N 4

N4

(структура)

1962

Pings C. J.;
Paalman H. H.
„Molec. Phys. 1962, 5,
N5, 531-34

N_4^+ (и.с)

1967

Asundi R.K.; Schulz G.J.
Chantry P.J.
„J. Chem. Phys. 1967, 47,
N5, 1584-91

1968

N_4^+

) 12 Б897. **Константа равновесия и скорости для обратимой реакции $N_4^+ \rightleftarrows N_2^+ + N_2$.** Varney R. N. Equilibrium constant and rates for the reversible reaction $N_4^+ \rightleftarrows N_2^+ + N_2$. «Phys. Rev.», 1968, **174**, № 1, 165—172 (англ.)

В области давлений (P_0) 0,63—1,24 *мм* измерена константа равновесия процесса $N_4^+ \rightleftarrows N_2^+ + N_2$ как функция E/P_0. (E — напряженность электрич. поля). Скорости прямой и обратной р-ции измерялись как функция E/P_0 в области от 40 до 70 $сек^{-1} \cdot мм^{-1}$. Энергия диссоциации N_4^+ составляет 0,87 *эв*. В указанной области изменений E/P_0 равновесие сильно сдвигается слева направо.

Л. Русин

Vp

X · 1969 · 12

1973

N_4^+

(K_p)

150153x **Ion-molecule equilibriums in mixtures of molecular nitrogen and argon.** Teng, Harry H.; Conway, D. C. (Dep. Chem., Texas A and M Univ., College Station, Tex.). *J. Chem. Phys.* 1973, 59(5), 2316–23 (Eng). Equil. consts. for the reactions $2N_2 + N_2^+ = N_4^+ + N_2$ (I); $N_4^+ + Ar = ArN_2^+ + N_2$ (II); $ArN_2^+ + Ar = Ar_2^+ + N_2$ (III) were detd. mass spectrometrically. The reactions were studied as a function of *E/P* (where *E* is in volts/cm and *P* is in torr) and temp. in a drift tube. It was found that entropy change for reaction I $\Delta S_I° =$ −16.2 ± 2.9 eu (entropy units) and enthalpy change $\Delta H_I° =$ −24.4 ± 2.1 kcal/mole at 723°K. By extrapolation of enthalpy data to 0°K, the bond energies, $D_0(AB^+)$, are 25.9 ± 2.1, 26.2 ± 2.2, and 27.8 ± 2.2 kcal/mole for N_2-N_2^+, Ar-N_2^+, and Ar-Ar$^+$, resp. When presumably more accurate literature data for Reac-

(+5) N_2^+; N_2; ArN_2^+ (K_p

$(N_2-N_2^+)$; $(Ar-Ar^+)$

$(Ar-N_2^+)$ D_0

C. A. 1973, N26, 79

tion (I) were used, the $D_0(AB^+)$ for the same series are 24.3, 24.5, and 26.3 kcal/mole. With literature data for Reaction (I) $\Delta S_{II}° = 3.57 \pm 0.06$ eu, $\Delta H_{II}° = -0.549 \pm 0.026$ kcal/mole, $\Delta S_{III}° = 1.87 \pm 0.08$ eu and $\Delta H_{III}° = 2.16 \pm 0.03$ kcal/mole at 298°K. Various models were used to det. the model dependence of the quantities derived from the equil. const. data. The $\Delta H_n°$, $\Delta S_n°$ and $D_0(AB^+)$ values are only weakly dependent on the assumed bond length and weak mode vibrational frequency distribution of the ion-mol. complex. However, $D_0(\text{Ar-N}_2^+)$, $\Delta S_n°$, and $\Delta H_n°$ (n = II or III) would be significantly different if Ar-N_2^+ were T shape rather than linear as assumed.

1973

N_2-N_2

(D_0)

Teng, Harry H., et al;
J. Chem. Phys.,
1973, 59(5), 2316-23.

(см. N_4^+; $\underline{I}$)

$N_2^+ + N_2 = N_4^+$ 1984

Stephan K., Maerk T.D., et al.

(ΔH) J. Chem. Phys. 1984, 80(7), 3185-8.

