

Si - Br

7577

(AsH₃; AsD₃; DSiCl₃; DSiBr₃)

1936

Delfosse J.M.

Nature 1936, 137, 368

"Raman spectra of "heavy" arsine,
silicochloroform and silicobromoform"

C.A., 1936, 5498⁶

SiBr₃D

W

SiBr_2F_2

Spitzer R.
Howell W. J.,
Schomaker V.

1942

J. Am. Chem. Soc.,
86, 64, 62

сир-ра
мол-м
методом
дифракции
электронов.



5755 2

1950

SiF_4 , SiF_3CH_3 , LiF , Cl , SiF_3Br
(mol. wt.)

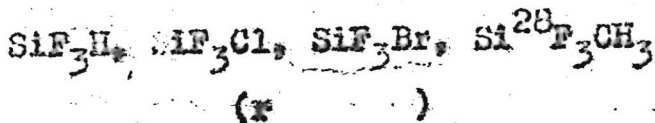
Sheridan J., Gordy S.
Phys. Rev., 1950, 77, 110

Microscopic spectra and ...

SiBrF_3

5759

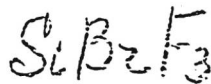
1957



Sheridan J., Gordy W.
J. Chem. Phys., 1951, 19, 965-970

The microwave spectra...

J



1953

5789

SiCl_4 , SiBr_4 , SiJ_4 , SiCl_2Br_2 , SiCl_3Br ,
 SiClJ_3 , SiCl_2J_2 , SiCl_3J ,

Kakiuti Y.

Bull.Chem.Soc. Japan., 1953, 26, N 5,
260-261

The normal vibrations of some...

J

SiBrCl_3

Si Cl₃ Br

⁵⁴⁸³
[BP - ~~2879~~ - IV]

1954

Si Cl Br₃

Si Cl₂ Br₂

Schneider B, et al,
Chem. Listi, 48, 336,

и.и.
суктрас.

coll. Czechosl. Chem.
Comm., 19, N4, 653.

1958.

5790

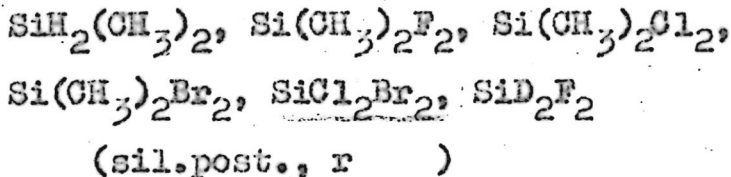
SiCl_4 , SiFCl_3 , SiBrCl_3 , SiJCl_3
(*vi*, sil.post.)

Stokr J., Schneider B.
Chem. Listy, 1958, 52, N 6, 985-995

SiBr_2Cl_3

1963

8693



Radhakrishnan M.
 Z.phys.Chem. (DDR), 1963, 222, N 3-4,
 211-216

Potential constants...



J

M759 - IV

1965

SiH_3F ; SiH_3Cl ; SiH_3Br ; SiH_3J ;

SiD_3F ; SiD_3Cl ; SiD_3Br ; SiD_3J ; ($\checkmark$)

Bald D.F., Buttler M.J., McKean D.C.
Spectrochim. Acta, 1965, 21, N 3,
451-64

Frequency shifts from gas ...

J

PX, 1966, 2 101

orig.

From original

1965

SiD_3H , SiH_3F , SiH_3J , SiF_3H , SiF_3D , SiCl_3H ,

SiBr_3H , SiBr_3Cl , SiJ_3Cl , SiCl_3Br , SiCl_3J

(M , vib , vib , vib , vib , vib)

Venkateswarly K., Devi V.M.,

Current sci (India), 1965, 34(12), 373-4

Mean amplitudes of vibrationi XY_3Z
type of silicon compounds

CA., 1965, 63, N 9, 10843h

M 1191

1966

CH_3F , CD_3F , SiH_3F , SiD_3F (mixture norm.)

$\text{X} = \text{F}, \text{Cl}, \text{Br}, \text{J}, \quad \text{CH}_3\text{Cl}, \text{CD}_3\text{Cl}, \text{SiH}_3\text{Cl}, \text{SiD}_3\text{Cl},$
 $\text{CH}_3\text{Br}, \text{CD}_3\text{Br}, \text{SiH}_3\text{Br}, \text{SiH}_3\text{J}, \text{SiD}_3\text{J}, \text{SiD}_3\text{Br},$
 $\text{CH}_3\text{J}, \text{CD}_3\text{J}$

Pulay P., Torok F.

Acta Chim. Acad. Sci. Hung. 1966, 47(3),
273-9

Paratemer form of matrix F.II. Assignment
with the aid the parameter form (short
communication)

F

J

CA., 1966, 65, N 2, 1397g

$(\text{SiBr}_3)_2$ 0

ν_i
см. пост.

