

Si-H-Cl

7577
1936

(AsH₃; AsD₃; DSiCl₃; DSiBr₃)

Delfosse J.M.

Nature 1936, 137, 868

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

C.A., 1936, 5498⁶

SiCl₃D 1

5823

1953

SiD_3Cl (mol.str.)

Bak B., Bruhn J., Rastrup-Andersen J.
J.Chem.Phys., 1953, 21, N 4,
753-4

Microwave spectrum and...

J

SiClD_3

5822

1984

SiD_3Cl , SiH_3F , SiD_3F ()

Andersen F.A., Bak B.
Acta chem.scand., 1954, **L**, N 5,
738-743

Infrared ...

SiClD_3

J

5824

1954

SiD_3Cl , SiD_3F (mol.str.)

Back B., Bruhn J., Rastrup-Andersen
Acta Chem.Scand., 1954, 8, 367-73

Stereochemistry of ...

J

SiClD_3

1959

5758

SiF_3H , SiF_3D , SiD_3F , SiD_3Cl ()

Hewson G., Polo E.R., Wilson M.E.
Spectrochim. acta., 1959, N 10, 793-99

Infrared spectrum...

J



SiClD_3

1962

7753

V, (GeCl_4 , SiCl_4 , GeHCl_3 , GeDCl_3 ,
 SiHCl_3 , SiDCl_3)

Freeman D.E., Wilson, M.K.

J. phys. Chem., (BRD), 1962, 35, w4-6, 335-34.
 (ann).

The inclusion of intramolecular
 tension in certain simple valence force
 fields. SiCl_4

10

Proc 9ms, 1963, 9D 66.

1962

8497

SiH_3F , SiD_3F , SiH_3Cl , SiD_3Cl , SiH_3J , SiD_3J
(mol. konst., t.d.f.)

Nagarajan G.

J. Scient. and Industr. Res. 1962,

B21, N 10, 463-467

Potential constants and ...

Re



SiClD₃

1963

9667

HSiCl_2 , DSiCl_2 , HSiBr , (mol. post.)

Herzberg G., Verna R.D.
Sympos. Molec. Struct. and Spectrosc.,
Columbus, 1963, Columbus, Ohio, s.a.
49-50

Spectra of the free...

J

M759

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

Frequenc_y shifts from gas...

J

PX, 1966, 2 101

orig.

CONFIDENTIAL

CH_3F , CD_3F , SiH_3F , SiD_3F (cyclic mon.)

X = F, Cl, Br, J, CH_3Cl , CD_3Cl , SiH_3Cl , SiD_3Cl ,
 CH_3Br , CD_3Br , SiH_3Br , SiH_3J , SiD_3J , SiD_3Br ,
 CH_3J , CD_3J

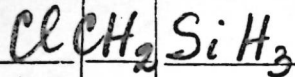
Pulay P., Torok F.

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

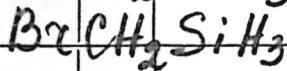
Parameter form of matrix F. II. Assignment
with the aid the parameter form (short
communication)

F

1973.



Ohno Kiichi

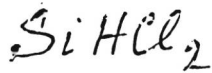
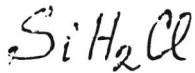


et al.

Ji; cur. no. i

J. Sci. Hiroshima Univ.
Ser. A; 1973, n. 2
345-56

(cur. BrCH₂BeH₃; III)



(м.н.)

Витам М 2 У

1974

исследования термодина-
мические свойства проме-
жуточные продуктов высоки
температурных р-ций

отв. Фусин А.Д.

Коттев Т.С.

SiHCl_2

1974.
Руденко А.Р.; Контев Т.С.,
и др.

(м.н)

Отчет Хим. гр-та МГУ
за 1973-74г по готов.

N 74/154, между
Хим. гр-том и ГИИХ.

Исследование термоз. св-в
промежуточных продуктов в широком
температ. диапазоне

1974.

SiH_2Cl

Русин А.Д., Контев Т.С.

и др.

Отчет Лим. ф-та ИТУ
за 1973-74 г., дог. 74/154
между Лим. ф-том и ГИИХ.

(м.п.)

