Si-H-Cl

7577

1936

(AsH_3; AsD_3; $DSiCl_3$; $DSiBr_3$)

Delfosse J.M.
Nature 1936, 137, 868

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

C.A., 1936, 5498[6]

$SiCl_3D$ 1

p

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

$SiClD_3$

1954

5822

SiD_3Cl, SiH_3F, SiD_3F ( )

Andersen F.A., Bak B.
Acta chem.scand., 1954, 8, 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 ( )

Kerrem C., Polo S.R., Wilson M.K.
Spectrochim.acta., 1959, N 10, 793-99

Infrared spectrum...

J

$SiClD_3$

7753

1962

ν_i ($GeCl_4$, $SiCl_4$, $GeHCl_3$, $GeDCl_3$, $SiHCl_3$, $SiDCl_3$)

Freeman D.E., Wilson M.K.

J. phys. chem., (BRD), 1962, 35, N 4-6, 385-39
(aus)

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

$SiCl_3D$

10

Proc Phys, 1963, 9066.

8497

1962

SiH_3F, SiD_3F, SiH_3Cl, SiD_2Cl_2, SiH_3J, SiD_3J

(mol.konst., t.d.f.)

Negarajan C.

J.Scient.and Industr.Res. 1962,
B21, N 10, 463-467

Potential constants and ...

Ne

$SiCl_2D_3$

1963

9667

HSiCl, DSiCl, HSiBr, (mol.past.)

Herzberg G., Verma 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; ( )

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.

M 1191

1966

CH_3F, CD_3F, SiH_3F, SiD_3F (Matrix 100°K.)

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

J

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

1973.

$ClCH_2SiH_3$ Ohno Kiichi
$BrCH_2SiH_3$ et al.

Vibr. spectra" J. Sci. Hiroshima Univ. Ser. A; 1973, v 2 345-56

(cm. $BrCH_2GeH_3$; III)

SiH_2Cl
$SiHCl_2$

(II, VI)

Отчет И 29 1974

Исследование термодинамические свойств промежуточных продуктов высокотемпературных р-ций

отв. Фуфин А.Д.
Коптев Т.С.

1974.

$SiHCl_2$

Рудин А.Р., Контев Т.С., и др.

(м.н)

Отчет Хим. ф-та МГУ за 1973-74 г по договор. № 74/154, между Хим. ф-том и ГИИХ. Исследование термод. св-в промежуточ. продуктов высоко температ. р-ций

1974.

SiH_2Cl		Русина А.Р., Коптев Т.С. и др.
		Отчет Хим. ф-та МГУ за 1973-74 г., договор 74/154
(м.п)		между хим. ф-том и ГИИХ. стр 19
		Исследование теплоз. св-в пром. продуктов высоко-хим. р-ций

SiH_2Cl Яковлев О.П. 1977

Автореферат диссертации на соиск. ученой степени к.х.н.

м.п

номер

Термодин. анализ и исследов. равновесий..

MSiCl | оттиск 12815 | 1981

обзор, теорий. расчий. молекул. орбиталей, геометрий

Bohm M.C., Gleiter R.

Theor. chim. acta, 1981, 59 (2), 153 – 179.

$H_3Si^{35}Cl$,
$H_3Si^{37}Cl$

1981

Vi, M·N;

12 Д491. Колебательные спектры и силовые постоянные симметричных волчков: вращательный анализ полос ν_2 и $2\nu_3$ молекул $H_3Si^{35}Cl$ и $H_3Si^{37}Cl$. Vibrational spectra and force constants of symmetric tops: rotational analysis of ν_3 and $2\nu_3$ of $H_3Si^{35}Cl$ and $H_3Si^{37}Cl$. 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 $см^{-1}$ 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.

Ф. 1981, 18, N 12.

SiH_3Cl^-

1981

Clark Timothy

J. Chem. Soc. Chem.

(AE, Do) Commun.; 1981, N 11,

575-576.

(сеч. CH_3F^-; I)

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

$(SiH_2Cl_2)^+$,

$(SiCl_2H_2)^+$

SiH_3Cl

структура,

кв. мех.

расчёт.

Glidewell Ch.

THEOCHEM 1981,

2 (1-2), 87-98.