(см. N_3^+; I)

Nп

1987

106: 183547h Thermodynamic properties and homogeneous nucleation of molecular clusters of nitrogen. Pal, P.; Hoare, M. R. (R. Holloway Bedford New Coll., Univ. London, Surrey, UK TW2 0EX). *J. Phys. Chem.* 1987, 91(10), 2474-9 (Eng). A theor. model for the dynamics of N microclusters, based on the assumed free rotation of N_2 mols. within a solidlike harmonic vibrating structure, is described. This approach allows the known morphol. of rare-gas-type at. clusters to be adopted to account for the statistical thermodn. of nonpolar diat. species with considerable simplification. As judged by the prediction of thermodn. parameters related to homogeneous nucleation, the approxn. would appear to be justified in a favorable temp. range.

термод. св-ва

C.A. 1987, 106, N22

N_4 1990

Francl, Michelle M.,
Chesick, John P.,

J. Phys. Chem., 1990,
(ΔH_f) 94 (2), 526-8.

The nitrogen (N_4) molecule and its metastability.

C.A. 1990, 112, N8, 62956

N_4^+

1990

колебат. спектр в матрице, Ne

113: 180514d The vibrational spectra of molecular ions isolated in solid neon. III. The nitrogen tetraatomic monopositive ion. Thompson, Warren E.; Jacox, Marilyn E. (Natl. Sci. Found., Washington, DC 20550 USA). *J. Chem. Phys.* 1990, 93(6), 3856-62 (Eng). When a $Ne:N_2$ = 100 or 200 mixt. is codeposited at 5 K with a beam of Ne atoms excited by a microwave discharge, a weak to moderately intense IR absorption appears at 2237.6 cm^{-1} which is assigned to the N_4^+ mol. ion. The anal. of the IR spectra of the ^{15}N substituted species N_4^+ supports the conclusion from earlier ab initio calcns. and ESR observations that N_4^+ has a linear, centrosym. ground-state structure. For the N_4^+ species with noncentrosym. isotopic substitution, the in-phase end-atom stretching fundamental becomes IR active and has also been obsd. Although the anion responsible for overall charge neutrality of the deposit has not been definitively identified, secondary photolysis studies provide some information regarding its properties.

С.А. 1990, 113, N 20

$(N_2)_2$

1993

119: 235175a Computed gas-phase thermodynamics of nitrogen (N_2) association. Uhlik, Filip; Slanina, Zdenek; Hinchliffe, Alan (Department of Chemistry, UMIST, P.O. Box 88, Manchester, UK M60 1QD). *Thermochim. Acta* 1993, 223(1-2), 1-6 (Eng). The thermodn. of the gas-phase N_2 dimerization was computed in terms of partition functions constructed on the basis of ab initio quantum-chem. computations. Two different evaluations of the dimerization energetics were used, indicating four and three $(N_2)_2$ min. energy structures. In both sets, two particular structures coexist at temps. relevant for atm. conditions. Enhancement of heat capacity through this isomerism is felt at very low temps. only. For the dimerization equil. const., an interval in which the true value should be present is suggested. These data are important for the study of the earth atm., and also for cometary and planetary atmospheres.

термодинамика димеризации N_2

C. A: 1993, 119, N 22

N_4

2001

ab initio рас
чт осн. и перво
го возб. сост.
$^1B_{3u}$

135: 322980h Ab initio study of the ground state and the first excited state of the rectangular (D_{2h}) N_4 molecule. Bittererova, Martina; Ostmark, Henric; Brinck, Tore (Physical Chemistry, Royal Institute of Technology, SE−100 44 Stockholm, Swed.). *Chem. Phys. Lett.* 2001, 347(1,2,3), 220−228 (Eng), Elsevier Science B.V. The dissocn. pathway of D_{2h} N_4 has been investigated at the CASSCF level of theory. A new C_{2v} transition state to dissocn. was found and characterized on the potential energy surface. The effective barrier of dissocn. from D_{2h} N_4 to $2N_2$ is estd. to be 6.5 kcal/mol from MR−AQCC/VTZ//CAS-(12,12)/VTZ calcns. Vertical excitation energies and oscillator strengths for the lowest 20 singlet states of D_{2h} N_4 have been calcd. using the EOM−CCSD method. The geometry of the first excited state $^1B_{3u}$, considered as the lowest optically accessible state, has been optimized and characterized at various computational levels. This state might be useful for detection of D_{2h} N_4 by means of laser−induced fluorescence spectroscopy.

C.A. 2001, 135, N22