стр 19

Исследования термод. св-в
происходят. ● продукты
высоко-темн. р-ции

SiH_2Cl

Яковлев О.П.

1977

и.п.
номер

Автоматизированная
система на базе
учебной программы КХН

термодинам. анализ и
переходов - равновесия...

MSiC

Оммуек 12815

1981

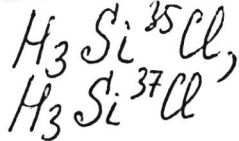
обзор,
теории.
расши.
молеку.
орбитали,
электроны

Bohm M. P., Gleiter R.

Theor. chim. acta, 1981,

59 (2), 153 - 179.

1981



Vi, m.n.

12 Д491. Колебательные спектры и силовые постоянные симметричных волчков: вращательный анализ полос ν_2 и $2\nu_3$ молекул $\text{H}_3\text{Si}^{35}\text{Cl}$ и $\text{H}_3\text{Si}^{37}\text{Cl}$. Vibrational spectra and force constants of symmetric tops: rotational analysis of ν_3 and $2\nu_3$ of $\text{H}_3\text{Si}^{35}\text{Cl}$ and $\text{H}_3\text{Si}^{37}\text{Cl}$. Bürger H., Cichon J., Dobos S., Eujen R., Schulz P., Ruoff H. «J. Mol. Spectrosc.», 1981, 86, № 2, 298—309 (англ.)

С помощью фурье-спектрометра исследованы спектры ИК-поглощения H_3SiCl в газообразной фазе в области колебательно-вращательных полос ν_3 и $2\nu_3$. (550 и 1100 см^{-1}). Измерения проведены с разрешением $0,04 \text{ см}^{-1}$ на образцах естественного состава и образцах, обогащенных изотопом ^{35}Cl . Обнаружены «горячие» полосы, обусловленные переходами с возбужденных колебательных уровней ν_3 и ν_6 , а также тонкая структура, связанная с изотопами ^{28}Si , ^{29}Si , ^{30}Si , ^{35}Cl и ^{37}Cl . Определены значения молекулярных вращательных постоянных.

фр. 1981, 18, N 12.

SiH_3Cl^-

1981

Clark Timothy

J. Chem. Soc. Chem.

(4E, D₀) Commun.; 1981, N 11,
575-576.

(an. CH_3F^- ; $\bar{\Gamma}$)

$(SiH_3Cl)^+$, $(SiCl_3H)^+$, $(SiCl_3F)^+$ 1981

$(SiH_2Cl_2)^+$ Glidewell Ch.

$(SiCl_2H_2)^+$ * THEOCHEM 1981,

SiH_3Cl
структура,
кв. мех.
расшир.

2(1-2), 87-98.

●
(см. $(SiH_4)^+$; III)

Оммуек 12784

Cl_2SiH_2

1981

Cl_3SiH

Нордман В.Ч. и др.

мех.
кв. ~~кв.~~
расчет.

Всесен. ЛТУ. Химия,
1981, 22, № 6, 602-604.

(сер. $(\text{CH}_3)_3\text{SiH}$; III)

SiHCl_3

[Dmmuck 12908] 1981

crkmp
& mampuse

Miller F.H., Andrews L.

Vi

J. Mol. Struct., 1981,
77, 65-73

Хлорсиланы

1982

/ 97: 30621y Spectroscopic properties of chlorosilanes. Dernova, V. S.; Kovalev, I. F. (USSR). *Spektroskopich. Svoistva Soedin. Elementov IV B Gruppy, Saratov* 1981, 3-10 (Russ). From *Ref. Zh., Khim.* 1982, Abstr. No. 8B212. Title only translated.

Чекмп

C.A. 1982, 97, N4

SiCl_3OH

1982

9 Д503. Реакции атомов кислорода с SiHCl_3 в твердом аргоне. ИК-спектр SiCl_3OH . Oxygen atom reactions with SiHCl_3 in solid argon: the infrared spectrum of SiCl_3OH . Shirk Amy E., Shirk James S. «J. Mol. Spectrosc.», 1982, 92, № 1, 218—228 (англ.) |

Показано, что основным продуктом реакций при УФ-фотолизе (излучением ртутной лампы) смеси $\text{SiHCl}_3/\text{O}_3$ и ВУФ-фотолизе (излучением H_2 -лампы) смеси $\text{SiHCl}_3/\text{O}_2$ в Ar -матрице является SiCl_3OH . Получены ИК-спектры нормальных и изотопзамещенных молекул SiCl_3OH , и построено обобщенное силовое поле.