Отпуск 12784

(см. $(SiH_4)^+$; III)

Cl_2SiH_2
Cl_3SiH

1981

Логгин В.И. и др.
Вестн. МГУ. Химия,
1981, 22, №6, 602-604.

кв. мех. ~~хим.~~ расчет.

(см. $(CH_3)_3SiH$; III)

$SiHCl_3$ | Оттиск 12908 | 1981

спектр в матрице

Di

Miller F.H., Andrews L.,
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.

Спектр

C.A. 1982, 97, N 4

$SiCl_3OH$

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 $SiHCl_3/O_3$ и ВУФ-фотолизе (излучением H_2-лампы) смеси $SiHCl_3/O_2$ в Ar-матрице является $SiCl_3OH$. Получены ИК-спектры нормальных и изотопзамещенных молекул $SiCl_3OH$, и построено обобщенное силовое поле.

спектр, сил. по ст.

ф. 1982, 18; 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

$SiHCl_2$

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 $SiHCl_3$ and SiH_2Cl_2 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.

Н. спектр

(X) (A) SiH_2Cl_2

C.A. 1983, 99, N20

$SiH_{4-x}Cl_x$ (ОП. 20554) 1984

Aron J., Burnell J., Ford T. A.,

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

Оп. 18388 1984

$H(SiCl_2)_n H$
$n = 3-7$

Hengge E., Mixlauß.,
Z. anorg. und allg.
Chem., 1984, 508, N1,
43 – 49.

масс-спектр.

$SiCl_4 + H_2$

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. l., s. a., 311—314 (нем.)

термодин. расчеты состава

Проведены термодинамич. расчеты состава системы $SiCl_4+H_2$ при т-ре 1000 К (Cl/H=0,1) и 1300 К (Cl/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 $SiCl_4+3{,}5\%$ 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 т-ры. Проведено сравнение с расчетом.

Ю. А. Лебедев

Х. 1986, 19, №9

$SiH_4 - HCl$ 1984

6 Л327. **ИК-лазерная фотохимия смеси SiH_4—HCl.** Infrared laser photochemistry of SiH_4—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 ($\lambda_{возб.}$ = = 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 Si_2H_5Cl. Фотолиз смеси SiH_4—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, N 6.

Si Hy Cly

1985

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

M. n.

J. Phys. Chem., 1985,
89, N 21, 4647-4657.

(см. SiH_n (n=1,2,3,4)) III

$Cl_3Si-SiCl_3$ Дел. 22296 1985

М Гр. Stölevik R., Bakken P.

геометр.,
спрукт.,
сп. носит.,
Но;

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

(см. $F_3Si-SiF_3$; III)

$SiHCl_3$ | ом 26267 | 1986

Smith J.C.,

(ув спектр) J. Mol. Spectrosc.,
1986, 120, N1, 110-117.

$Si^{35}Cl_3H$ (Dm. 26288) 1987

Carpenter J.H., Smith J.G.,

ли-волно вой спектр J. Mol. Spectrosc., 1987, 121, N2, 270-277.

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

SiH_2Cl_2
$SiHCl_3$

оиг. 28100

1987

Weaving J. S.,
Ford T. A.
J. Mol. Struct.,
1987, 161, 245–
– 264.

колебан.
волновые
числа,
теор. расчёт,
распредел.
потенц.
энергии

D_3SiCl 1988

Thiel Walter,
Yamaguchi Yukio, et al.

Спектр. исслед., м. п.

J. Mol. Spectrosc. 1988, 132 (1), 193–206.

(спектр H_3SiF; III)

$SiH_nCl^-_{(3-n)}$

1990

Hopkinson A.C.,
Rodriquez C.F. et al.
Can. J. Chem. 1990,
68 (8), 1309-16.

расчёт
структур.

(см. $SiH_nF^-_{(3-n)}$; III)

$H_3SiCl_2SiH_3$
$H_3SiCl_2SiCl_3$ Jenicher A., 1992

спектры Monatsh. Chem. 1992,
и свойства, 123 (1-2), 17-24.
de cristo
racem

(cell. H_3Si ● F_2SiH_2, III)

SiH_2Cl 1992

Rodriquez C. F.
Hopkinson A. C.

