C3 N4

$(CN)_2CNN$

$C(CN)_2$

ν_i

Smith W.H.

1967

Diss. Abstr.,
B27, N7, 2319

ИК- и Раман- исследование
нек-рых линейных мол-л.

(см. C_3S_2) III

1969

$(CN)_2CNN$

8013t Vibrational spectra of dicyanodiazomethane $(NC)_2$-(CNN) and the dicyanomethylene free radical [$:C(CN)_2$]. Smith, William Hayden; Leroi, George E. (Michigan State Univ., East Lansing, Mich.). *U.S. Clearinghouse Fed. Sci. Tech. Inform., AD* 1969, AD-682230, 29 pp. (Eng). Avail. CFSTI. From *U.S. Govt. Res. Develop. Rep.* 1969, 69(7), 72. Ir spectra were obtained for $(CN)_2CNN$ in the solid state and isolated in inert matrixes. Crude Raman spectra of dicyanodiazomethane in MeCN soln. were also obtained. The vibrational anal. has been performed on the basis of C_{2v} symmetry and correlated with the spectra of a no. of related mols. Photolysis of matrix isolated $(CN)_2CNN$ yields sufficient $:C(CN)_2$ (dicyanomethylene), stabilized in situ, to permit observation of the ir spectrum. The results of the vibrational anal. indicate that the linear diradical has an extremely low central carbon bending frequency, analogous to those of C_3O_2 and C_3S_2.

TCVL

спектр

C. A. 1969. 71. 2

[$(CN)_2CNN$] 1969

ν_i

11 Б410. Инфракрасные спектры дицианодиазометана [$(CN)_2CNN$] и свободного радикала дицианометилена [$:C(CN)_2$]. Smith W. Hayden, Leroi G. E. Infrared spectra of dicyanodiazomethane [$(CN)_2CNN$] and the dicyanomethylene free radical [$:C(CN)_2$]. «Spectrochim. acta», 1969, A25, № 12, 1917—1927 (англ.)

Получены ИК-спектры (область 30—3500 *см*$^{-1}$) $(CN)_2CNN$ в тв. состоянии при т-ре 77° K, а также его ИК-спектры в матрицах из Ar и CCl_4 при т-рах 4, 63, 77, кроме того получены предварительные данные по спектру КР при комнатной т-ре (спектр КР возбуждали He—Ne-лазером). Произведено отнесение наблюденных ча-

См. также C_3N_2

(+1)

☒

X. 1970. 11

стот к различным типам колебаний, молекуле прописана симм. C_{2v}, отнесение контролировалось соответствующим расчетом частот нормальных колебаний. При фотолизе матрично-изолированного $(CN)_2CNN$ образуются радикалы $\cdot CN$ и $:C(CN)_2$, для последнего выполнен соответствующий расчет колебаний и дано отнесение частот (проведено также сопоставление с частотами колебаний C_3O_2 и C_3S_2, радикалу при этом прописана симм. $D_{\infty h}$).

А. Бобров

$N(CN)_3^-$
$C(CN)_3^-$

1978

89: 33643c Analysis of the vibrational spectra cyanocyanamide [$N(CN)_2^-$] and methanetricarbonitrile [$C(CN)_3^-$]. Kireeva, I. K.; Kharitonov, Yu. Ya.; Knyazeva, N. A.; Keller, H. (Inst. Obshch. Neorg. Khim. im. Kurnakova, Moscow, USSR). *Zh. Neorg. Khim.* 1978, 23(5), 1183–9 (Russ). The frequencies and shape of the normal vibrations of the model ions $N(CN)_3^-$ and $C(CN)_3^-$ ions were calcd. The force consts. were also calcd. The spectral characteristics of the $N(CN)_2^-$ and $C(CN)_3^-$ ions were compared with a series of other pseudohalide ions.

Сил.кон.,

ν_i

C.A., 1978, 89, N4

p– C_3N_4(K)

1995

123: 93689c **Relative stability of hexagonal and planar structures of hypothetical C_3N_4 solids.** Ortega, Jose; Sankey, Otto F. (Dep. Phys. Astronomy, Arizona State Univ., Tempe, AZ 85287 USA). *Phys. Rev. B: Condens. Matter* 1995, 51(4), 2624–7 (Eng). A first-principles electronic-structure study is presented of a planar structural form of a hypothetical C_3N_4 solid comparing its energy to a fully three dimensional form. A mixed basis of pseudoat. orbitals and low-kinetic-energy plane waves are used to det. the single-particle Kohn-Sham wave functions. These results are tested against fully converged plane-wave-basis calcns. The proposed planar form of C_3N_4 (p–C_3N_4) is lower in energy than the hexagonal form β–C_3N_4. However, the energy difference between the two phases is small. The hexagonal β–C_3N_4 phase is insulating, with an indirect gap, while the planar form p–C_3N_4 has a semimetallic electronic structure.

относительн
стабильность

☒ (41) β – C_3N_4(K)

C.A. 1995, 123, N 8

C_3N_4

1997

127: 71130u Ab initio calculations of the structures and energies of gas phase isomeric C_3N_4 molecules. BelBruno, Joseph J. (Department of Chemistry, Burke Chemical Laboratory, Dartmouth College, Hanover, NH, USA). *Chem. Phys. Lett.* **1997**, 270(1,2), 99–102 (Eng), Elsevier. Ab initio calcns., including electron correlation, have been performed with split–valence plus polarization basis sets for isomeric C_3N_4 gas phase structures. The min. energy configuration at the MP2(FC)/6–31G* level of theory is a linear chain rather than the tricyanoamine structure suggested in the literature. The latter, a planar structure, is predicted to lie 8.55 kcal mol^{-1} higher in energy, while a pyramidal configuration is 5.13 kcal mol^{-1} above the planar isomer. This is the first reported comparison of the possible gas phase C_3N_4 isomers, which could be important to the current efforts in the prodn. of the cryst. material β–C_3N_4.

ab initio
расчет
структуры
и стабильн.

C.A. 1997, 127, N 5

F: C3N4
P: 3

1999

131:121065 Electronic structure of six phases of C3N4. A theoretical appr Molina, B.; Sansores, L. E. (Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, Mexico 04510, Mex.). Mod. Phys. B, 13(6 & 7), 193-201 (English) 1999

A systematic study of the structural properties and electronic structure of six phases of C3N4 is presented. The phases under study are the .beta .alpha., cubic, pseudocubic and two graphitic with different space group. structural anal. shows that only in .beta. and graphitic phases the N ato behave in a pure sp2 configuration. In the other phases, .alpha., cubic pseudocubic, the N with its 3 C neighbors form a pyramid. The band struc for each of the six phases is presented indicating with .beta., .alpha. a cubic phases have an indirect gap while the pseudocubic and the two graph phases have a direct gap. Also charge d. contours are presented and anal

C. A. 1999, 131