спектр,
сил. поле.

ф. 1982, 18; и 9

кулы SiCl_3OH для модели симметрии C_s и обобщенного валентного силового поля. Сделан вывод, что SiCl_3OH является главной водородсодержащей примесью в SiCl_4 в процессе изготовления оптич. волокна.

А. Н. Курский

SiHCl₂

1983

99: 166165b High vibrational overtones in trichlorosilane and dichlorosilane. Bernheim, R. A.; Lampe, F. W.; O'Keefe, J. F.; Qualey, J. R., III (152 Davey Laboratory, Pennsylvania State Univ., University Park, PA 16802 USA). *Chem. Phys. Lett.* 1983, 100(1), 45-50 (Eng). The absorption spectra at 12,000-18,000 cm⁻¹ were recorded for gaseous SiHCl₃ and SiH₂Cl₂ by using intracavity photoacoustic detection and dye lasers. The obsd. transitions correspond to the $\Delta\nu = 6, 7, 8$ and 9 overtones of the Si-H stretch and are adequately interpreted in terms of a local mode description of the vibration.

M. Crexmyr

~~1~~(7) SiH₂Cl₂

c. A. 1983, 99, N20

$\text{SiH}_4\text{-xCl}_x$

(OM-20554)

1984

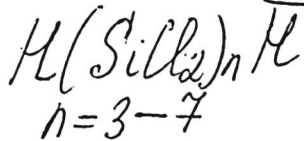
Aron J., Bunnell J., Ford
T. A.,

men.

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

[Am. 18388]

1984



Hengge E.; Mixtaub;

mac-camp.

Z. anorg. und allg.
Chem.; 1984, 508, N1,
43 - 49.



1984

9 Б4629. Кинетическое и термодинамическое исследование химического осаждения из паровой фазы и из плазмы в системе SiCl_4/H_2 . Reaktionskinetische und thermodynamische Untersuchungen zur Mederdruck- und Plasma-CVD aus dem System SiCl_4/H_2 . Klaus M., Hecht G., Cebulla H., Weißmantel Chr. «Beitr. 8. Tag. Hochvac., Grenzflächen/Dünne Schichten, Dresden, 5—7 März, 1984. Bd 2». S. 1., s. a., 311—314 (нем.)

Проведены термодинамич. расчеты состава системы $\text{SiCl}_4 + \text{H}_2$ при t -ре 1000 К ($\text{Cl}/\text{H} = 0,1$) и 1300 К ($\text{Cl}/\text{H} = 0,01$) в диапазоне давл. $10^2 \div 10^5$ Па. Даны равновесные конц-ии H_2 , SiCl_4 , SiHCl_3 , SiH_2Cl_2 , SiH_3Cl , SiH_4 , SiCl_3 , SiCl_2 , SiCl , Cl . Приведены эксперименты по получению Пл аморф. кремния в системе $\text{SiCl}_4 + 3,5\% \text{H}_2$ при давл. 1,33 кПа в ВЧ-разряде и без него. Измерены скорости роста Пл в таких условиях и получены их зависимости от t -ры. Проведено сравнение с расчетом.

Ю. А. Лебедев

термодин.
расчет
состава

х. 1986, 19, №9

$\text{SiH}_4 - \text{HCl}$

1984

6 Л327. ИК-лазерная фотохимия смеси $\text{SiH}_4 - \text{HCl}$.

Infrared laser photochemistry of $\text{SiH}_4 - \text{HCl}$ mixtures.

Moore C. B., Biedrzycki J., Lampe F. W. «J. Amer. Chem. Soc.», 1984, 106, № 25, 7761—7765 (англ.)

