Si-D

SiH_3D Polo, Wilson, 1954

Спектр. J. Chem. Phys. 22, 1559

Вращ. постоянные SiH_3D

1470-1680 $см^{-1}$

Изучалась структура полосы ν_2.

$\nu_0 = 1594,4 \pm 0.1$ $см^{-1}$

$B'' = 2,11 \pm 0,01$ $см^{-1}$

$B'' - B' = 0.019$ $см^{-1}$.

$r_{Si-H} = 1,47_7 \pm 0.003$ Å

1957

5712a

SiH_4. SiH_3D. SiH_3D_2

Ковалев И.Ф.
Оптика и спектроскопия. 1957. 2. № 3.
310-316

Колебательные спектры...

J

$SiDH_3$

SiH_3D

Thyagarajan G. | 1962

J. Mol. Spectrosc., 8, 73

Постоянные центробежного растяжения для аксиально симметрических молекул ZX_3Y ($Z = Si, Ge$; $X, Y = H, D, T$); знак постоянных в некоторых молекулах

(См. SiH_4) III

1971

SiH_3D
SiD_3H
SiH_2D_2

Wilde R.E.,
Srinivasan T.K.K., и др.

„J. Chem. Phys"., 1971, 55, №12,
5681-92.

(Vi)

(см. SiH_4, III).

70301.8460
TC, Ch, Ph

41125

1976
XIV-7793

SiH_2F (sub. fluor. nocta)

Robiette A.G., Georghiou C.,
Baker J.G. Microwave spectra of
SiH_2DF and $SiHD_2F$. Harmonic force field
and molecular structure.
"J. Mol. Spectrosc.", 1976, 63, N 3,
391-401 (англ.)

0821 ЕЖЖ

765 786 612

ВИНИТИ

Si_2HD_5 1982

Mc Kean D.C., et al.

J. Phys. Chem., 1982,

Vi, ee. n. 86, N 3, 307-309.

(см. PH_2D_2, III)

$SiHD_3$

1983

Halonen L., Child M. S.

Di;

J. Chem. Phys., 1983, 79, N9, 4355-4362.

(cm. CH_3D; III)

SiH_3D 1983

$SiHD_3$ Halonen L., Child M. S.

J. Chem. Phys., 1983, 79, N 9, 4355–4362.

(сер. CH_3D; III)

H_3SiD

1985

12 Л193. Вращательные константы H_3SiD в основном состоянии. The Ground State Rotational Constants of H_3SiD. Bürger H., Rahner A., Kauppinen J. «Z. Naturforsch.», 1985, **A40**, № 4, 386—388 (англ.)

С помощью фурье-спектрометра высокого разрешения получены спектры ИК-поглощения газообразного H_3SiD в области 660—1070 $см^{-1}$. Эффективное разрешение, определяемое прибором, доплеровским и ударным уширением, составляло 0,005 $см^{-1}$. С точностью лучше 10^{-4} $см^{-1}$ измерены частоты колебательно-вращательных линий и выполнено их отнесение к полосам ν_3 (912,9 $см^{-1}$), ν_5 (951,4 $см^{-1}$) и ν_6 (784,3 $см^{-1}$). По комбинационным разностям частот этих линий найдены вращательные постоянные молекулы в основном состоянии вплоть до секстичных. Константы A_0 и $D_K°$ определены по частотам линий полосы ν_6, разрешенных за счет внутримолекулярных возмущений. М. В. Т.

м.п.; Di;

Ф. 1985; 18, N 12

SiH2

1985

Fredin Leif, Hauge R. H.,
et al.

ИК спектр
в
матрице

J. Chem. Phys. 1985,
82(8), 3542-5.

(см. SiH_2; III)

