Si N2

70317.4218
Ph, Ch, TC

40771
SiN_2 *

1977
5-17401

Lembke R.R., Ferrante R.F., Weltner W., Jr. SiCO, SiN_2 and $Si(CO)_2$ molecules: electron spin resonance and optical spectra at 4 K. (см. SiCO; III)
"J. Amer. Chem. Soc.", 1977, 99, N 2, 416-423 (англ.) 0831 ГПНК

806 815 ВИНИТИ

SiN_2 30353 1988

Краснов К.С.,
Филиппенко Н.В.,

м.п.
(обзор)

ОНИИТЭХИМ.
Деп. N 378-ХП-86,
Черкассы, 1988.

SiNN Om 31349 1988

De Kock R. L., Grev R. S., et al.,

ИК спектр, структура

J. Chem. Phys., 1988, 89, N 5, 3016-3027.

SiNN

1992

7 Б1033. Неэмпирическое исследовние низколежащих электронных состояний радикала SiNN. Ab initio study of low-lying electronic states of the SiNN radical /Cai Z.-L. //47th Ohio State Univ. Int. Symp. Mol. Spectrosc., Columbus, Ohio, June 15—19, 1992 .—Columbus (Ohio) ,1992 .—С. 104 .—Англ.

На основе расчетов потенциальных поверхностей основного и возбужденных электронных состояний молекулы SiNN методами конфигурац. вз-вия с несколькими исходными конфигурациями определены равновесные геометрич. параметры, энергии возбуждения, силовые постоянные и гармонич. частоты колебаний. Найденные величины, а также х-ки радиац. перехода $A^3\pi$—$X^3\Sigma^-$ удовлетворительно согласуются с эксперим. данными.

А. В. Немухин

М. П.

Х. 1993, N7

SiNN

1992

7 Б1032. Неэмпирическое исследование низколежащих электронных состояний радикала SiNN. Ab initio study of low-lying electronic states of the SiNN radical /Cai Z.-L., Wang Y.-F., Xiao H.-M. //J. Chem. Soc. Faraday Trans .—1992 .—88 ,№ 12 .—С. 1611—1613 .—Англ.

Методами конфигурац. вз-вия с несколькими исходными конфигурациями и с базисами типа двухэкспонентных с поляризац. АО рассчитаны фрагменты потенциальных поверхностей молекулы SiNN в состояниях $X^3\Sigma^-$, $a^1\Delta$, $A^3\pi$ и $^1\pi$. Результаты для равновесных расстояний сопоставлены с данными прежних расчетов методами ССП и многоконфигурац. методом ССП. В частности, для основного состояния равновесное расстояние Si—N в новом расчете составляет 1,9 А, а не 3,2, как сообщалось ранее (см. //J. Chem. Phys .—1988 .—С. 3016). Таким образом, нет необходимости характеризовать молекулу SiNN как вандерваальсов комплекс. Приведены рассчитанные гармонич. частоты колебаний, энергии возбуждения в высшие электронные состояния, а также радиац. время жизни возбужденного состояния $A^3\pi$, равное 345 нс.

А. В. Немухин

М·П·

Х·1993, № 7

SiNN 1992

121: 286800z Ab initio study of low-lying electronic states of the SiNN radical. Cai, Z.-L.; Wang, Y.-F.; Xiao, H.-M. (Dep. Chem., East China Inst. Technol., Nanjing, Peop. Rep. China 210014). *J. Chem. Soc., Faraday Trans.* 1992, 88(12), 1611-13 (Eng). The equil. geometries, excitation energies, force consts. and vibrational frequencies for the low-lying electronic states $\tilde{X}^3\Sigma^-$, $\tilde{a}^1\Delta$, $\tilde{A}^3\Pi$ and $\tilde{1}^1\Pi$ of the SiNN radical have been calcd. at the MRSDCI level with a double-zeta plus polarization basis set. Our calcns. imply that SiNN is a bonding and not a van der Waals mol. Our calcd. excitation for $\tilde{X}^3\Sigma^- \rightarrow \tilde{A}^3\Pi$ and vibrational frequencies for these tow states are in good agreement with expt. Electronic transition dipole moment, oscillator strength for the $\tilde{A}^3\Pi \rightarrow \tilde{X}^3\Sigma^-$ transition, radiative lifetime for the $\tilde{A}^3\Pi$ state and the spin properties for the $\tilde{X}^3\Sigma^-$ state are calcd. based on the MRSDCI wavefunctions, predicting results in reasonable agreement with available exptl. data.