В диапазонах давлений газов 28—60 Тор и т-р 295—414 К изучено фотохимич. поведение смеси SiH_4 с HCl под действием ИК-излучения лазера на CO_2 ($\lambda_{\text{возб.}} = 10,6$ мкм). В качестве газообразных продуктов фотолиза такой системы обнаружены H_2 , Si_2H_6 , SiH_3Cl , SiH_2Cl_2 и SiHCl_3 , а также следы Si_3H_8 и $\text{Si}_2\text{H}_5\text{Cl}$. Фотолиз смеси $\text{SiH}_4 - \text{HCl}$ приводил также к образованию твердых фотопродуктов, содержащих Si, H и Cl. Рассмотрены возможные механизмы фотолиза смеси. Предположено, что его первичной реакцией является фоторазложение SiH_4 на SiH_2 и H_2 , за которым следует конкурирующее взаимодействие SiH_4 и HCl с молекулами SiH_2 . Библ. 23.

Т. А. Ш.

Ф. 1985, 18, № 6.

SiH_4Cl_4

1985

Ho P., Coltrin M. E.,
et al.

u. n. J. Phys. Chem., 1985,
89, n 21, 4647-4657.

(cur.  SiH_n ($n=1,2,3,4$)) III

$\text{Cl}_3\text{Si}-\text{SiCl}_3$ деп. 22296 1985

и гр. Stölevik R., Bakken P.

реценз.
структ.,
ссыл. посыл.,
во;

J. Mol. Struct., 1985,
124, N1-2, Suppl.:
Theochem., 25, N1-2,
133-142.

(ссыл. $\text{F}_3\text{Si}-\text{SiF}_3$; III)

SiHCl_3

[om 26267]

1986

Smith J. F.,

(yb cnekmp)

J. Mol. Spectrosc.,
1986, 120, N1, 110-117.

$\text{Si}^{35}\text{Cl}_3\text{H}$

(Om. 26288)

1987

Carpenter J.H., Smith J.B.,

mm-wave
wave spectrum J. Mol. Spectrosc., 1987, 121,
N2, 270-277.

Analysis of the Quadrupole
Coupling in the Millimeter-Wave
Spectrum of Trichlorosilane.

SiH_2DCl
 $SiHD_2Cl$

ser. 28100 1987

Weaving J. S.,
Ford T. A.

J. Mol. Spect.,
1987, 161, 245-
● - 264.

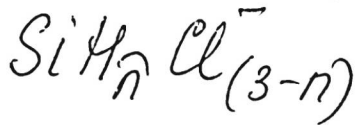
колебаний.
волновое
число,
теор. расчёт,
распредел.
потенц.
функции

1988

$D_3 SiCl$ Thiel Walter,
Yamaguchi Yukio, et al.

Chem.
noceir., *J. Mol. Spectrosc.* 1988,
ser. n. 132(1), 193-206.

(^{29}Si $H_3 SiF$; III)

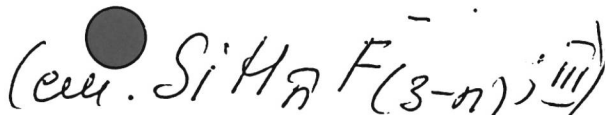


1990

Hopkinson A.C.,
Rodríguez C. F. et al.

Can. J. Chem. 1990,
68 (8), 1309-16.

расчёт
сверхжидк.



$H_3SiCl_2SiH_3$
 $H_3SiCl_2SiCl_3$ Jericho A.,

1992

список а Monatsk. Chem. 1992,
и соединений, 123 (1-2), 17-24.
ab initio
расчет

(all. $H_3Si \bullet F_2SiH_2$, III)

SiH_2Cl

1992

Rodriguez C. F.

Hopkinson A. C.

(He)

Can. J. Chem. 1992,
70 (8), 2234 - 40.

(see SiH_3 ; 11)



1993

Bonazzola L.,
Michael J. P. et al.

JCP,
New. J. Chem. 1993,
ссылка. 17(4), 271-4.

