watson theories applied to the deformable planar rotor. Bellet, Jean; Deldalle, Alain; Samson, Claude; Steenbeckeliers, Guy (Lab. Spectrosc. Hertzienne, Fac. Sci., Lille, Fr.). *C. R. Acad. Sci., Paris, Ser. A B* 1969, 268B (7), 560–3 (Fr, The rotational spectrum of the asym. top, DCOOD, has been measured between 7.5 and 145 GHz. Comparison between the calcd. and observed frequencies leads to the identification of ~80 transitions. The calcns. were made by using on the one hand, the theory of Kivelson (K. Kivelson and E. B. Wilson, 1952), simplified by improvements introduced by J. M. Dowling (1961), and on the other hand, by the theory recently introduced by J. K. G. Watson (1968). The calcns. based on these 2 theories describe the exptl. spectrum closely and give the same rotational and centrifugal distortion consts. DWJF

брауш. спектр

C.A. 1969. 71. 2

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(См. CH_2O_2) III

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Caillet P., Forel M.T, Spectres de vibrations et champ de force de valence de l'acide formique monomère et de ses dérivés deutériés. "Ann.chim."(France), 1975,10,N 6, 311-315 (франц.;рез.англ.)

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Microwave spectrum of formic acid and its isotopic species in D, C and O. Study of coriolis resonances between ν_7 and ν_9 vibrational excited states.

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F: DCOOD

P: 3\131:65084 FTIR Spectrum of the .nu.4 Band of DCOOD.

Tan, T. L.; Goh, K. L.; Ong, P. P.; Teo, H. H. (Department of Physics, Faculty of Science, National University of Singapore 119260, Singapore). J. Mol. Spectrosc., 195(2), 324-327 (English) 1999 The FTIR spectrum of the .nu.4 band of deuterated formic acid (DCOOD) was measured with a resoln. of 0.004 cm-1 in the frequency range of 1120 1220 cm-1. A total of 1866 assigned transitions were analyzed and fitted using a Watson's A-reduced Hamiltonian in the Ir representation

to derive rovibrational consts. for the upper state (v4 = 1) with a std. deviation 0.00036 cm-1. In the anal., the consts. for the ground state were improv by a simultaneous fit of microwave frequencies and combination difference from the IR measurements. Due to the relatively unperturbed nature of th band, the consts. can be used to accurately calc. the IR line positions f the whole band. Although the band is a hybrid type A and B, only a-type transitions were strong enough to be obsd. The band center is at 1170.79980 .+-. 0.00002 cm-1.

F: DCOOD
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132:243309 High resolution FTIR spectrum of the .nu.1 band of DCOOD. Goh, K. L.; Ong, P. P.; Teo, H. H.; Tan, T. L. Faculty of Science, Department Physics, National University of Singapore Singapore, Singapore Spectrochim. Acta, Part A, 56A(5), 991-1001 (English) 2000 The IR absorption spectrum of the .nu.1 band of deuterated formic acid (DCOOD) was measured on a Bomem DA3.002 Fourier transform spectrometer at 2560-2690 cm-1 with a resoln. of 0.004 cm-1. A total of 292 IR transitio were assigned in this hybrid type A and B band centered at 2631.8736 .+-. 0.0004 cm-1. The assigned transitions were fitted to give a set of 8 rovibrational consts. for the v1 = 1 state with a std. deviation of 0.000 cm-1.

C.A. 2000, 132

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F: D2CO
P: 3

134:272909 **The v2 band of formaldehyde-d2.** Lohilahti, J.; Alanko, S. Department of Physical Sciences, University of Oulu, Oulu, Finland. J. Mol. Spectrosc. (2001), 205(2), 248-251. in Engl.

High-resoln. FTIR spectrum of the v2 band (1590-1780 cm-1) of D2CO was recorded. More than 2500 rovibrational transitions were assigned up to Jmax = 52 and Kdmax = 17. The upper state v2 = 1(A1) is perturbed by a ΔKa = 2 interaction with the v3 = 2(A1) state. To explain the resonance perturbation in the v2 = 1 state, some lines of the 2v4 band (the band center at .apprx.1868 cm-1) were assigned. Both bands were fitted simultaneously to the Watson-type rotational Hamiltonian using I' representation in a redn., and the mutual interaction was taken into account. The rotation parameters of the v2 = 1 state ≤8th order and the interaction parameter were obtained.