

Si-D

SiH₃D
чиреп.

Polo, Wilson,

1954

J. Chem. Phys. 22, 1559

Вращ. переходные SiH₃D

1470-1680 cm⁻¹

изучение спектра водое ν₂

ν₀ = 1594,4 ± 0.1 cm⁻¹

ν_{Si-H} = 1,47 ± 0.03 Å

B'' = 2,11 ± 0,01 cm⁻¹
B'' - B' = 0.013 cm⁻¹

1957

5712a



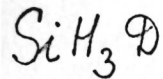
Ковалев И.Ф.

Оптика и спектроскопия, 1957, 2, № 3,
310-316

Колебательные спектры...

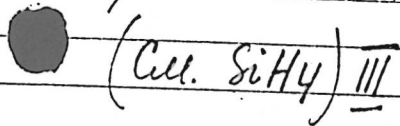
J





Thyagarajan G. 1962.
J. Molec. Spectrosc., 8, 73

Постоянные центробежно-ного расщепления для аксиально симметрических молекул ZX_3Y ($\text{Z} = \text{Si, Ge}$; $\text{X, Y} = \text{H, D, T}$); знак постоянных в некоторых молекулах



SiH_3D
 SiD_3H
 SiH_2D_2

(vi)

Wilde R.E.,
Srinivasan T.K.K., 4 pp.

1971

"J. Chem. Phys.", 1971, 55, v12,
5681-92.

• (cor. SiH_4 , III).

70301.8460

TC, Ch, Ph

41125

SiH₂D₂F / м. в. (фрагм. по сд.)

1976
XIV-7793

Robiette A.G., Georghiou C.,

Baker J.G. Microwave spectra of
SiH₂DF and SiHD₂F. Harmonic force field
and molecular structure.

"J. Mol. Spectrosc.", 1976, 63, N 3,
391-401 (англ.)

0821

10

785 786 812

ВИНИТИ

Si₂MD₅

1982

Mc Kean D.C., et al.

J. Phys. Chem., 1982,

V_i, ser. n.

86, N3, 307-309.

●
(ser. PHD₂; 11)

SiMD₃

1983

Malonen L., Child
M.S.

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

Vi;

([•]Car. CH₃ D; III)

SiH_3D

1983

SiHD_3

Halonen L., Child M.
S.

ν_i ;

J. Chem. Phys., 1983,
79, n 9, 4355 - 4362.

(comp. 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 $660\text{--}1070\text{ см}^{-1}$. Эффективное разрешение, определяемое прибором, доплеровским и ударным уширением, составляло $0,005\text{ см}^{-1}$. С точностью лучше 10^{-4} см^{-1} измерены частоты колебательно-вращательных линий и выполнено их отнесение к полосам ν_3 ($912,9\text{ см}^{-1}$), ν_5 ($951,4\text{ см}^{-1}$) и ν_6 ($784,3\text{ см}^{-1}$). 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. В. Т.

ср. 1985, 18, N12

SiH₂

1985

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

UK chemist
6

main purpose

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

(see SiH₂; III)

Si₂HD₅

OM. 24628

1986

105: 180694x 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.; Craddock, S. (Dep. Chem., Univ. Aberdeen, Old Aberdeen, UK AB9 2UE). *J. Mol. Struct.* 1986, 145(3-4), 225-42 (Eng). IR spectra of Si₂HD₅, SiHD₂Me, SiH₃CHD₂, SiHD₂X (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 (A₀-B₀) const., from which the A₀ rotational const. may be obtained. When combined with all known Raman and microwave const., 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 C-Si 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.

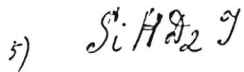
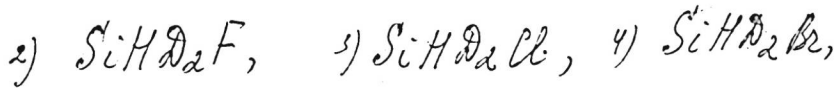
(UK chem)

15



C.A. 1986, 105,
N20

HQ of



DOSi^+

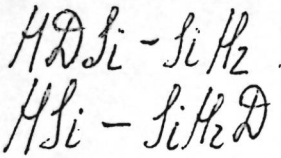
1989

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

ser. n.,
 Vi^+ ; J. Chem. Phys. 1989,
91 (9), 5310-12.