Si_2HD_5 OM 24628 1986

105: 180691x **The ground state structures of disilane, methylsilane and the silyl halides, and an silicon-hydrogen bond length correlation with stretching frequency.** Duncan, J. L.; Harvie, J. L.; McKean, D. C.; Cradock, S. (Dep. Chem., Univ. Aberdeen, Old Aberdeen, UK AB9 2UE). *J. Mol. Struct.* 1986, 145(3-4), 225-42 (Eng). IR spectra of Si_2HD_5, $SiHD_2Me$, SiH_3CHD_2, $SiHD_2X$ (X = F, Cl, Br, I) were recorded at 0.05 cm^{-1} resoln. Analyses of perpendicular fundamentals of these very slightly asym. top mols. permit the accurate detn. of their ground state (A_0–$\bar{B}_0$) consts., from which the A_0 rotational consts. may be obtained. When combined with all known Raman and microwave consts., this enables the ground state structures to be detd. with precision, allowance being made for the shortening of SiH(CH) bonds on deuteration. For disilane, this work represents the 1st spectroscopic detn. of a complete structure, while for the silyl halides it demonstrates overestimates in the SiH bond length of ~1% by previous workers. For methylsilane, comparison with a recent ab initio structure calcn. reveals a considerable overestimate of the CSi bond length in the latter. A correlation between isolated SiH stretching frequency and ground state bond length over 15 mols. reveals a somewhat reduced sensitivity compared with the corresponding CH correlation. Nevertheless, a predictive capability of better than ±0.003 Å seems possible from the isolated SiH stretching frequency, at least for mols. with fully satd. bonding.

(UK exemp)

(15)

C.A. 1986, 105, N20

HR of

1) $SiHD_2CH_3$, SiH_3CHD_2

2) $SiHD_2F$, 3) $SiHD_2Cl$, 4) $SiHD_2Br$,

5) $SiHD_2J$

DOSi+

1989

Warner H.E., Fox A., et al.

e.n., J. Chem. Phys. 1989, 91 (9), 5310-12.

Vi;

(cer. HOSi+; III)

HDSi-SiH2
HSi-SiH2D

1990

16 Б1147. **Теоретическое исследование изомеризации синглетный дисилен — силилсилилен — анализ динамики и термодинамики на неэмпирическом уровне** / Ju Guan-Zhi, Ma Wan-Yong, Deng Cong-Hao // Хуасюэ сюэбао = = Acta Chim. Sin.— 1990.— 48, № 2.— С. 105—109.— Кит.; рез. англ.

Неэмпирическим методом ССП с использованием базисных наборов 3—21 ГФ и 3—21 ГФ* изучена ПВ потенциальной энергии для р-ции изомеризации синглетного силилена $HXSi\text{-}SiH_2$ (I) в $HSi—SiH_2X$ (II), при (X = D). Для стационарных точек ППЭ рассчитаны частоты колебаний в интервале т-р от 100 до 1200 К оценены термодинамич. ф-ции, константы равновесия и скорости для р-ции изомеризации I в II. Показано, что р-ция изомеризации экзотермична и в исследованном интервале т-р протекает самопроизвольно. Это хорошо согласуется с эксперим. данными (см. // Int. J. Chem. Kinet.— 1979.— 11.— С. 1167). Показано, что поправка на энергию нулевых колебаний в данном случае существенна и ее необходимо учитывать при рассмотрении такого типа процессов. Результаты расчетов сопоставлены с данными др. неэмпирич. расчетов. И. Н. Сенченя

И.П.

Х. 1990, N 16

$D_8Si_8O_{12}$ 1991

Baertsch M., Bornhauser P., et al.,

Spectrochim Acta, Part A, 1991, 47A (11), 1627–9

IR, calc, (Di)

Call: ● $H_8Si_8O_{12}$; III)

$D_3Si^{79}Br$

1997

128: 94711u **High-resolution infrared spectrum of $D_3Si^{79}Br$ in the ν_1/ν_4 region: the structure of silyl bromide.** Demaison, J.; Cosleou, J.; Burger, H.; Mkadmi, E. B. (Laboratoire de Spectroscopie Hertienne, URA CNRS 249, Universite de Lille 1, F-59655 Villeneuve d'Ascq, Fr.). *J. Mol. Spectrosc.* 1997, 185(2), 384-391 (Eng), Academic Press. FTIR spectra of monoisotopic $D_3Si^{79}Br$ covering the bands ν_1 (a_1, 1580.637 cm^{-1}) and ν_4 (e, 1615.085 cm^{-1}) have been recorded with a resoln. of 3 $\times 10^{-3}$ cm^{-1}. The rovibrational anal. revealed severe perturbations of the $-5 \leq K\Delta K \leq 4$ series of ν_4 while ν_1 and the high-K subbands of ν_4 are almost unperturbed and served to det. the parameters of the $\nu_1 = 1$ and $\nu_4 = 1$ states, with σ(Fit) ca. 5×10^{-4} cm^{-1}. Equil. rotational consts. of $H_3Si^{79}Br$ and $D_3Si^{79}Br$ were deduced with the help of the vibrational corrections α_i. The r_0, r_s, r_m^P, and r_e structures of silyl bromide have been detd. The exptl. values of the HSiH angle and of the Si-H distance are found in excellent agreement with their ab initio predictions. The r_e structure is r_e(Si-H) = 1.470(2) Å, r_e(Si-Br) = 2.207(1) Å, and α_e-(HSiH) = 110.5(2)°.