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

(see SiH_3; II)

$HSiCl_3^-$ 1993

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

ЭСР, New. J. Chem. 1993,
спектрум. 17(4), 271-4.

(спец. $Cl_3SiSiCl_3^-$, III)

Si_2H_5Cl

1993

119: 169469w **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 Si_2H_5X, Si_2D_5X, 1,1-$Si_2H_4X_2$ and 1,1-$Si_2D_4X_2$ 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 $Si_2D_4X_2$ samples but only two from the Si_2D_5X 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 C_2H_5Cl, Si_2H_5Cl and 1,1-$Si_2H_4Cl_2$ 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)

(H) Si_2H_5Br

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 calcns. 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.

$H_n SiCl^+$ 1994

Sana M., Decrem M., et al.

$\Delta_f H$, структ., теор. расчёт

J. Chem. Soc., Faraday Trans. 1994, 90 (23), 3505-11.

(см. $H_n SiN^+$; III)

$SiH_{5-n}Cl_n^-$ (DM · 37531) 1994

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

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

Theoretical Study of Pseudorotation of ● Pentacoordi-

nated Silicon Anions: $SiH_{5-n}X_n^-$
(X = F, Cl)

$SiH_4 \cdot HCl$ 1995

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

ab initio pacem THEOCHEM 1995, 338,
141-53

(coll. $CH_4 \cdot HF$, III)

$SiH_4 \cdot HCl$ 1995

Govender, Maganthran G., et al.,

ab initio расчет стр-ры, стабильн. св-ва

S. Afr. J. Chem., 1995, 48 (3/4), 98-107;

(См. $CH_4 \cdot HF$, III.)

1995

F: Si-H-Cl
P: 3
14Б167. Симметрично замещенные силаны (XH[2]C)[2]SiH[2], (XH[2]C)[2]SiX[2], (X[2]HC)[2]SiH[2] и (X[2]HC)[2]SiX[2] с X=F, Cl, или Br. Конформационные энергии, структура и торсионные силовые постоянные, полученные методом молекулярной механики. Symmetrically substituted silanes: (XH[2]C)[2]SiH[2], (XH[2]C)[2]SiX[2], (X[2]HC)[2]SiH[2] and (X[2]HC)[2]SiX[2] with X=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.

РЖХ 1997

Si_2H_5Cl

1995

⊕ **19Б1233. ИК-спектры поглощения и спектры комбинационного рассеяния монохлор- и монобромдисиланов, масштабированное неэмпирическое силовое поле, интенсивности, атомные полярные тензоры и эффективные заряды для Si_2H_5Cl.** Infrared and Raman spectra of monochloro- and monobromodisilanes, a scaled ab initio force field, intensities, atomic polar tensors and effective charges for Si_2H_5Cl / 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.

М.Л.

Исследованы ИК-спектры поглощения и спектры КР Si_2H_5Cl (I), Si_2D_5Cl (II), Si_2H_5Br (III) и Si_2D_5Br (IV),

Х. 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 ν(SiH) для III—IV рассчитан набор из 14 масштабирующих множителей, обсуждены различия между первоначальными и масштабированными результатами.

Г. М. Курамшина

Si_2H_5Cl
Si_2D_5Cl

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 Si_2H_5Cl.** 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 Si_2H_5Cl, Si_2D_5Cl, Si_2H_5Br and Si_2D_5Br. These include approx. IR intensities for Si_2H_5Cl. 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 Si_2H_5Cl were calcd. ab initio using a 6–31G* basis set, and the force field scaled to fit the d_0, d_5 and ν^{is}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–Si_2H_5Cl. These identify significant effects by Cl on the gauche SiH bond, but virtually none on the trans one.

UK, СКР, сил. пост., Vi

(H) (IX)

C.A. 1995, 122, N 16.

Si_2H_5Br, Si_2D_5Br

$Si_2H_4Cl_2$
$Si_2D_4Cl_2$

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-$Si_2H_4Cl_2$ and 1,1-$Si_2D_4Cl_2$. 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 Si_2H_5Cl. SiH bonds gauche to Cl become more polar (SiH^-), while those in trans positions remain unaffected. Torsional structure obsd. in the νSiH region may permit the anal. of torsional levels and provide an est. of barrier height.