($X^3\Sigma^-$, $a^1\Delta$, $A^3\Pi$, $1^1\Pi$)

теор. расчет

структ. парам., Ei, сил. пост.

C.A. 1994, 121, N24

SiNN

1992

4 Д64. Неэмпирическое исследование низколежащих электронных состояний радикала SiNN. Ab initio study of low-lying electronic states of the SiNN radical / Cai Z.-L., Wang Y.-F., Xiao H.-M. // J. Chem. Soc. Faraday Trans. .— 1992 .— 88 , № 12 .— С. 1611—1613 .— Англ.

С использованием метода НИК-КВ рассчитаны равновесные геометрии, энергии возбуждения, силовые постоянные и колебательные частоты низколежащих электронных состояний $\tilde{X}^3\Sigma^-$, $\bar{a}^1\Delta$, $\tilde{A}^3\Pi$ и $\tilde{1}^1\Pi$ радикала SiNN.

М·П·

Ф. 1993, N 4

SiNN 1992

Dixon D.A., DeKock Roger L.

структ. параметры, теор. расчёт

J. Chem. Phys. 1992, <u>97</u>(2), 1157-61.

(см. CNN; <u>III</u>)

SiNN Ом 36913 1992

117: 137976b Diazasilene (SiNN): a comparison of coupled cluster methods with experiment and local density functional methods. Ignatyev, Igor S.; Schaefer, Henry F., III (Cent. Comput. Quantum Chem., Univ. Georgia, Athens, GA 30602 USA). *J. Phys. Chem.* 1992, 96(19), 7632–4 (Eng). Ab initio quantum mech. methods were applied to the $^3\Sigma^-$ electronic ground state of the diazasilene mol. Higher level electron correlation methods are found to significantly effect the predicted equil. geometry. The SCF and single- and double-excitation CI (CISD) methods predict a loosely bound Si···N:N structure. The single and double excitation coupled cluster method (CCSD) predicts both the loose structure and a tightly bound Si–N_2 structure, with the latter lying 2.3 kcal/mol lower in energy. The highest level theor. method, CCSD(T), includes all connected triple excitations and predicts only the tight Si–N_2 structure. The CCSD(T) vibrational frequencies are in close agreement with expt. and in qual. agreement with local d. functional methods.

теор. расчет структ. и энергетики

С. А. 1992, 117, N 14

SiNN

1993

9Д111. Структура и колебательные частоты CNN и SiNN с использованием теории функционала нелокальной плотности. Structure and vibrational frequencies of CNN and SiNN using nonlocal density functional theory / Murray Christopher W., Laming Gregory J., Handy Nicholas C., Amos Roger D. // J. Phys. Chem.. — 1993. — **97**, № 9. — C. 1868—1871. Англ.

Density functional calculations with accurate quadrature and large basis sets are reported on SiNN and CNN using the gradient corrected exchange-correlation functionals, B-LYP. For CNN the symmetric stretch and bending frequencies are in good agreement with infrared values. The asymmetrics stretch frequency agrees with the recently determined value from laser-induced fluorescence experiments. These results are in qualitative agreement with local density functional results, although the use of the non-local functional appears to be an improvement. For SiNN, B-LYP gives good results which are close to the experimental frequencies and high level ab initio results.

М.П.