(ссыл.  $\text{Cl}_3\text{SiSiCl}_3$; III)

Si₂H₅Cl

1993

119: 109469w Vibrational spectra in the ν (silicon-hydrogen) and ν (SiD) regions of chloro and bromodisilanes and ab initio geometry studies of chloroethane, chlorodisilane and dichlorodisilane. McKean, D. C.; McPhail, A. L.; Edwards, H. G. M.; Lewis, I. R.; Mastryukov, V. S.; Boggs, J. E. (Dep. Chem., Univ. Aberdeen, Aberdeen, UK AB9 2UE). *Spectrochim. Acta, Part A* 1993, 49A(8), 1079-94 (Eng). IR measurements in the gas phase are reported for the ν (SiH) and ν (SiD) regions of Si₂H₅X, Si₂D₅X, 1,1-Si₂H₄X₂ and 1,1-Si₂D₄X₂ species where X = Cl, Br. Incomplete Raman data were also obtained. All three possible isolated SiH stretching frequencies are obsd. in the spectra of the Si₂D₄X₂ samples but only two from the Si₂D₅X ones. The missing ν (SiH) values are obtained by use of the frequency sum rule, and by harmonic local mode force field treatments of all the available ν (SiH) and ν (SiD) data, using a procedure previously tested on disilane. Ab initio calcns. of the geometries of C₂H₅Cl, Si₂H₅Cl and 1,1-Si₂H₄Cl₂ using the 6-31G* basis set are reported. Trends in r_e (CH) or r_e (SiH) values reflect trends in ν (CH) or ν (SiH) ones. The alpha, trans and

(UK)

Δ

④ Si₂H₅Br

C.A. 1993, 119, N 16

gauche effects of halogen are similar in CH and SiH compds., although smaller in the latter. In both cases, ab initio calcs. predict larger effects than are obsd. in the spectra, esp. for the α effect of halogen. A kinetic isotope effect in the halogenation of disilane may occur. Reassignment of earlier spectra of disilyl iodide species is proposed.

$\text{SiH}_{5-n}\text{Cl}_n^-$

(DM-37531)

1994

$n=0-5$ Windus T.H., Gordon M.S.,
et al.,

ab initio g. Amer. Chem. Soc.,
paper 1994, 116, 3568-3579.

Theoretical study of
Pseudorotation of  Pentacoordi-

rated Silicon Anions: $\text{SiH}_{5-n}\text{X}_n^-$
(X = F, Cl)

SiH₄·HCl

1995

Govender, M.B.; Ford T.A.,

ab initio
pacem THEOCHEM 1995, 338,

141-53

(all.

● CH₄·HF; III)

Si H₄ · HCl

1995

Goverder, Maganthran &
et al.,

ad initio
pacem
CMP-PC,
CMAC with
M. Cb-PA

S. Adv. J. Chem.,
1995, 48 (34), 98-107;

(all. ● CH₄ · HF; III.)

1995

F: Si-H-Cl

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.

РМХ 1997

Si₂H₅Cl

1995

⊕ 19B1233. ИК-спектры поглощения и спектры комбинационного рассеяния моноклор- и монобромдисиланов, масштабированное неэмпирическое силовое поле, интенсивности, атомные полярные тензоры и эффективные заряды для Si₂H₅Cl. Infrared and Raman spectra of monochloro- and monobromodisilanes, a scaled ab initio force field, intensities, atomic polar tensors and effective charges for Si₂H₅Cl / McKean D. C., McPhail A. L., Edwards H. G. M., Lewis I. R., Murphy W. F., Mastryukov V. S., Boggs J. E. // Spectrochim. acta. A.— 1995.— 51, № 2.— С. 215-235.— Англ.

Исследованы ИК-спектры поглощения и спектры КР Si₂H₅Cl (I), Si₂D₅Cl (II), Si₂H₅Br (III) и Si₂D₅Br (IV),

X. 1997, № 19

для I проведены измерения абс. интенсивностей ИК-полос. Предложена интерпретация спектров I—IV, идентифицированы фундаментальные колебания, составные полосы и обертоны. Выполнен неэмпирич. квантово-механич. расчет для I на теор. уровне ХФ/6-31ГФ*, оптимизирована геометрия и рассчитано гармонич. силовое поле. С использованием данных для II, а также включением спектральных данных для колебаний $\nu(\text{SiH})$ для III—IV рассчитан набор из 14 масштабирующих множителей, обсуждены различия между первоначальными и масштабированными результатами.