Х. 1969. 2

1968
✓ 2 Б193. Колебательные спектры гексабромдисилоксана и гексабромдисилазана. Bürger Hans, Schulze Manfred. Die Schwingungsspektren von Hexabromdisiloxan und Hexabromdisilazan. «Z. Chem.», 1968, 8, № 7, 256—257 (нем.)

Исследованы ИК-спектры (33—4000 см^{-1}) и спектры КР жидких $\text{Br}_3\text{SiOSiBr}_3$ (I) и $\text{Br}_3\text{SiNHSiBr}_3$ (II). Спектры сопоставлены с ранее исследованными кол. спектрами SiBr_4 и HSiBr_3 . Произведен расчет силовых постоянных I и II и дано отнесение полос сим. и асим. вал. кол. SiOSi , отнесены соответственно полосы 693,5 и 1094 см^{-1} ; SiNHSi —726 и 955,5 см^{-1} . В области (315—530 см^{-1}) лежат вал. кол. SiBr , а в области ниже 230 см^{-1} —деф. кол. SiBr . Из различия спектров I и II в области вал. кол. SiBr сделан вывод о понижении локальной симметрии C_3 групп SiBr_3 в II. Анализ нормальных колебаний приводит к предположению что ниже 80 см^{-1} для I и II должна лежать еще одна ненаблюдавшаяся фундаментальная частота. А. Александров



Si-Br

Maijs, L.

1968

(cbez6) "Z. anorg. allgem. Chem.",

273, 170, 1953.

Jensovsky "Z. Chem." 2, 334, 1962;

3, 453, 1963.

(cur Si-F, III)

B9- XIV-625

1968

SiFBr₃

3

72638g Microwave spectrum and structure of fluorotribromosilane and methyltribromosilane. Mitzlaff, M.; Holm, R.; Hartmann, Hermann (Univ. Frankfurt/Main, Frankfurt/M., Ger.). *Z. Naturforsch. A* 1968, 23(11), 1819-21 (Ger). Microwave absorption spectra (30-40 GHz.) were recorded for SiFBr₃ and MeSiBr₃. Si-Br bond lengths 2.171 and 2.175 Å., and Br-Si-Br bond angles 111.36 and 111.09° were detd. for SiFBr₃ and MeSiBr₃, resp., by least sqs. anal. of the rotational consts. of the ⁷⁹Br and ⁸¹Br species with assumed values 1.56, 1.90, 1.093 Å., and 109.35° for bond lengths Si-F, Si-C, and C-H, and the H-C-H bond angle, resp. Measured and calcd. rotational consts. are tabulated. The SiBr₃ group has the same structure in SiFBr₃, SiHBr₃, and MeSiBr₃. A 1-kcal./mole barrier to internal rotation in MeSiBr₃ was detd. from the intensity ratios of the rotational lines of mols. in the torsional ground state to those of mols. in the 1st excited torsional state.

FBJG

u. b. check

C.A. 1969. 40. 16

ВГХ-ХІІ-625

1968

 SiFBr_3 м.в. спектр,
структура,
V.

4 Д353. Микроволновый спектр и структура фтор-трибромсилана и метилтрибромсилана. Mitzlaff M., Holm R., Hartmann H. Mikrowellenspektrum und Struktur von Fluortribromsilan und Methyltribromsilan. «Z. Naturforsch.», 1968, 23a, № 111, 1819—1821 (нем.; рез. англ.)

В области 30—40 Гц исследованы микроволн. спектры молекул SiFBr_3 (I) и CH_3SiBr_3 (II). Определены структурные параметры $d_{\text{Si-Br}}$, равные $2,171 \pm 0,001$ (для I) и $2,175 \pm 0,01$ Å (для II) и углы Br—Si—Br, равные $(111,36 \pm 0,15)^\circ$ (для I) и $(111,09 \pm 0,15)^\circ$ (для II). Найден барьер внутреннего вращения $V_3 \approx 1$ ккал/моль.

9. 1969.

49

X

B-9-XIV-625

1968

SiFBr₃

10 Б273. Микроволновый спектр и структура фтор-трибромсилана и метилтрибромсилана. Mitzlaff M., Holm R., Hartmann H. Mikrowellenspektrum und Struktur von Fluortribromsilan und Methyltribromsilan. «Z. Naturforsch.», 1968, 23a, № 11, 1819—1821 (нем.; рез. англ.)