(corr. HOSi^+ ; iii)

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.

М.Н.

Неэмпирическим методом ССП с использованием ба-
 зисных наборов 3—21 ГФ и 3—21 ГФ* изучена ПВ
 потенциальной энергии для р-ции изомеризации синглет-
 ного силилена $\text{HXS}\text{Si-SiH}_2$ (I) в $\text{HSi-SiH}_2\text{X}$ (II), при
 (X=D). Для стационарных точек ППЭ рассчитаны ча-
 стоты 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 сущест-
 венна и ее необходимо учитывать при рассмотрении та-
 кого типа процессов. Результаты расчетов сопоставлены
 с данными др. неэмпирич. расчетов. И. Н. Сенченя

Х. 1990, N 16

D₈ Li₈ O₁₂

1991
Baertsch M., Bornhauser P.,
et al.,

lek, CK₁,
(Di)

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

Call:



H₈ Li₈ O₁₂; III)

D₃Si⁷⁹Br

1997

128: 94711u High-resolution infrared spectrum of D₃Si⁷⁹Br in the ν_1/ν_4 region: the structure of silyl bromide. Demaison, J.; Cosleou, J.; Burger, H.; Mkadmi, E. B. (Laboratoire de Spectroscopie Heriotienne, 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 D₃Si⁷⁹Br covering the bands ν_1 (a₁, 1580.637 cm⁻¹) and ν_4 (e, 1615.085 cm⁻¹) have been recorded with a resolu. of 3×10^{-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 $\sigma(\text{Fit})$ ca. 5×10^{-4} cm⁻¹. Equil. rotational consts. of H₃Si⁷⁹Br and D₃Si⁷⁹Br 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 $r_e(\text{Si-H}) = 1.470(2)$ Å, $r_e(\text{Si-Br}) = 2.207(1)$ Å, and $\alpha_e(\text{HSiH}) = 110.5(2)^\circ$.

UK,
Cmpey.
Hapam,
Di

C.A. 1998, 128, N 8

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 resolu. 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 $\nu_1 = 1$ and $\nu_4 = 1$ states, yielding a std. deviation of each fit of $\sim 0.0004\text{ cm}^{-1}$, which may be compared with the exptl. precision ($\sim 0.0001\text{ cm}^{-1}$). Improved ground state parameters also were obtained by ground state combination differences.

(ν_i (Si-H))

C. A. 1997, 127, N 22

H. Si D₃

1998

129: 10091b High resolution FTIR study of the ν_3 bands of HSiD_3 and $\text{H}^{120}\text{SnD}_3$. Burger, Hans; Jerzembeck, Wolfgang; Ruland, Helmut; Halonen, Lauri (FB 9, Anorganische Chemie, Universität-GH, D-42097 Wuppertal, Germany). *J. Mol. Spectrosc.* 1998, 189(1), 8-15 (Eng), Academic Press. High resolu. Fourier Transform spectra of HSiD_3 and monoisotopic $\text{H}^{120}\text{SnD}_3$ were recorded in the region of the ν_3 fundamental at 850.68 and 646.90 cm^{-1} with a resolu. of 3.3 and $2.8 \times 10^{-3} \text{ cm}^{-1}$, resp. About 2000 rovibrational transitions of each species were assigned and fitted to 2 different redns. of the effective Hamiltonian, with $\sigma(\text{Fit}) = 1.2 \times 10^{-4}$ (HSiD_3) and $1.4 \times 10^{-4} \text{ cm}^{-1}$ ($\text{H}^{120}\text{SnD}_3$). The 2 sets of parameters are equiv., and relations between parameters belonging to different redns. are perfectly fulfilled. Also the ground state consts. C_0 and D_{K0} were detd. for the 1st time. For consistency the previously measured data belonging to the ν_3 band of $\text{H}^{70}\text{GeD}_3$ were refitted, $\sigma(\text{Fit}) = 1.6 \times 10^{-4} \text{ cm}^{-1}$, from improved ground state parameters including the h_3 term accounting for the splitting of the $K = 3$ level.

UK CHEM

M.A.

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□

 $\text{H}^{120}\text{SnD}_3$

C.A.

1998,

129,

N 1

H₃SiD

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.