Г. М. Курамшина

$\text{Si}_2\text{H}_5\text{Cl}$
 $\text{Si}_2\text{D}_5\text{Cl}$

UK, CLP,
CML, NOCM,
Pi

(H)IX

C. A. 1995, 122, N 16.

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

1995
122: 199817n Infrared and Raman spectra of monochloro- and monobromodisilanes, a scaled ab initio force field, intensities, atomic polar tensors and effective charges for $\text{Si}_2\text{H}_5\text{Cl}$. McKean, D. C.; McPhail, A. L.; Edwards, H. G. M.; Lewis, I. R.; Murphy, W. F.; Mastryukov, V. S.; Boggs, J. E. (Chem. Dep., Aberdeen Univ., Aberdeen, UK AB9 2UE). *Spectrochim. Acta, Part A* 1995, 51A(2), 215-35 (Eng). IR and Raman spectra are reported for $\text{Si}_2\text{H}_5\text{Cl}$, $\text{Si}_2\text{D}_5\text{Cl}$, $\text{Si}_2\text{H}_5\text{Br}$ and $\text{Si}_2\text{D}_5\text{Br}$. These include approx. IR intensities for $\text{Si}_2\text{H}_5\text{Cl}$. All the fundamentals of the chloro compds., except the torsion, are securely assigned, and nearly all those of the bromo ones. The force field and spectral intensities of $\text{Si}_2\text{H}_5\text{Cl}$ were calcd. ab initio using a 6-31G* basis set, and the force field scaled to fit the d_0 , d_5 and V°SiH data, using 14 independent scale factors. Significant changes in normal coordinate occur on scaling. The SiH stretching part of this force field agrees well with an earlier harmonic local mode force field, although differences occur in the normal coordinates. The 6-31G* at. polar tensors for the H and Cl atoms indicate that the dipole derivs. for the SiH and SiCl bonds lie close to the bond directions. Both H and Cl atoms behave as if neg. charged in all motions. Comparisons of νSiH intensities and frequencies, effective charges and Mulliken at. charges are made across the series SiH_4 - Si_2H_6 - $\text{Si}_2\text{H}_5\text{Cl}$. These identify significant effects by Cl on the gauche SiH bond, but virtually none on the trans one.

Si₂H₄Cl₂
Si₂D₄Cl₂

1995

124: 130090u Infrared and Raman spectra of 1,1-dichlorodisilane species: a scaled ab initio force field, atomic polar tensors, dipole derivatives and atomic charges. McKean, D. C.; Edwards, H. G. M.; Lewis, I. R.; Murphy, W. F.; Mastryukov, Vladimir S.; Boggs, James E. (Chemistry Dep., Univ. Edinburgh, Edinburgh, UK EH9 3JJ). *Spectrochim. Acta, Part A* 1995, 51A(13), 2237-47 (Eng). IR and Raman spectra are reported for 1,1-Si₂H₄Cl₂ and 1,1-Si₂D₄Cl₂. All fundamentals except the silyl torsion are firmly assigned. A scaled ab initio force field is calcd. at the HF/6-31G* level, embodying eleven scale factors. Calcd. IR and Raman intensities, at. polar tensors, King effective and Mulliken at. charges are all listed. These confirm the α and β effects on SiH bonds of Cl substitution found earlier in Si₂H₅Cl. SiH bonds gauche to Cl become more polar (SiH⁻), while those in trans positions remain unaffected. Torsional structure obsd. in the ν SiH region may permit the anal. of torsional levels and provide an est. of barrier height.

(UK, CKP)
Gul. NOCM,
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C.A. 1996, 124, N 10