В диапазоне 30—40 Гц исследованы вращательные спектры молекул SiFBr₃ (I), CH₃SiBr₃ (II) и их изотопич. разновидностей по Br. Определены значения вращательной постоянной B_0 и постоянных центробежного искажения D_J и D_{JK} . Из значений B_0 при предположении, что Si—F=1,56, Si—C=1,90, C—H=1,093 Å и $\angle HCH=109,35^\circ$, определены длины связи Si—Br=2,171±0,001 в I, 2,175±0,001 Å в II и вал. угла $\angle BrSiBr=111,36\pm0,15^\circ$ в I и $111,09\pm0,15^\circ$ в II. Барьер внутреннего вращения группы SiBr₃ $V_3\approx 1$ ккал/моль.
М. Р. Алнев

М. Р. Алнев,
структура

+1

X. 1969. 10

X

1969

 SiBr_3F SiBr_2F_2 SiF_3Br

Раман -

чек

C. A. 1969.

H. 22

(107331b) Raman spectra of silicon fluorobromides. Dubois, Marie L.; Delhay, Marie B.; Wallart, Francis (Lab. Spectrosc. Raman, Fac. Sci., Lille, Fr.). *C. R. Acad. Sci., Ser. B* 1969, 269(5), 260-2 (Fr). Si fluorobromides, prep'd. by the reaction of AlBr_3 and Na^+ or Ba^{2+} fluorosilicates at 270° , were condensed in 2 fractions: 1 fraction at 20° , rich in SiBr_4 and SiBr_3F ; and another fraction at -78° , rich in SiF_2Br_2 and SiF_3Br . By studying temp. dependence (room temp. to 77°K .) of the He-Ne laser-excited Raman spectra, and by considering changes predicted by symmetry changes on exchange of F and Br atoms, assignment of the fundamental frequencies of each of the 4 mols. was accomplished without isolating the compds. in pure form.

FBIF

SiBrCl₃

1971.

Aleshonkova, Yu. A.; et al

Dokl. Nauch.-Tekh. Konf. Ivanov.

Khim.-Tekhnol. Inst. 1971, 15-17.

Chem.
Notes.

(see ClBrCl₃ ; III)

SiClBr₃
GeClBr₃

1971.

Aleshonkova, Yu. A.; et al

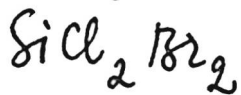
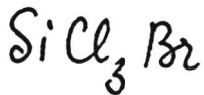
Dokl. Nauch.-Tekh. Konf. Ivanov.

Khim.-Tekhnol. Inst. 1971, 15-17.

Синтез
и анализ

• (ср. CClBr₃; III)

Si-Mal XIV-334 1971

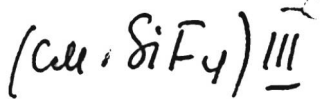


Heöfler F.

Z. Naturforsch., 26a
(3), 547.

$\checkmark_i$

M.H.



40115.1275
Ch, Ph, TE, Ex-C

SiF_3Br

29848, 15-3030

1973

Cradock Stephen, Ebsworth E.A.V.,
Whiteford R. Alastair. Photoelectron
spectra of some simple fluorosilanes.
"J. Chem. Soc. Dalton Trans.", 1973,
N 22, 2401-2404 (англ.)

0022

(см SiF_3H ; III)

008 009

- 015

ВИНИТИ

1978

Sig Br₆

Sahini V.E., et al

Chem.
noct.

Rev. Roum. Chim., 1978,
23, 15, 643-9



(See Sig F6) III

1978

12 Б235. Колебательные спектры и силовые константы перхлорированных и пербромированных цикло-
силанов. Hassler K., Kovar D., Hengge E.
Schwingungsspektren und Kraftkonstanten perchlorierter
und perbromierter Cyclosilane. «Spectrochim. acta», 1978,
A34, № 12, 1199—1203 (нем.)

Исследованы ИК-спектры в области $50-700\text{ см}^{-1}$ и
спектры КР Si_5X_{10} (I) и Si_6X_{12} (II) ($\text{X}=\text{Cl}, \text{Br}$). Про-
веден расчет частот и силовых констант I и II с ис-
пользованием модифицированного валентно-силового
поля. Силовые константы связей (f) SiX и SiSi I и II
сопоставлены с соотв-щими силовыми константами SiX_4
(III) и Si_2X_6 (IV). Показано, что $f(\text{SiX})$ и $f(\text{SiSi})$ в
I и II уменьшаются по сравнению с константами диси-
ланов IV и остаются практич. неизменными при пере-
ходе от I к II: $f(\text{SiCl})$ ($\text{N}/\text{см}$) = 3,11, 2,9, 2,6, 2,6;
 $f(\text{SiBr})$ ($\text{N}/\text{см}$) = 2,45, 2,3, 2,2, 2,25 в III, IV, I и II
соотв., $f(\text{SiSi})$ ($\text{N}/\text{см}$) = 2,4, 2,2, 2,2 (для хлорсиланов),
2,1, 1,85, 1,85 (для бромсиланов) в IV, I и II, соот-
ветственно.