(UK, CKP) Gui. noch., Di

C.A. 1996, 124, N 10

$Si_2H_4Cl_2$

Si_2H_5Cl

$Si_2H_3Cl_3$

$Si_2H_2Cl_4$

1996

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 νSiH region obsd. in mixts. of chlorodisilanes are assigned by the joint use of substituent effects, detd. earlier in Si_2H_5Cl and 1,1–$Si_2H_4Cl_2$, and ab initio calcns. for 1,2–$Si_2H_4Cl_2$, 1,1,2–$Si_2H_3Cl_3$ and SiH_3SiCl_3, which together with 1,1,2,2–$Si_2H_2Cl_4$ were identified as being present. νSiH 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–$Si_2H_4Cl_2$ at HF/tzvp and MP2/tzvp levels. Alpha or gauche Cl substitution shortens both SiH and SiCl bonds, the former reflecting νSiH changes. Trans Cl substitution shortens SiCl bonds slightly, but has no effect on SiH bonds. The local mode behavior of νSiH 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.

Ik спектр,

ν_{Si-H}

C. A. 1996, 124, N 18

$Si_2H_4Cl_2$
Si_2H_5Cl
$Si_2H_3Cl_3$

1996

124: 245204b **Ab initio calculations of vibrational properties and conformer stabilities in 1,2-$Si_2H_4Cl_2$, 1,1,2-$Si_2H_3Cl_3$ and 1,1,1-$Si_2H_3Cl_3$, 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 calcns. of vibration frequencies and intensities were made for 1,2-$Si_2H_4Cl_2$ (conformers 12G, 12T), 1,1,2-$Si_2H_3Cl_3$ (conformers $112C_s$, $112C_1$) and 1,1,1-$Si_2H_3Cl_3$ (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-$Si_2H_4F_2$ 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-$Si_2H_4Cl_2$, 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 $112C_1$ conformer, an HF/6-31G* calcn. gives $X(C_1)$ ≈0.9, a likely upper limit.

ab initio

C.A. 1996, 124, N 18

1998

$Si_2H_nCl_{4-n}$

мол. ранет структ., Di и стабилн.

C.A. 1998, 128, N10

128: 119829d **Ab Initio Molecular Orbital Study of the Thermochemistry and Reactions of the Chlorinated Disilenes and Their Isomers ($Si_2H_nCl_{4-n}$).** 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 $H_nCl_{3-n}SiSiCl$ 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 $Si_2H_nCl_{4-n}$ 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.,

Ж. бен. Хим. 1998, 68(3), 411-413.

теорем. расчет Di, спектр.

(all. $ClSi$●$(CH_3)_3$; III)

F: Cl2HSi-SiHCl2
P: 3
DM39923 1999
131:248508 1,1,2,2-Tetrachlorodisilane (Cl2HSi-SiHCl2): molecular structu 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.(HSiSiH) = 180.degree., and gauche, with a tors angle .phi.(HSiSiH) .apprxeq. 60.degree.. The gauche conformer predomina occupying approx. 80% of the gas compn. at 23.degree.C. Some structural parameter values obtained from the GED refinements, using results from th earlier spectroscopic work and ab initio MO calcns. as constraints, are a follows (gauche conformer with estd. 2.sigma. uncertainties): bond length r(Si-Si) = 2.310(8) A, r.ltbbrac.(Si-Cl).rtbbrac. = 2.039(2) A (av. value r(Si-H) = 1.511 A (assumed value). Bond angles (.angle..alpha.): .angle..ltbbrac.SiSiCl.rtbbrac. = 108.9(4).degree. (av. value), .angle.Cl 109.7(3).degree., .angle.SiSiH = 111.5.degree. (assumed value).

1999

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

C.A. 2000, 132

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.

HSiCl | Оп. 41304 | 2002

Vazquez J. et al.,

вращ.
пост.
эксп.
и
расч. констант.

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

волн. чисел

Theoretical Investigation of the Structure and Vibrational Spectrum of the

Electronic ground state
$\tilde{X}$ ($1A'$) of HSiCl.

$LiHCl_3$ (On 41862) 2003

ab initio racem

Jing-Jing Zheng et al., Mol. Phys., 2003, 101, N8, 1165-70.

An ab initio anharmonic force field of $LiHCl_3$