1996

Si₂H₄Cl₂
 Si₂H₅Cl
 Si₂H₃Cl₃
 Si₂H₂Cl₄

UK CRYST,
 Si-H

C. A. 1996, 124, N 18

124: 245203a SiH stretching frequencies in chlorodisilanes and (ab initio calculations of geometry, stretching frequency, vibrational intensity and Mulliken and King effective atomic charges. McKean, D. C.; Palmer, M. H.; Guest, M. F. (Department of Chemistry, University of Edinburgh, West Mains Road, Edinburgh, UK EH9 3JJ). *J. Mol. Struct.* 1996, 376, 289-303 (Eng). IR frequencies in the ν SiH region obsd. in mixts. of chlorodisilanes are assigned by the joint use of substituent effects, detd. earlier in Si₂H₃Cl and 1,1-Si₂H₄Cl₂, and ab initio calcs. for 1,2-Si₂H₄Cl₂, 1,1,2-Si₂H₃Cl₃ and SiH₃SiCl₃, which together with 1,1,2,2-Si₂H₂Cl₄ were identified as being present. ν SiH frequencies for all the staggered conformers are predicted using harmonic local mode theory. Ab initio geometries were obtained for the >3 compds. at the HF/6-31G* level, and for both conformers of 1,2-Si₂H₄Cl₂ at HF/tzvp and MP2/tzvp levels. Alpha or gauche Cl substitution shortens both SiH and SiCl bonds, the former reflecting ν SiH changes. Trans Cl substitution shortens SiCl bonds slightly, but has no effect on SiH bonds. The local mode behavior of ν SiH vibrations extends to both IR and Raman intensities. Ab initio-based at. polar tensors are used to obtain dipole derivs., $d\mu/dr$, for the SiH and SiCl bonds and King effective at. charges, ξ , for all atoms. The changes in the latter are compared with changes in the Mulliken at. charges and a close connection is found in the case of gauche Cl substitution.

Si₂H₄Cl₂
Si₂H₅Cl
Si₂H₃Cl₃
~~Si₂H₄Cl₂~~

~~ab initio~~

ab initio
param

C.A. 1996, 124, 18

1996
(124: 245204b) Ab initio calculations of vibrational properties and conformer stabilities in 1,2-Si₂H₄Cl₂, 1,1,2-Si₂H₃Cl₃ and 1,1,1-Si₂H₃Cl₃, and comparisons with observed infrared and Raman spectra. McKean, D. C.; Palmer, M. H.; Edwards, H. G. M.; Lewis, I. R.; Guest, M. F. (Chemistry Department, University of Edinburgh, West Mains Road, Edinburgh, UK EH9 3JJ). *J. Mol. Struct.* 1996, 376, 305-15 (Eng). Ab initio calcs. of vibration frequencies and intensities were made for 1,2-Si₂H₄Cl₂ (conformers 12G, 12T), 1,1,2-Si₂H₃Cl₃ (conformers 112C₅, 112C₁) and 1,1,1-Si₂H₃Cl₃ (111), at an HF/6-31G* level. Energies and abundances of both conformers were obtained for 12 and 112 at this level, and for 12 also at HF/tzvp, MP2/6-31G* and MP2/tzvp levels. Similar energies are also reported for 1,2-Si₂H₄F₂ at HF/6-31G* and HF/tzvp levels. A simple method of scaling the HF/6-31G* frequencies permits assignment of a no. of bands obsd. in the IR and Raman spectra of 1,2-Si₂H₄Cl₂, and of a few in IR spectra of 112 and 111. Positions of unobserved bands are predicted to within an expected accuracy of ≈10 cm⁻¹. The T conformer is slightly more stable than the G 1 in both 1,2-dichloro and 1,2-difluoro compds., unlike the situation in the corresponding haloethanes. However, the relative stability of the 12G and 12T conformers is somewhat sensitive to basis set and level of treatment. The best est. for the abundance X(G) of 12G is ≈0.6, in rough agreement with obsd. spectra. For the 112C₁ conformer, an HF/6-31G* calcn. gives X(C₁) ≈0.9, a likely upper limit.

1998

 $\text{Si}_2\text{H}_n\text{Cl}_{4-n}$ моф. продукт
структур, Di
и стабильн.C.A. 1998,
128, N10