Е. Б. Назарова

 $\text{Si}_5\text{Br}_{10}$ $\text{Si}_6\text{Br}_{12}$

сил. конст.

I.

☒

2.1079, N12

SiBz_3Cl

1981

Aleshonkova Yu. A.,
Volkov N. V., et al.

Russ. Deposited Doc. 1981,
no. VINITI 2717-81, 11 pp.

(Ser. CF₃Cl; III)

$\text{SiCl}_3 \text{ Bz}$

1981

Aleshonkova Yu. A.,
Volkov N. V., et al.

Vi, clev.
noeii.

Deposited Dec. 1981,
VINITI 2717-81, 11 pp.

($\text{C}_{60}\text{F}_3 \text{ ce; III}$)

SiBr₃F

1981

SiF₃Br

Alesonkova Yu. A.,
Volkov N. V., et al.

Vi, cer.

uocer.

Deposited Dec. 1981,
VINITI 2717-81, 11 pp.

(Cer. CF₃ Cl; III)

SiH_2FBz

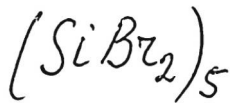
1982

SiH_2Alk Bureš et al., Černý Č.,
Pavliček Z.

Vi, cer.
nocm.

Chem. listy, 1982,
76, N4, 375-388.

●
(cer. SiH_4 ; III)



1982

Hörig M., et al.

eur. month. Monatsh. Chem.,

A E. 1982, 113, N 2, 129-
-138.

• (eur. $(\text{SiCl}_2)_6$; III)

$(\text{SiBr}_2)_4$

1982

Mönnig M., et al.

Monatsh. Chem.,

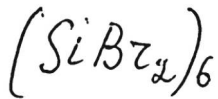
ссыл. номер.

1982, 113, N 2, 129-

Δ F.

-138.

●
(ссыл. $(\text{SiCl}_2)_6$; III)



1982

Hörig M., et al.

Monatsh. Chem.,

Chem. USSR.

Δ E.

1982, 113, N2, 129 -
- 138.

●
(1 Chem. $(\text{SiCl}_2)_6$; III)

SiBr₃Cl

1983

Dhanalakshmi A.,
Kornala P.

Vi;

Bull. cl. sci. Acad. roy.
Belg., 1983, 69, N2, 110-116.

● (cur. CF₃H; III)

SiBr_3O

1983

Dhanalakshmi A.,
Kamala P.

Ni;

Bull. cl. sci. Acad. roy.
Belg., 1983, 69, n2, 110-116.

● (ex. CF_3H ; III)

SiH₄-xBr_x

(OM-20554)

1984

Aron Z., Bunnell Z., Ford
T.A.,

Z. Mol. Struct., 1984,
110, N3-4, 361-379.

U.A.

Om. 22296

1985

$\text{Br}_3\text{Si}-\text{SiBr}_3$ и др.

Stölevik R., Bakken P.,

рацем
структура,
глицерин.
барьера,
син. рацем.

J. Mol. Struct., 1985,
124, N 1-2, 133-142.

SiH₃Br

DM-26612

1986

Dobbs K.D., Mehre W.F.,

un. J. Comput. Chem., 1986,
7, N 3, 359-378.

SiH₂D₂ Bz

1986

Duncan J. L., Harvie J. L.,
et al.

UK
cncmp

J. Mol. Spect. 1986,
145 (3-4), 225-42.

(cor.  Si₂H₂D₅; III)

$\text{Br}_2\text{HSi}-\text{SiHBr}_2$ (om. 25234) 1986

Thomassen H., Hasen K.,
Stølevik R., et al.,

J. Mol. St

молекул.
структура,
электроно-
граф. ис-
следован.

SiF₃Br

1987

4 Л203. Микроволновый спектр, структура, постоянные квадрупольной связи и дипольный момент молекулы бромтрифторсилана. Microwave spectrum, structure, quadrupole coupling constants, and dipole moment of bromotrifluorosilane. Cox A. Peter, Ewart Ian C., Gayton Tim R. «J. Mol. Spectrosc.», 1987, 125, № 1, 76—90 (англ.)

В диапазоне 8—40 ГГц исследованы МВ-спектры четырех изотопных форм молекулы SiF₃Br. Идентифицированы линии вращательных переходов с $J \leq 12$ и их квадрупольная СТС в основном колебательном состоянии и в первых возбужденных состояниях вырожденных колебаний ν_5 и ν_6 . Определены значения вращательных и квартичных центробежных постоянных, q -постоянных l -удвоения, постоянных квадрупольной связи ядер ^{79}Br (344 МГц) и ^{81}Br (287 МГц) и дипольного момента (0,835 ед. Дебая). Для $^{28}\text{SiF}_3^{79}\text{Br}$ $B_0 = 1550,06$ МГц; $D_J = 0,166$, $D_{JK} = 1,245$ кГц; $q_5 = 0,30$, $q_6 = 1,17$ МГц.