(Н)

Ф. 1993, N9

SiN_2

1998

Davy R.D., Schaefer H.F. III

стабильн;
структура

Chem. Phys. Lett.,
1996, 255, N 1,2,3,
p. 171-178

1996

F: SiN2
P: 3

16Б143. Трехатомные 14-электронные молекулы с открытой цепочкой и циклической формы. Молекулярная структура и колебательные частоты P[2]Si, P[2]C, SiN[2] и Si[2]S. [Исследование неэмпирическими методами ХФ, КВ и связанных кластеров]. Open chain versus cyclic 14-electron triatomics: Molecular structures and vibrational frequencies of P[2]Si, P[2]C, SiN[2] and Si[2]S / Davy Randall D., Schaefer Henry F. (III) [Chemical Physics Letters] // Chem. Phys. Lett. - 1996. - 255, N 1 - 3. - C. 171-178. - Англ.

РЖХ 1997

SiN_2
SiN_4

1997

127: 25151d SiN_2 and SiN_4 molecules: ab initio study of molecular and electronic structure, stability, and IR activity. Janoschek, Rudolf (Inst. Theoretische Chemie, Karl-Franzens-Univ. Graz, A-8010 Graz, Austria). *Adv. Quantum Chem.* 1997, 28, 235-245 (Eng), Academic. The geometries, vibrational wave nos. and absorption intensities, and complexation energies of SiN_2 and SiN_4 have been calcd. by second order Moeller-Plesset perturbation theory, the single and double excitation coupled cluster method, and the gradient cor. exchange-correlation d. functionals (B3LYP). The electronic structures have been studied applying the natural bond orbitals anal. A hitherto ignored pair of strong bands near 2000 cm^{-1} in the IR spectrum of SiN_2 is assigned to the NN stretching modes of the novel compd. SiN_4.

ab initio
расчет,
стр-ра,
Di

C.A. 1997, 127, N2

SiNN

1997

126: 191190q Diazasilene (SiNN): is there a conflict between experiment and theory? Ornellas, Fernando R.; Ueno, Leonardo T.; Iwata, Suehiro (Inst. Quim., Univ. Sao Paulo, 05599-970 Sao Paulo, Brazil). *J. Chem. Phys.* **1997**, 106(1), 151-157 (Eng). American Institute of Physics. The mol. SiNN was investigated with the highly correlated coupled cluster method with single and double excitations and corrections for the connected triples [CCSD(T)], and with the multiref. single and double excitations CI approach (MR-CI). A series of basis sets ranging from the simple 6-31G*, 6-311G*, and Dunning's double-zeta (DZ) plus polarization basis sets to the more extended correlation consistent cc-pVTZ and cc-pVQZ ones were employed to check the dependence of the geometry optimization and of the frequency evaluation on the basis sets. The highest level result of 1859 cm^{-1} for the harmonic stretching frequency of the NN bond differs considerably from a previous CCSD(T)/DZ prediction of 1726 cm^{-1}. In fact, most of the results analyzed in this study point to a frequency value greater than 1810 cm^{-1}. Reexamg. the scant exptl. evidence, the authors est. the harmonic frequency to be very close to 1830 cm^{-1}. Surprisingly, an extended internally contracted MR-CI calcn. with the cc-pVTZ basis

(теор. расчет)

C. A. 1997, 126, N 14

predicts a frequency 144 cm^{-1} higher than the corresponding CCSD(T)/cc-pVTZ result. Comparison with existing d.-functional studies and with a previous MR-CI calcn. are also carried out. At the CCSD(T)/cc-pVTZ level, other isomers of SiN_2 are further investigated for the first time. One sym. linear ($^3\Sigma_g^-$), and one sym. bent ($^1A_1$) structure are found to lie relatively high in energy: 84.60 and 102.23 kcal/mol, resp., relative to SiNN ($^3\Sigma^-$). However, one cyclic $^1A_1$ and the singlet asym. isomer SiNN ($^1\Sigma^+$) are only 6.09 and 15.81 kcal/mol above the global min. Although the higher frequencies of the former isomers do not fall in the region of relevance to the exptl. assignment discussed in this work, that of the lowest lying $^1A_1$ state (1850 cm^{-1}) is practically identical to the CCSD(T)/cc-pVTZ frequency computed for the $^3\Sigma^-$ state.