128: 119829d Ab Initio Molecular Orbital Study of the Thermochemistry and Reactions of the Chlorinated Disilenes and Their Isomers ($\text{Si}_2\text{H}_n\text{Cl}_{4-n}$). Swihart, Mark T.; Carr, Robert W. (Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455 USA). *J. Phys. Chem. A* 1998, 102(4), 785-792 (Eng), American Chemical Society. Structures, vibrational frequencies, and energies for the chlorinated disilenes, their dibridged isomers, and the transition states connecting the chlorinated disilenes to the corresponding silylsilylenes are presented. Geometries and frequencies were obtained at the MP2/6-31G(d,p) level, and energetics were calcd. at the G2, G2(MP2), MP4/6-31+G(2df,p), and/or MP2/6-31+G(2df,p) levels of theory, depending on the no. of chlorine atoms in the mol. The silylsilylene isomer with the structure $\text{H}_n\text{Cl}_{3-n}\text{SiSiCl}$ was found to be lowest in energy for all of the chlorinated compds. The dibridged structures are all significantly higher in energy than the silylsilylene and disilene structures. Barriers for isomerization by H transfer and Cl transfer ranged from 5-18 kcal/mol and 9-23 kcal/mol above the disilene, resp. Energies along paths for decompn. of the chlorinated disilenes to pairs of silylenes are presented, confirming that the reverse reactions are barrierless. Finally, energetics of various decompn. products of the $\text{Si}_2\text{H}_n\text{Cl}_{4-n}$ compds. are considered. It is shown that for the species with two or more chlorines, decompn. to a pair of silylenes should be the dominant reaction path based on the energetics of competing paths. The isomerization barriers are much smaller than decompn. barriers, so the isomerization reactions will be fast compared to decompn.

ClSiH_2

1998

Feshin V.P., Kon'shin, M.Yu.,

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J. Gen. Chem. 1998, 68(3),
411-413.

$(\text{Cu} \cdot \text{ClSi} \bullet (\text{CH}_3)_3; \text{III})$

F: Cl₂HSi-SiHCl₂

P: 3

DM 39923

1993

131:248508 1,1,2,2-Tetrachlorodisilane (Cl₂HSi-SiHCl₂): molecular structure conformation and torsional potential as determined by gas-phase electron diffraction, vibrational spectroscopic data and ab initio molecular orbit calculations. Johansen, T. H.;
Hagen, K.; Stolevik, R. NTNU, Department o
Chemistry, Norwegian University of Science and
Technology Trondheim N-703 Norway J. Mol. Struct.,
485-486, 121-133 (English) 1999 The mol.
structure, conformational compn. and torsional potential
of 1,1,2,2-tetrachlorodisilane (TCDS), Cl₂HSi-SiHCl₂,
were studied using gas electron diffraction (GED) data
at 23.degree.C, together with earlier rec spectroscopic
data and normal coordinate and ab initio MO calcns. The
ti compd. exists in the gas phase at room temp. as a

mixt. of two conformers with a torsion angle
 $\phi(\text{HSiSiH}) = 180^\circ$, and gauche, with a torsion
 angle $\phi(\text{HSiSiH}) \approx 60^\circ$. The gauche
 conformer predominates, occupying approx. 80% of the gas
 compn. at 23°C . Some structural parameter values
 obtained from the GED refinements, using results from the
 earlier spectroscopic work and ab initio MO calcns. as
 constraints, are as follows (gauche conformer with estd.
 2-sigma uncertainties): bond length $r(\text{Si-Si}) = 2.310(8)$
 Å, $r(\text{Si-Cl}) = 2.039(2)$ Å (av. value
 $r(\text{Si-H}) = 1.511$ Å (assumed value). Bond angles
 (α): $\angle(\text{SiSiCl}) = 108.9(4)^\circ$ (av. value), $\angle(\text{ClSiSiH}) =$
 $109.7(3)^\circ$, $\angle(\text{SiSiH}) = 111.5^\circ$ (assumed
 value).

F: HClSi₂

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 substituted disilynes a their isomers HYSi₂ and Y₂Si₂ (Y = F, Cl, Br, Li).
The effect of substit 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 disilenyldiene structures and double-bridged structures have the lowest energy and can be experimentally detectable, while the classical linear structures have high energy and are thus unstable.

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[Om. 41304]

2002

Vazquez J. et al.,

Trans.

Proc.

Chem.

J. Phys. Chem. 2002,
A106, N17, 4429-34.

Trans. Chem.

Theoretical

the structure and
spectrum of

Investigation of
Vibrational
the

Electronic Ground State
 $\tilde{X}(1A')$ of HCl.

LiHCl_3

(DM 41862)

2003

ab initio
pacem

Ling-Ling Zheng et al.,
Nat. Phys., 2003, 101,
N8, 1185-70.

An ab initio anharmonic
force field of LiHCl_3