М. Р. Алиев.

М.П.

ф. 1988, 18, 44

SiF_3Br

1987

7 Б1349. Микроволновый спектр, структура, постоянные квадрупольного взаимодействия и дипольный момент бромтрифторсилана. Microwave spectrum, structure, quadrupole coupling constants, and dipole moment of bromotrifluorosilane. Cox A. P., Ewart I. C., Gayton T. R. «J. Mol. Spectrosc.», 1987, 125, № 1, 76—90 (англ.)

На штарковском микроволновом (МВ) спектрометре с использованием РЧ—МВ двойного резонанса в обл. частот 12—38 гГц измерены вращат. спектры 4 изотопич. образцов бромтрифторсилана $^{28}\text{SiF}_3^{79}\text{Br}$, $^{28}\text{SiF}_3^{81}\text{Br}$, $^{30}\text{SiF}_3^{79}\text{Br}$ и $^{30}\text{SiF}_3^{81}\text{Br}$ в основном и двух возбужденных колебат. состояниях. Анализ МВ-данных позволил существенно уточнить значения молек. постоянных, опубликованных ранее. Существенно уточнены значения ^{79}Br - и ^{81}Br -ядерных квадрупольных постоянных $eQq=344,0(1)$ и $287,4(1)$ МГц, соотв. Определены полный дипольный момент $\mu=0,835(7)D$ и структурные параметры $r(\text{SiBr})=2,1559(37)$ А,

Уб спектр;
структура,
У, м.п.

Х. 1988, 19, № 7

$r(\text{SiF}) = 1,5591(52) \text{ \AA}$, $\angle \text{FSiB} = 110,38(19)^\circ$, $\angle \text{FSiF} =$
 $= 108,55(19)^\circ$.
С. Н. Мурзин



SiH_2NBr
 SiHN_2Br

acc. 28100

1987

Weaving J.S.,
Ford T.A.

колебание.
волевоое
чужа,

J. Mol. Street,
1987, 161, 245-
- 264.

теор. расчёт,
распредел.
номеров.
Исследования.

$\text{BrF}_3 \text{Si}^+$
($\text{SiF}_3 \text{Br}^+$)

com. 30490
Jacox M.E.,

1988

Ti, Vi;

J. Phys. and Chem. Ref.
Data, 1988, 17, N2, 460.

)

F-Li-Cl

om. 33714

1990

у термод.
данные

Binnemies M.,
Schnöckel M.,
Chem. Rev. 1990, 90,
N1, 321-330.



Li_xOyBr_z (OM 34803) 1990

Kornick A., Binnemiek,

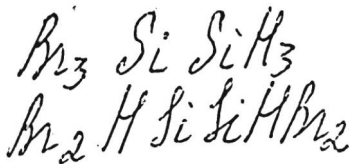
Z anorg. allg. Chem.

1990, 587, 157-166.

Über die Bildung von
Kalsgenosiloxanen bei

Reaktion von SiH_4 ($X=\text{Cl}$,
b) mit Sauerstoff.

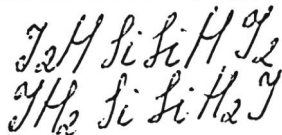
1991



115: 377097 IR and Raman spectra of some bromodisilanes and iododisilanes. Hassler, K.; Poeschl, M. (Inst. Anorg. Chem., T. U. Graz, A-8010 Graz, Austria). *Spectrochim. Acta, Part A* 1991, 47A(3-4), 439-44 (Ger). IR and Raman spectra of the disilanes X_3SiSiH_3 , $\text{X}_2\text{HSiSiHX}_2$ ($\text{X} = \text{Br}, \text{I}$) and $\text{IH}_2\text{SiSiH}_2\text{I}$ and their deuterated deriva. are reported and assigned. The measured H/D isotope shifts were used for a normal coordinate anal.

UK - a Pa -
 МАМ. СРЕДН.
 Di

(41) 



C.A. 1991, 115, N 4

H_2SiBr

Дм 35983

1991

№ 24 Б1343. Инфракрасный спектр высокого разрешения $H_3Si^{79}Br$ в области от 21 до 233 cm^{-1} . Фундаментальные частоты ν_1 и ν_4 . The high-resolution infrared spectrum of $H_3Si^{79}Br$ from 2100 to 2330 cm^{-1} . The ν_1 and ν_4 fundamentals / Lattanzi F., di Lauro C., Bürger H. // Mol. Phys.— 1991.— 72, № 3.— С. 575—592. — Англ.