ИК, спектр. парам., Di

C.A. 1998, 128, N8

H_3SiD

1997

127: 312506d **The Si–H stretching fundamentals of $H_3{}^{28}SiD$.** Fusina, L.; Cane, E.; Escribano, R.; Burger, H. (Dipartimento di Chimica fisica e Inorganica, Universita di Bologna, I–40136 Bologna, Italy). *J. Mol. Spectrosc.* **1997**, 184(2), 385–394 (Eng), Academic. The $\nu_1(A_1)$ and $\nu_4(E)$ Si–H stretching fundamentals of H_3SiD were recorded at an effective resoln. of 0.006 cm^{-1} between 2050 and 2300 cm^{-1}. A total of ~2500 rovibrational transitions of the $H_3{}^{28}SiD$ isotopomer were assigned with J' up to 27 and K' up to 22. A large no. of perturbation allowed $\Delta k = \pm 3$ transitions were identified in both the ν_1 and ν_4 bands. The assigned transitions were analyzed using two different theor. models, which took into account several rovibrational interactions between and within the $v_1 = 1$ and $v_4 = 1$ states, yielding a std. deviation of each fit of ~0.0004 cm^{-1}, which may e compared with the exptl. precision (~0.0001 cm^{-1}). Improved ground state parameters also were obtained by ground state combination differences.

(Si–H)

C. A. 1997, 127, N 22

$HSiD_3$ 1998

129: 10091b **High resolution FTIR study of the ν_5 bands of $HSiD_3$ and $H^{120}SnD_3$.** Burger, Hans; Jerzembeck, Wolfgang; Ruland, Helmut; Halonen, Lauri (FB 9, Anorganische Chemie, Universitat–GH, D–42097 Wuppertal, Germany). *J. Mol. Spectrosc.* 1998, 189(1), 8–15 (Eng), Academic Press. High resoln. Fourier Transform spectra of $HSiD_3$ and monoisotopic $H^{120}SnD_3$ were recorded in the region of the ν_5 fundamental at 850.68 and 646.90 cm^{-1} with a resoln. of 3.3 and 2.8 × 10^{-3} cm^{-1}, resp. About 2000 rovibrational transitions of each species were assigned and fitted to 2 different redns. of the effective Hamiltonian, with σ(Fit) = 1.2 × 10^{-4} ($HSiD_3$) and 1.4 × 10^{-4} cm^{-1} ($H^{120}SnD_3$). The 2 sets of parameters are equiv., and relations between parameters belonging to different redns. are perfectly fulfilled. Also the ground state consts. C_o and D_{Ko} were detd. for the 1st time. For consistency the previously measured data belonging to the ν_5 band of $H^{70}GeD_3$ were refitted, σ(Fit) = 1.6 × 10^{-4} cm^{-1}, from improved ground state parameters including the h_3' term accounting for the splitting of the K = 3 level.

ИК спектр, м-л.

(+) $H^{120}SnD_3$

C. A. 1998, 129, N 1

H_3SiD

2001

135: 159429z **The (n00A_1/E), n=3, 4, and 6, local mode states of H_3SiD: Fourier transform infrared and laser photoacoustic spectra and ab initio calculations of spectroscopic parameters.** Burger, H.; Lecoutre, M.; Huet, T. R.; Breidung, J.; Thiel, W.; Hanninen, V.; Halonen, L. (Anorganische Chemie, Universitat-GH, D-42097 Wuppertal, Germany). *J. Chem. Phys.* 2001, 114(20), 8844-8854 (Eng), American Institute of Physics. The rotational structure of the local mode Si-H stretching vibrational bands (n00 A_1/E), n = 3, 4, and 6, of $H_3{}^{28}SiD$ were studied by high-resoln. FTIR and by photoacoustic laser spectroscopy. The recorded bands were rotationally analyzed with a Hamiltonian model which makes use of simple arithmetic relations between some of the rovibrational parameters. While the (300 A_1/E) states are unperturbed, severe perturbations by unknown dark states affect the (400 A_1/E) and (600 A_1/E) states for J values exceeding 8. Ab initio calcns. were performed to form the quadratic and the cubic potential energy surfaces which were used to calc. spectroscopic parameters for the Si-H stretching fundamentals. These results, together with the local mode relations, were successfully used to model the vibrational dependence of effective rovibrational parameters in the excited local mode states.