Исследован фурье-ИК-спектр высокого разрешения $H_3^{28}Si^{79}Br$ в области фундаментальных полос ν_1 и ν_4 (21—233 cm^{-1}). В спектре наблюдался ряд ангармонич. резонансов. Отмечено наличие нескольких сильных колебательно-вращат. возмущений, особенно в области низких значений K . Объяснены некие аномалии вращат. структуры спектра. С помощью МНК с использованием итерационной процедуры найдены значения колебательно-вращат. параметров. Б. С. Авербух

М. П.

Х. 1991, № 24

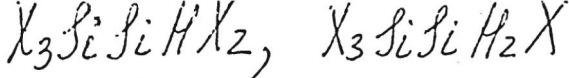
$\text{Si}_2\text{H}_5\text{Br}$

1993

McKean D.C., McPhail A.L.,
et al.,

(UK) Spectrochim. Acta, Part A
1993, 49A(8), 1079-94.

(Cell. $\text{Si}_2\text{H}_5\text{Cl}$,  III)

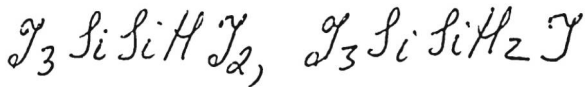


1994



120: 230246k Vibrational spectra and normal coordinate analysis of penta- and tetrahalodisilanes $X_3SiSiHX_2$ and X_3SiSiH_2X , $X = Br$ and I . Hasler, K. (Inst. Anorg. Chem., TU, A-8010 Graz, Austria). Spectrochim. Acta, Part A 1994, 50A(2), 243-9 (Ger). The IR and Raman vibrational spectra of the title compds. were measured and assigned with the aid of normal coordinate analyses. SiSi-force consts. were calcd. They increase with increasing electronegativity of the halogen X.

UK, CKP,
Cul. NCM,
Vi



(H)

18

C.A. 1994, 120, 118

1995

F: Si-H-Br

P: 3

14Б167. Симметрично замещенные силаны $(\text{XH}[2]\text{C})[2]\text{SiH}[2]$, $(\text{XH}[2]\text{C})[2]\text{SiX}[2]$, $(\text{X}[2]\text{HC})[2]\text{SiH}[2]$ и $(\text{X}[2]\text{HC})[2]\text{SiX}[2]$ с $\text{X}=\text{F}$, Cl , или Br . Конформационные энергии, структура и торсионные силовые постоянные, полученные методом молекулярной механики. Symmetrically substituted silanes: $(\text{XH}[2]\text{C})[2]\text{SiH}[2]$, $(\text{XH}[2]\text{C})[2]\text{SiX}[2]$, $(\text{X}[2]\text{HC})[2]\text{SiH}[2]$ and

$(\text{X}[2]\text{HC})[2]\text{SiX}[2]$ with $\text{X}=\text{F}$, Cl or Br . Conformational energies, structures and torsional force constants obtained by molecular-mechanics calculations / Johansen Tore H., Stolevik Reidar [Journal of Molecular Structure] // J. Mol. Struct. - 1995. - 372, N 2 - 3. - С. 275-284. - Англ.

РНИХ 1997

1995

F: Si₃H₂Br₆

P: 3

14B168. 1,1,1,3,3,3-Гексабромтрисилан. Структура и конформация, определенные методами газовой электронографии, колебательной спектроскопии, а также с использованием расчетов неэмпирическим методом МО и методом молекулярной механики. 1,1,1,3,3,3-Hexabromotrisilane: Structure and conformation determined by gas-phase electron diffraction, ab initio molecular orbital and molecular mechanics calculations, and vibrational spectroscopy / Johansen Tore H., Hagen Kolbjorn, Stolevik Reidar, Ernst Margot, Hassler Karl [Journal of Molecular Structure] // J. Mol. Struct. - 1995. - 372, N 2 - 3. - С. 161-172. - Англ.

РМХ 1997



M. gugg.

C. A. 1996, 124, N 8

1995

124: 98233e The 1,1,1,3,3,3-Hexabromotrisilane: structure and conformation determined by gas-phase electron diffraction, ab initio molecular orbital and molecular mechanics calculations, and vibrational spectroscopy. Johansen, Tore H.; Hagen, Kolbjorn; Stolevik, Reidar; Ernst, Margot; Hassler, Karl (Department of Chemistry, AVH, University of Trondheim, N-7055 Trondheim, Norway). *J. Mol. Struct.* 1995, 372(2-3), 161-72 (Eng). The mol. structure of 1,1,1,3,3,3-hexabromotrisilane at 140°C was studied using gas-phase electron diffraction. The two SiBr_3 groups are both staggered relative to the central SiH_2 group, but a twist of about 13° of the SiBr_3 groups relative to the exactly staggered position reduces the symmetry to C_2 . From the vibrational spectra a distinction between C_2 or C_{2v} symmetry is possible, and point group C_{2v} can be ruled out by arguments based on the selection rules. Bond lengths (r_g) and valence angles ($\angle_a$) are: $r(\text{Si}-\text{Si}) = 2.344(18)\text{\AA}$, $r(\text{Si}-\text{Br}) = 2.205(4)\text{\AA}$, $\angle(\text{SiSiSi}) = 112.9(19)^\circ$, $\angle(\text{BrSiBr}) = 109.6(6)^\circ$ (av. BrSiBr angle), and $\angle(\text{SiSiBr}) = 109.3(6)^\circ$ (av. SiSiBr angle). Error limits are given as 2σ where σ includes ests. of uncertainties in voltage/height measurements and correlation in the exptl. data. The IR and Raman vibrational spectra are assigned using normal coordinate calcns. as well as ab initio calcns.; harmonic force consts. are reported. In addn. mol. mechanics and ab initio (RHF/SBK and RHF/STO-3G) calcns. were performed to assist the structural anal. and to compare with the diffraction results.

$\text{Si}_2\text{H}_5\text{Br}$

$\text{Si}_2\text{D}_5\text{Br}$

UK, CKP
еес. ноеес.,
 Vi

1995
McKean D. C.,
McPhail A. L. et al.
Spectrochim. Acta.
Part A 1995, 51A
(2), 215-35.

(еес. $\text{Si}_2\text{H}_5\text{Cl}$; III)

D₃SiBr

1997

126: 322559s Millimeter-wave and high resolution infrared spectra of D₃SiBr. Buerger, H.; Cosleou, J.; Demaison, J.; Mkadmi, E. B.; Paplewski, M. (Anorganische Chemie, Univ.-Gesamthochschule Wuppertal, D-42097 Wuppertal, Germany). *J. Mol. Spectrosc.* 1997, 182(1), 205-214 (Eng), Academic. The mm-wave (mmw) spectra of D₃-Si⁷⁹Br and D₃Si⁸¹Br in the vibrational ground state were recorded at 150-650 GHz. The mmw spectra of D₃Si⁷⁹Br in the $\nu_3 = 1$ and $\nu_6 = 1$ states were studied in some limited spectral ranges. FTIR spectra of

(mm crkcp) monoisotopic D₃Si⁷⁹Br covering the bands $\nu_3(a_1, 418.650 \text{ cm}^{-1})$, $\nu_6(e, 464.254 \text{ cm}^{-1})$, $\nu_5(e, 685.367 \text{ cm}^{-1})$, and $\nu_2(a_1, 686.373 \text{ cm}^{-1})$ were recorded with resolns. of $(2.5-3.5) \times 10^{-3} \text{ cm}^{-1}$. J-dependent ground state parameters up to sextic terms were detd. from the mmw spectra, and $A_0 = 1,425263(12) \text{ cm}^{-1}$ for D₃Si⁷⁹Br was derived from fits of several $(\Delta k - \Delta l) = \pm 3$ interactions obsd. in the ν_2/ν_5 band system. While ν_3 and ν_6 interact weakly by Coriolis x, y resonance, the Coriolis resonance of the almost degenerate ν_2 and ν_6 bands (~6000 IR lines) supplemented by mmw data and of the ν_2 and ν_5 bands (~8000 lines) were obtained with root-mean-square deviations of 0.28 and $0.37 \times 10^{-3} \text{ cm}^{-1}$ for the IR data. Some hot bands of ν_3 were detected and analyzed.

C.A. 1997, 126, N24

SiFCl

1997

127: 363628c Detection of a new halosilylene, SiFCl, by microwave spectroscopy. Fujitake, Masaharu; Hirota, Eizi (The Institute for Molecular Science, Okazaki, Japan 444). *J. Mol. Struct.* 1997, 413-414, 21-30 (Eng), Elsevier. The rotational spectrum of SiFCl in the ground vibronic state was obsd. at 340-356 GHz. The anal. of the obsd. spectrum, which consisted of both a-type and b-type transitions, yielded rotational consts. and centrifugal distortion consts. of the ^{35}Cl and ^{37}Cl isotopic species in the ground state. The harmonic force field of SiFCl was derived from the centrifugal distortion consts. and the inertial defects detd. for both isotopic species and was used to calc. the vibrational frequencies of the mol. The av. structure in the ground vibrational state is $r_z(\text{Si-F}) = 1.5960 \text{ \AA}$, $r_z(\text{Si-Cl}) = 2.0714 \text{ \AA}$, $\theta_z(\text{F-Si-Cl}) = 100.85^\circ$ and $\delta r_z(\text{Si-Cl})$ [^{35}Cl - ^{37}Cl difference] = $0.000065 \text{ \AA}$ by using the obsd. rotational consts. and the harmonic force field derived.

Мб сиемф,
структурн.
параметры

C.A. 1997, 127, N 26

BrLiO

1998

Br_2LiO

Alikhani, M.E; et al,

comp-pa, Di,
meop. paper

J. Comput. Chem.
1998, 19 (11), 1205-14.

(cm. $\text{ClLiO}^\bullet$; III).

1999

F: HBrSi₂

P: 3

132:127981 Effect of substituents on the
structure and stability of the disilyne isomers.

Bei, Yi-Ling; Feng, Sheng-Yu Department of
Chemistry, Shandong University Jinan 250100,
Peop. Rep. China Huaxue Xuebao, 57(12),
1306-

1312 (Chinese) 1999 The 6-31G** level of quantum
chem. ab initio calcns. was used in the theor.
research on the structure and stability of

C. H. 2000, 132

substituted disilynes a their isomers HYSi_2 and Y_2Si_2 ($\text{Y} = \text{F}, \text{Cl}, \text{Br}, \text{Li}$). The effect of substit on the stability of various isomers, esp. that of Si-Si bond, is discusse detail. The results show that among various substituted disilyne isomers disilenylidene structures and double-bridged structures have the lowest e and can be exptl. detectable, while the classical linear structures have energy and are thus unstable.

1999

F: Br₂Si₂

P: 3

132:127981 Effect of substituents on the
structure and stability of the disilyne isomers.

Bei, Yi-Ling; Feng, Sheng-Yu Department of
Chemistry, Shandong University Jinan 250100,
Peop. Rep. China Huaxue Xuebao, 57(12),
1306-

1312 (Chinese) 1999 The 6-31G** level of quantum
chem. ab initio calcns. was used in the theor.

C.A. 2000, 132

research on the structure and stability of substituted disilynes and their isomers HYSi_2 and Y_2Si_2 ($\text{Y} = \text{F}, \text{Cl}, \text{Br}, \text{Li}$). The effect of substituent on the stability of various isomers, esp. that of Si-Si bond, is discussed in detail. The results show that among various substituted disilyne isomers disilenylidene structures and double-bridged structures have the lowest energy and can be experimentally detectable, while the classical linear structures have higher energy and are thus unstable.

F: Si_2Br_6

P: 31:65144 Studies on vibrational spectra and normal coordinate analysis of hexabromodisilane.

Xu, Xue-Jun; Xue, Ying; Xie, Dai-Qian; Yan, Guo-Sen (Dep. Chem., Sichuan Univ., Chengdu 610064, Peop. Rep. China). Gaodeng Xuexiao Huaxue Xuebao, 20(6), 941-944 (Chinese) 1999 The optimized geometries, IR intensities, Raman activities and fundamental vibrational frequencies and PEDs are reported for D_{3d} symmetr of Si_2Br_8 using HF/6-31G and B3LYP/6-31G method. The predicted value of Si-Si torsional vibrational frequency is given. A

normal coordinate anal was carried out and HF force field is scaled with scale factor of 0.9 pertinent to all vibrational modes. The av. error between the predicted frequencies obtained from HF/6-31G SQM force field and the obsd. fundamental vibrational frequencies is 9.4 cm⁻¹; the av. error between th predicted value from unrefined DFT force field and the obsd. result is 8. cm⁻¹. The fundamental vibrational frequencies obtained from DFT calcn. with B3LYP/6-31G.bul. are in good agreement with the exptl. results.

SiBr₄⁺

2000

X²T₂, A²T₁,
B²E, C²T₂

(3)

C.A. 2001, 134, N12

134: 170314h Observation of different ionic state of SiBr₄ - photoelectron spectroscopic and theoretical studies. Sun, Zheng; Zheng, Shi-jun; Wang, Dian-xun (State Key Lab. for Structural Chemistry of Unstable and Stable Species, Institutes of Chemistry, Chinese Academy of Sciences, Beijing, Peop. Rep. China 100080). *Huaxue Xuebao* 2000, 58(12), 1645-1648 (Ch), Kexue Chubanshe. The Photoelectron Spectroscopy (PES) and different ionic state of SiBr₄ were reported. The ionic states of SiBr₄⁺ are X ²T₂, A ²T₁, B ²E, C ²T₂ resp. The adiabatic ionization potential of the compd. is I_a(X ²T₂ ← X ¹A₁) = 10.532 eV. A frequency of 450 ± 30 cm⁻¹ was obsd. in the PES band of X ²T₂ ionic state. The assignment of the PE spectrum was performed with the help of theor. calcns. and band characters. Obvious spin-orbital coupling split was obsd. in X ²T₂ and A ²T₁ states, and the splitting space are 0.27 and 0.53 eV. The comparison of different calcns. shows that the outer valence Green's function method gives good results in ionization potential calcns.